**ΠΑΝΕΠΙΣΤΗΜΙΟ ΑΘΗΝΩΝ**

**ΜΕΤΑΠΤΥΧΙΑΚΟ ΔΙΠΛΩΜΑ ΒΙΟΣΤΑΤΙΣΤΙΚΗΣ**

**ΜΑΘΗΜΑ: ΜΠΕΫΖΙΑΝΗ ΣΥΜΠΕΡΑΣΜΑΤΟΛΟΓΙΑ**

**ΔΙΔΑΣΚΟΝΤΕΣ: Ι. Ντζούφρας, Π. Τσιαμυρτζής**

ΔΙΔΑΚΤΙΚΟ ΥΛΙΚΟ ΓΙΑ ΤΟ ΜΑΘΗΜΑ

# ΜΠΕΫΖΙΑΝΗ ΣΥΜΠΕΡΑΣΜΑΤΟΛΟΓΙΑ:

## *Βιοστατιστική κατά Bayes με τη χρήση του Λογισμικού BUGS*

*(Μέρος ΙΙ: Επιλογή Μοντέλων και Μεταβλητών κατά Bayes, Διαγνωστικά Τεστ)*

*ΙΩΑΝΝΗΣ ΝΤΖΟΥΦΡΑΣ*


*Χίος, Μάιος 2004*
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# Bayesian Biostatistics Using BUGS


## Βιο-Στατιστική κατά Bayes με τη χρήση του Λογισμικού BUGS

**ΜΑΘΗΜΑ 4:** ***ΕΙΣΑΓΩΓΗ ΣΤΟΝ ΕΛΕΓΧΟ ΥΠΟΘΕΣΕΩΝ, ΕΠΙΛΟΓΗ ΜΟΝΤΕΛΩΝ ΚΑΙ ΜΕΤΑΒΛΗΤΩΝ ΚΑΤΑ BAYES ΜΕ ΤΟ WINBUGS***

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## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.1. Εισαγωγή: Εκ-των-Υστερων Λόγος Πιθανοτήτων των Μοντέλων*

Ξαναγυρίζουμε στο Παράδειγμα της Εστριόλης

- Green & Touchston (1963, *Am.Jour. Of Obsterics & Gynecology*)
- Μελέτη σχέσης
  - Y : Βάρος γέννησης (birthweight) ενός παιδιού
  - X : Επίπεδο εστριόλης (estriol) των εγκύων γυναικών
- $Y_i \sim \text{Normal}(\mu_i, \sigma^2)$
- $\mu_i = \eta_i = \alpha + \beta X_i$

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.1. Εισαγωγή: Εκ-των-Υστερων Λόγος Πιθανοτήτων των Μοντέλων*

Ξαναγυρίζουμε στο Παράδειγμα της Εστριόλης

Μας ενδιαφέρει να ελέγξουμε την υπόθεση

**$H_0$: β=0 vs. $H_1$ β ≠0**

Το οποίο ειναι ισοδύναμο με τη σύγκριση των μοντέλων

$m_0$ : $Y \sim N(\alpha, \sigma^2)$

$m_1$ : $Y \sim N(\alpha+\beta X, \sigma^2)$

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.1. Εισαγωγή: Εκ-των-Υστερων Λόγος Πιθανοτήτων των Μοντέλων*

Εκ-των-Υστέρων Λόγος Πιθανοτήτων (Posterior Model Odds) του μοντέλου $m_0$ έναντι του μοντέλου $m_1$:

$$PO_{01} = \frac{f(m_0 \mid \mathbf{y})}{f(m_1 \mid \mathbf{y})} = \frac{f(\mathbf{y} \mid m_0)}{f(\mathbf{y} \mid m_1)} \times \frac{f(m_0)}{f(m_1)}$$

**$B_{01}$: Bayes Factor**
**(Παράγοντας Bayes)**

**Prior Model Odds**
**(Εκ-των-Προτέρων Λόγος Πιθανοτήτων των Μοντέλων)**

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.1. Εισαγωγή: Εκ-των-Υστερων Λόγος Πιθανοτήτων των Μοντέλων*

- *f*(m): Εκ-των-Προτέρων Πιθανότητα του μοντέλου m (Prior model probability)
- *f*(m|**y**): Εκ-των-Υστέρων Πιθανότητα του μοντέλου m (Posterior model probability)
- f(**y**|m): Περιθωριακή Πιθανοφάνεια των Δεδομένων στο μοντέλο m (marginal likelihood of model m)

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.1. Εισαγωγή: Εκ-των-Υστερων Λόγος Πιθανοτήτων των Μοντέλων*

- $\frac{f(m_0)}{f(m_1)}$ : Εκ-των-προτέρων λόγος πιθανοτήτων του μοντέλου $m_0$ έναντι του μοντέλου $m_1$ (Prior model odds of $m_0$ vs. $m_1$)
- $B_{01} = \frac{f(\mathbf{y} \mid m_0)}{f(\mathbf{y} \mid m_1)}$ : Παράγοντας Bayes του μοντέλου $m_0$ έναντι του μοντέλου $m_1$ (Bayes Factor of model $m_0$ vs. $m_1$)
- $PO_{01} = \frac{f(m_0 \mid \mathbf{y})}{f(m_1 \mid \mathbf{y})}$ : Εκ-των-υστέρων λόγος πιθανοτήτων του μοντέλου $m_0$ έναντι του μοντέλου $m_1$ (Posterior model odds of $m_0$ vs. $m_1$)

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

Στο BUGS μπορούμε να εκτιμήσουμε τη *εκ-των-υστερων πιθανότητα f(m|y)* εισάγωντας την λανθάνουσα (latent) δίτιμη μεταβλητή γ:

$$Y \sim Normal(\alpha + \beta X, \sigma^2).$$

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

Στο BUGS μπορούμε να εκτιμήσουμε τη *εκ-των-υστερων πιθανότητα f(m|y)* εισάγωντας την λανθάνουσα (latent) δίτιμη μεταβλητή γ:

$$Y \sim Normal(\alpha + \gamma \times \beta X, \sigma^2).$$

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

Για λεπτομέρειες παραπέμπουμε στα ακόλουθα

- **Katsis, A. and Ntzoufras, I. (2003).** Testing Hypotheses for the Distribution of Insurance Claim Counts Using the Gibbs Sampler.
- **Ntzoufras, I. (2002).** Gibbs Variable Selection Using BUGS. *Journal of Statistical Software,* Volume **7,** Issue 7, 1 – 19 .
- **Dellaportas, Forster and Ntzoufras (2002).** On Bayesian Model and Variable Selection Using MCMC. *Statistics and Computing*, **12**, 27–36.
- **Dellaportas, Forster and Ntzoufras (2000).** On Bayesian Model and Variable Selection Using MCMC. In *Generalized Linear Models: A Bayesian Perspective*, 271–286.
- **MY BUGS TUTORIAL PAGE:** `http://stat-athens.aueb.gr/~jbn/bugs_tutorial/home.html`
- **Ntzoufras (2002).** Tutorial on Bayesian Model Selection (Msc Hand outs)

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

Η κατανομή $f(\beta|\gamma=0)$ ονομάζεται και *ψευδο-prior (pseudo-prior)* ή or *κατανομή πρότασης (proposal distribution)*.

- Δεν επηρεάζει την *εκ-των-υστέρων κατανομη* δηλ. την $f(\alpha, \beta, \gamma|\, \mathbf{y})=f(\alpha, \beta|\, \gamma, \mathbf{y})\, f(\gamma\,|\,\mathbf{y})$.
- Επηρεάζει την *σύγκλιση της αλυσίδας*
- Για να δουλέψει αποτελεσματικά πρέπει να είναι κοντά στην εκ-των-υστέρων κατανομή: $f(\beta|\, \mathbf{y}, \gamma=1)$ .
- Για λόγους απλούστευσης υποθέτουμε

$$f(\beta|\, \gamma=0)= f(\beta|\, \gamma=1)$$

[Δουλεύει καλά στο συγκεκριμένο παράδειγμα]

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

(1) $Birth_i \sim Normal(\mu_i, \sigma^2)$
(2) $\eta_i = \alpha + \beta \times Estriol_i$
(3) $\mu_i = \eta_i = \alpha + \beta \times Estriol_i$
for i=1,…,31

```
for (i in 1:n) {
  Birth[i]~dnorm(mu[i],tau)
  x[i]<-estriol[i]-mean(estriol[])
  mu[i] <-a+        b*x[i]
}
```

PRIORS

- $f(\alpha)=Normal(0, 10^4)$
- $f(\beta)=Normal(0, 10^4)$
- $f(\tau^2)=Gamma(10^{-4},10^{-4})$
- $\sigma^2=1/\tau$

```
a~dnorm(0.0,1.0E-04)
b~dnorm(0.0,1.0E-04)
tau~dgamma(1.0E-04,1.0E-04)
s2<-1/tau
```

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

(1) $Birth_i \sim Normal(\mu_i, \sigma^2)$
(2) $\eta_i = \alpha + \gamma \times \beta \times Estriol_i$
(3) $\mu_i = \eta_i = \alpha + \beta \times Estriol_i$
for i=1,…,31

```
for (i in 1:n) {
  Birth[i]~dnorm(mu[i],tau)
  x[i]<-estriol[i]-mean(estriol[])
  mu[i] <-a+ gamma*b*x[i]
}
```

PRIORS

- $f(\alpha)=Normal(0, 10^4)$
- $f(\beta)=Normal(0, 10^4)$
- $f(\tau^2)=Gamma(10^{-4},10^{-4})$
- $\sigma^2=1/\tau$
- $\gamma \sim$ **Bernoulli (0.5)**

```
a~dnorm(0.0,1.0E-04)
b~dnorm(0.0,1.0E-04)
tau~dgamma(1.0E-04,1.0E-04)
s2<-1/tau
gamma~dbern(0.5)
```

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

(1) $Birth_i \sim Normal(\mu_i, \sigma^2)$

(2) $\eta_i = \alpha + \gamma \times \beta \times Estriol_i$

(3) $\mu_i = \eta_i = \alpha + \beta \times Estriol_i$

for i=1,...,31

```
for (i in 1:n) {
  Birth[i]~dnorm(mu[i],tau)
  x[i]<-estriol[i]-mean(estriol[])
  mu[i] <-a+ gamma*b*x[i]
}
```

PRIORS

- $f(\alpha)=Normal(0, 10^4)$ — `a~dnorm(0.0,1.0E-04)`
- $f(\beta)=Normal(0, 10^4)$ — `b~dnorm(0.0,1.0E-04)`
- $f(\tau^2)=Gamma(10^{-4},10^{-4})$ — `tau~dgamma(1.0E-04,1.0E-04)`
- $\sigma^2=1/\tau$ — `s2<-1/tau`
- $\gamma \sim$ **Bernoulli (0.5)** — `gamma~dbern(0.5)`

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

Μετά από Burn-in 1000 επαναλήψεων και 20,000 επαναλήψεις ως δείγμα

$$f(\gamma=1|\mathbf{y}) = 0.6268$$

$$PO_{10}=BF_{10} = 1.68$$

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

- Δεν συζητήσαμε για τις εκ-των-προτέρων κατανομές των μοντέλων όταν κάνουμε επιλογή/σύγκριση μοντέλων [το θέμα είναι πολύ μεγάλο και σύνθετο για αυτό το μάθημα].
- Μεγάλες τιμές της εκ-των-προτερων διακύμανσης του β θα ενεργοποιήσει το παράδοξο των Bartlett - Lindley => $f(\gamma=1|\mathbf{y}) \rightarrow 0.0$
- Μία λύση: Η εκ-των-προτέρων (ΕτΠ) κατανομή της μοναδιαίας πληροφορίας (Unit information prior, BIC):

ΕτΠ Διακύμανση του β =

Μέγεθος Δείγματος **X** ΕτΥ Διακύμανση του β που παίρνουμε όταν χρησιμοποιούμε επίπεδη ΕτΠ κατανομή

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

Ας Ξανατρέξουμε το παράδειγμα με την ΕτΠ μοναδιαίας πληροφορίας.

- Τρέχουμε το παράδειγμα με μεγάλη ΕτΠ διακύμανση και βρίσκουμε

  ΕτΥ Διακύμανση= $(0.1431)^2$

- Παίρνουμε τώρα στη σύγκριση των 2 μοντέλων με

  ΕτΠ Διακύμανση του β = 31 X $(0.1431)^2$ = 0.6348

  ΕτΠ Ακρίβεια του β = 1/0.6348 = 1.575

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

Μετά από Burn-in 1000 επαναλήψεων και 20,000 προσομοιώμενες τιμές έχουμε ως αποτέλεσμα

$f(\gamma=1|\mathbf{y})= 0.9922$

$PO_{10}=BF_{10} = 127.20$

## 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

### *6.2. Εκ-των-Υστερων Πιθανοτήτες των Μοντέλων στο BUGS*

Αυτό το Παράδειγμα είναι μόνο για Επίδειξη

Μην προσπαθήσετε να τρέξετε σύγκριση μοντέλων στο BUGS αν δεν έχετε πρώτα κατανοήσει πολύ καλά την προσομοίωση των απλών μοντέλων και το τρόπο λειτουργίας των μεθόδων σύγκρισης μοντέλων.

Να είστε πολυ προσεκτικοί όταν επιλέγετε ΕτΠ (prior) και ψευδο-ΕτΠ (pseudo-prior) κατανομές

# 6… ΑΠΛΟΙ ΕΛΕΓΧΟΙ ΥΠΟΘΕΣΕΩΝ

## *6.3. Άλλοι Τρόποι Υπολογισμού του Παράγοντα Bayes*

**MCMC για Σύγκριση Μοντέλων**

- ***Reversible Jump MCMC*** (RJMCMC, Green, 1995) [Δεν μπορεί να εφαρμοστεί στο WINBUGS ακόμα]
- ***Δειγματολήπτης των Carlin και Chib*** (1995). Παράδειγμα 13 (Pines dataset) στο Bugs 0.5 Examples vol.**2**, σελ. 47-50 .

**Τρόποι Υπολογισμού της Περιθωριακής Πιθανοφάνειας**

- Εκτιμητής του ***Αρμονικού μέσου*** της Πιθανοφάνειας
- Ο Εκτιμητής των ***Newton και Raftery*** (1994).
- Ο Εκτιμητής των ***Gelfand και Dey*** (1994).
- Ο Εκτιμητής του ***Chib*** (1995, JASA).
- Ο Εκτιμητής ***Laplace-Metropolis*** (Lewis και Raftery, 1997)
- κ.α. Για Λεπτομέρειες προτείνω να δείτε το καλό review του *Lopes (2002).*

# 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

## *7.1. Κριτήρια Πληροφορίας (Information Criteria)*

Τα κριτήρια πληροφορίας γενικά ορίζονται ώς την μέγιστη πιθανοφάνεια στη οποία επιβάλλεται μια ποινή για κάθε επιπλέον παράμετρο που εκτιμούμε

- Deviance = -2 max{ log - likelihood }
- IC = -2 max{ log - likelihood } + parameters × penalty
- AIC= -2 max{ log - likelihood } + parameters × 2
- BIC= -2 max{ log - likelihood } + parameters × log(n)

## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.1. Κριτήρια Πληροφορίας (Information Criteria)*

Μπορούμε να ορίσουμε τις Bayesian versions των AIC/BIC και να βρούμε τις posterior και να τις συγκρίνουμε (Brooks 2002)

- B.Deviance(m) = -2 log{$f(\mathbf{y}|\boldsymbol{\theta},m)$} = -2 log - likelihood
- B.AIC(m) = -2 log{$f(\mathbf{y}|\boldsymbol{\theta}, m)$} + parameters × 2
- B.BIC(m) = -2 log{$f(\mathbf{y}|\boldsymbol{\theta}, m)$} + parameters × log(n)

## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.2. Bayesian AIC/BIC στο WINBUGS (Estriol Example)*

ΜΠΟΡΟΥΜΕ ΝΑ ΤΡΕΞΟΥΜΕ ΚΑΙ ΤΑ ΔΥΟ ΜΟΝΤΕΛΑ ΣΕ ΕΝΑ ΠΡΟΓΡΑΜΜΑ WINBUGS.

- 1… Ορίζουμε το λογάριθμο της Πιθανοφάνειας για κάθε παρατήρηση (μέσα στο `for`).
- 2… Υπολογίζουμε τη συνολική λογαριθμο - Πιθανοφάνεια
- 3… Υπολογίζουμε το AIC/BIC για κάθε μοντέλο
- 4… Υπολογίζουμε διαφορές των AIC/BIC που μας ενδιαφέρουν.(μονο σε παράλληλη δειγματοληψία)

# 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

## *7.2. Bayesian AIC/BIC στο WINBUGS (Estriol Example)*

**ΜΟΝΤΕΛΟ 1: BIRTHWEIGHT=α+β ESTRIOL**

```
model estriol_AIC_BIC;
{
(1) pi<-3.14
    for (i in 1:n) {
    birth[i]~dnorm( mu[i], tau );
    mu[i]<-a.star+b*(estriol[i]-mean(estriol[]));
(1) loglike1[i]<- -0.5*log(2*pi)+0.5*log(tau)
                  -0.5*pow( birth[i]-mu[i],2 )*tau
    }
```


# 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

## *7.2. Bayesian AIC/BIC στο WINBUGS (Estriol Example)*

**ΜΟΝΤΕΛΟ 1: BIRTHWEIGHT=α+β ESTRIOL**


```
#       prior distributions for model m1
        a.star~dnorm( 0, 1.0E-04 )
        b~dnorm( 0, 1.0E-04 ); # normal prior for b
        tau~dgamma( 1.0E-04 , 1.0E-04 );
        s2<-1/tau;
        a<-a.star-b*mean(estriol[]);
#       Bayesian versions of LogLikelihood
        L1<-sum( loglike1[] )                    (2)
#       Bayesian versions of BIC
        BIC1<- -2*L1 + 3*log(n)                  (3)
#       Bayesian versions of AIC
        AIC1<- -2*L1 + 3*2
}
```

# 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

## *7.2. Bayesian AIC/BIC στο WINBUGS (Estriol Example)*

**ΜΟΝΤΕΛΟ 0: BIRTHWEIGHT=α**

```
model estriol_AIC_BIC{
      pi<-3.14
      for (i in 1:n) {
#           definition of model m1
#           … … … … … … … … … … … … …
#           definition of model m0
            birth0[i]<-birth[i]
            birth0[i]~dnorm( mu0[i], tau0 );
            mu0[i]<-a0;
(1)         loglike0[i]<- -0.5*log(2*pi)+0.5*log(tau0)
                          -0.5*pow( birth0[i]-mu0[i],2)*tau0
      }
```

# 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

## *7.2. Bayesian AIC/BIC στο WINBUGS (Estriol Example)*

**ΜΟΝΤΕΛΟ 0: BIRTHWEIGHT=α**

```
#     prior distributions for model m1
#     … … … … … … … … … … … … … … … … …
#     prior distributions for model m0
      a0~dnorm( 0, 1.0E-04 );
      tau0~dgamma( 1.0E-04 , 1.0E-04 );
#     Bayesian versions of LogLikelihood
      L1<-sum( loglike1[] )                          (2)
      L0<-sum( loglike0[] )
#     Bayesian versions of BIC
      BIC1<- -2*L1 + 3*log(n)                        (3)
      BIC0<- -2*L0 + 2*log(n)
(4)   DBIC10<- BIC0-BIC1
#     Bayesian versions of AIC
      AIC1<- -2*L1 + 3*2                             (3)
      AIC0<- -2*L0 + 2*2
(4)   DAIC10<- AIC0-AIC1                          }
```

## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.2. Bayesian AIC/BIC στο WINBUGS (Estriol Example)*

- Αποτελέσματα

| node | mean | sd | MC error | 2.5% | median | 97.5% | start | sample |
|---|---|---|---|---|---|---|---|---|
| AIC0 | 189.4 | 2.003 | 0.032 | 187.5 | 188.8 | 194.8 | 1001 | 5000 |
| AIC1 | 178.2 | 2.533 | 0.03684 | 175.3 | 177.5 | 184.7 | 1001 | 5000 |
| BIC0 | 192.3 | 2.003 | 0.032 | 190.3 | 191.6 | 197.7 | 1001 | 5000 |
| BIC1 | 182.5 | 2.533 | 0.03684 | 179.6 | 181.8 | 189.0 | 1001 | 5000 |
| DAIC10 | 11.23 | 3.212 | 0.05295 | 4.246 | 11.48 | 17.65 | 1001 | 5000 |
| DBIC10 | 9.798 | 3.212 | 0.05295 | 2.812 | 10.04 | 16.22 | 1001 | 5000 |

- Υποστηρίζεται το μοντέλο με $\beta \neq 0$ και με το AIC και με το BIC

## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.3. Πληροφοριακό Κριτήριο Απόκλισης (Deviance Information Criterion)*

Το DIC είναι Γενίκευση του AIC
Spiegelhalter *et al.* (2002, RSSB)

- $DIC(m)= \overline{D}(\boldsymbol{\theta},m)+ p_D(m)$

- $\overline{D}(\boldsymbol{\theta},m)$ = posterior mean of deviance for model m
- $p_D(m)$ = effective number of parameters of model m

- $DIC(m)=2\overline{D}(\boldsymbol{\theta},m)-D(\overline{\boldsymbol{\theta}},m)$

- $D(\overline{\boldsymbol{\theta}},m)$: Deviance evaluated at the posterior mean of **θ** (ή άλλου εκτιμητή)

## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.3. Πληροφοριακό Κριτήριο Απόκλισης (Deviance Information Criterion)*

**ΜΕΡΙΚΑ ΣΧΟΛΙΑ ΓΙΑ ΤΟ DIC**

**1) Γενίκευση του AIC. Για τα μή ιεραρχικά μοντέλα $p_D$ είναι περίπου ίσο με τον πραγματικό αριθμό των παραμέτρων.**

**2) Μικρές αλλαγές της εκτίμησης του θ (που χρησιμοποιείται για τον υπολογισμό του $p_D$) μπορεί να οδηγήσει σε άλλο DIC (άρα επηρεάζεται και από prior, την παραμετροποίηση του μοντέλου και από την ασυμμετρία της posterior του θ).**

## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.3. Πληροφοριακό Κριτήριο Απόκλισης (Deviance Information Criterion)*

**ΜΕΡΙΚΑ ΣΧΟΛΙΑ ΓΙΑ ΤΟ DIC**

**3) Στο WINBUGS δεν δίδεται το Μόντε Κάρλο σφάλμα (MC error).**

**Το σφάλμα του Deviance μπορούμε να το βρούμε εύκολα επιβλέποντας (monitor) την posterior του Deviance (οριζουμε `D1<- -2L1` και `D0<- -2L0` στο παραδειγμα της Εστριόλης). Αυτό το σφάλμα γενικά είναι μικρό.**

**Ανησυχία υπάρχει για το $p_D$ (και $D(\theta,m)$ ) και γενικά θα πρέπει να κοιτάζουμε τη σταθερότητα αυτών των ποσοτήτων μετά από αρκετές επαναλήψεις.**

## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.3. Πληροφοριακό Κριτήριο Απόκλισης (Deviance Information Criterion)*

**ΜΕΡΙΚΑ ΣΧΟΛΙΑ ΓΙΑ ΤΟ DIC**

**4) Αν η λογαριθμο - πιθανοφάνεια είναι κοίλη ως πρός τις παραμέτρους της (στοχαστικούς κόμβους) τότε DIC>0. Παρόλα αυτά μπορούμε να πάρουμε αρνητικό DIC στις ακόλουθες περιπτώσεις**

**i) με μη κοίλες λογαριθμο-πιθανοφάνειας (π.χ. Student-t κατανομή) όπου υπάρχει μεγάλη διαφορά μεταξύ prior και δεδομένων.**

**ii) όταν η posterior μίας παραμέτρου είναι συμετρική και δικόρυφη και γενικά όταν ο εκ-των-υστέρων μέσος είναι φτωχός περιγραφικός δείκτης με μεγάλη εκ-των-υστέρων διακύμανση.**

## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.3. Πληροφοριακό Κριτήριο Απόκλισης (Deviance Information Criterion)*

**ΜΕΡΙΚΑ ΣΧΟΛΙΑ ΓΙΑ ΤΟ DIC**

**5) Το ελάχιστο DIC εκτιμάει ποιό μοντελο θα δώσει τις καλύτερες σύντομες (short-term) προβλέψεις στην ίδια λογική με το AIC.**

**Παρόλα αυτά άν η διαφορά των DIC είναι μικρότερη από 5 για μοντέλα που δίνουν τελείως διαφορετικά συμπεράσματα τότε είναι λάθος απλά να αναφέρουμε το μοντέλο με το μικρότερο DIC.**

**6) Το DIC (όπως και τα AIC/BIC) είναι συγκρίσιμα για μοντέλα με τα ίδια δεδομένα. Τα μοντέλα δε χρειάζεται να είναι «φωλιασμένα» το ένα μέσα στο άλλο (nested).**

## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.3. Πληροφοριακό Κριτήριο Απόκλισης (Deviance Information Criterion)*

**ΜΕΡΙΚΑ ΣΧΟΛΙΑ ΓΙΑ ΤΟ DIC**

**7) Το DIC διαφέρει σε στόχους και μορφή από το BIC και τον Παράγοντα Bayes.**

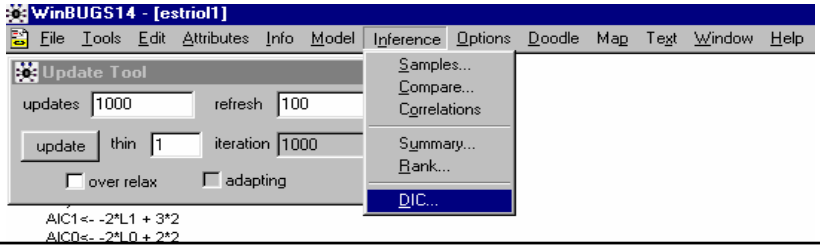
**8) Θα πρέπει να χρησιμοποιείτε με προσοχή το DIC μέχρι να υπάρξου πιο πολλά ερευνητικά αποτελέσματα. Σε μερικά μοντέλα το WINBUGS δεν μπορεί να υπολογιστεί το DIC. Για λεπτομέρειες παραπέμπουμε στην Ιστο-σελίδα του WINBUGS** http://www.mrc-bsu.cam.ac.uk/bugs/winbugs/contents.shtml

**9) Ο υπολογισμός των Bayesian BIC/AIC είναι πιο εύκολος και άμεσος (και μπορούμε να έχουμε και MC error).**

## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.4. Υπολογισμός του DIC στο WINBUGS (Estriol Example)*

- Δεν χρειάζεται να ορισουμε κάτι επιπλέον στο μοντέλο του WINBUGS.
- Μπορούμε να τρέξουμε παράλληλα όλα τα μοντέλα που θέλουμε να συγκρίνουμε μαζί.
- Αφού προσομοιώσουμε τις πρώτες παρατηρήσεις στην περίοδο Burn-in επιλέγουμε **INFERENCE>DIC**



## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.4. Υπολογισμός του DIC στο WINBUGS (Estriol Example)*

- Επιλέγουμε το κουτί **SET** .


- Προσομοιώνουμε το δείγμα από την posterior κατανομή (**MODEL>UPDATE**, συμπληρώνουμε στο **updates** τον αριθμό των επαναλήψεων).
- Επιλέγουμε το ***DIC TOOL*** (**INFERENCE>DIC**) και το κουτί **DIC**.


## 7… ΑΛΛΟΙ ΤΡΟΠΟΙ ΣΥΓΚΡΙΣΗΣ ΜΟΝΤΕΛΩΝ

### *7.4. Υπολογισμός του DIC στο WINBUGS (Estriol Example)*

- **ΑΠΟΤΕΛΕΣΜΑΤΑ**

**Dbar = post.mean of -2logL; Dhat = -2LogL at post.mean of stochastic nodes**

| | Dbar | Dhat | pD | DIC |
|---|---|---|---|---|
| birth | 172.201 | 169.086 | 3.115 | 175.316 |
| birth0 | 185.433 | 183.447 | 1.985 | 187.418 |
| total | 357.633 | 352.533 | 5.100 | 362.734 |

- Διαφορά = 13.23
- Μοντέλο 1 πάλι καλύτερο
- $p_D$ είναι περίπου ίσο με 3 και 2 (αριθμός παραμέτρων στα δύο μοντέλα).

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *ΠΕΡΙΕΧΟΜΕΝΑ*

- [BUGS manual: page 40]
- Κατάλοιπα (Residuals)
- Εκ-των-υστέρων Επίπεδο Σημαντικότητας (Posterior P-values)
- Προβλεπτικά Μέτρα Σύγκρισης Μοντέλων (Predictive Model Comparison Measures)
- Προβλεπτικά Μέτρα Πάραλληλης Δειγματολειψίας (Parallel Sampling Predictive Measures)

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *ΕΝΑ ΑΠΛΟ ΠΑΡΑΔΕΙΓΜΑ (LINE.BUG)*

```
model{
# Likelihood
  for( i in 1 : N ) {
     y[i] ~ dnorm(mu[i],tau)
     mu[i]<- alpha+ beta*( x[i]-mean(x[]) )
  }
# Prior distributions
  tau ~ dgamma(0.001,0.001)
  sigma <- 1 / sqrt(tau)
  alpha ~ dnorm(0.0,1.0E-6)
  beta ~ dnorm(0.0,1.0E-6)
}
```

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *ΕΝΑ ΑΠΛΟ ΠΑΡΑΔΕΙΓΜΑ (LINE.BUG)*

**Data (ΧΩΡΙΣ OUTLIER):**

```
list(x = c(1, 2, 3, 4, 5),
     y= c(1, 3, 3, 3, 5), N = 5)
```

**Data(2) (ΜΕ OUTLIER):**

```
list(x = c(1, 2, 3, 4, 5),
     y= c(1, 7, 3, 3, 5), N = 5)
```

**Inits:**

```
list(alpha = 0, beta = 0, tau = 1)
```

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.1. ΕΛΕΓΧΟΣ ΚΑΤΑΛΟΙΠΩΝ*

Εξετάζουμε την εκ-των-υστέρων κατανομή των καταλοίπων ($y_i$=data)

- Κατάλοιπα (Residual): $r_i = y_i - E(y_i)$

```
resid[i]<-y[i]-mu[i]
```

- Τυποποιημένα Κατάλοιπα (Standardized Residual): $sr_i = r_i/\sqrt{V(y_i)} = \{y_i - E(y_i)\}/\sqrt{V(y_i)}$

```
sresid[i]<-r[i]*sqrt(tau)
```

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.1. ΕΛΕΓΧΟΣ ΚΑΤΑΛΟΙΠΩΝ*

ΑΠΟΤΕΛΕΣΜΑΤΑ (DATA ΧΩΡΙΣ OUTLIER)

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| resid[1] | -0.38 | 1.1 | 0.023 | -2.3 | -0.4 | 1.6 |
| resid[2] | 0.82 | 0.71 | 0.017 | -0.42 | 0.81 | 2.1 |
| resid[3] | 0.027 | 0.65 | 0.016 | -1.0 | 0.013 | 1.1 |
| resid[4] | -0.77 | 1.0 | 0.022 | -2.0 | -0.79 | 0.51 |
| resid[5] | 0.43 | 1.5 | 0.031 | -1.4 | 0.42 | 2.3 |

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| sresid[1] | -0.49 | 0.83 | 0.018 | -2.1 | -0.49 | 1.1 |
| sresid[2] | 1.0 | 0.69 | 0.017 | -0.3 | 1.0 | 2.4 |
| sresid[3] | 0.013 | 0.45 | 0.0086 | -0.9 | 0.017 | 0.9 |
| sresid[4] | -1.0 | 0.7 | 0.018 | -2.4 | -0.98 | 0.32 |
| sresid[5] | 0.52 | 0.8 | 0.016 | -1.1 | 0.52 | 2.1 |

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.1. ΕΛΕΓΧΟΣ ΚΑΤΑΛΟΙΠΩΝ*

ΑΠΟΤΕΛΕΣΜΑΤΑ (DATA ΜΕ OUTLIER)

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| resid[1] | -2.0 | 3.7 | 0.066 | -8.3 | -2.0 | 4.5 |
| resid[2] | 3.6 | 2.4 | 0.046 | -0.69 | 3.6 | 8.0 |
| resid[3] | -0.72 | 2.1 | 0.04 | -4.3 | -0.75 | 2.9 |
| resid[4] | -1.1 | 3.2 | 0.051 | -5.3 | -1.1 | 3.3 |
| resid[5] | 0.53 | 4.7 | 0.072 | -5.6 | 0.48 | 6.8 |

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| sresid[1] | -0.73 | 0.85 | 0.017 | -2.4 | -0.74 | 0.86 |
| sresid[2] | 1.3 | 0.78 | 0.021 | -0.13 | 1.3 | 2.9 |
| sresid[3] | -0.28 | 0.47 | 0.0067 | -1.2 | -0.28 | 0.63 |
| sresid[4] | -0.42 | 0.58 | 0.009 | -1.6 | -0.42 | 0.72 |
| sresid[5] | 0.17 | 0.77 | 0.014 | -1.4 | 0.17 | 1.7 |

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.2. ΠΡΟΒΛΕΠΟΜΕΝΕΣ ΤΙΜΕΣ ΚΑΙ ΚΑΤΑΛΟΙΠΑ*

Εξετάζουμε τις τιμές που αναμένουμε (προβλέπουμε) με βάση το μοντέλο ($y_i^{pred}$)

```
y.pred[i]~dnorm( mu[i], tau)
```

Επίσης εξετάζουμε και τις αποστάσεις των προβλεπόμενων τιμών από τις παρατηρηρούμενες

- Τυποποιημένα Κατάλοιπα (Predicted Standardized Residual):

  $sr_i^{pred} = (y_i - y_i^{pred})/\sqrt{V(y_i)}$

```
sr.pred[i]<-(y[i]-y.pred[i])*sqrt(tau)
```

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.2. ΠΡΟΒΛΕΠΟΜΕΝΕΣ ΤΙΜΕΣ ΚΑΙ ΚΑΤΑΛΟΙΠΑ*

ΑΠΟΤΕΛΕΣΜΑΤΑ (DATA ΧΩΡΙΣ OUTLIER)

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| y.pred[1] | 1.4 | 1.6 | 0.03 | -1.5 | 1.4 | 4.3 |
| y.pred[2] | 2.2 | 1.4 | 0.022 | -0.33 | 2.2 | 4.8 |
| y.pred[3] | 3.0 | 1.3 | 0.022 | 0.31 | 3.0 | 5.5 |
| y.pred[4] | 3.9 | 1.4 | 0.025 | 1.3 | 3.8 | 6.7 |
| y.pred[5] | 4.6 | 1.6 | 0.026 | 1.8 | 4.6 | 7.6 |

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| sr.pred[1] | -0.5 | 1.3 | 0.024 | -3.1 | -0.48 | 2.1 |
| sr.pred[2] | 0.98 | 1.2 | 0.02 | -1.3 | 0.97 | 3.3 |
| sr.pred[3] | 0.02 | 1.1 | 0.019 | -2.1 | 0.014 | 2.0 |
| sr.pred[4] | -1.0 | 1.2 | 0.022 | -3.5 | -1.0 | 1.3 |
| sr.pred[5] | 0.49 | 1.3 | 0.024 | -2.0 | 0.49 | 3.0 |

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.2. ΠΡΟΒΛΕΠΟΜΕΝΕΣ ΤΙΜΕΣ ΚΑΙ ΚΑΤΑΛΟΙΠΑ*

ΑΠΟΤΕΛΕΣΜΑΤΑ (DATA ΜΕ OUTLIER)

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| y.pred[1] | 2.9 | 5.6 | 0.1 | -7.1 | 2.9 | 13.0 |
| y.pred[2] | 3.5 | 4.8 | 0.077 | -5.3 | 3.5 | 12.0 |
| y.pred[3] | 3.7 | 4.6 | 0.075 | -5.5 | 3.8 | 12.0 |
| y.pred[4] | 4.4 | 5.0 | 0.088 | -4.3 | 4.3 | 14.0 |
| y.pred[5] | 4.7 | 5.4 | 0.09 | -5.1 | 4.6 | 15.0 |

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| sr.pred[1] | -0.72 | 1.4 | 0.025 | -3.4 | -0.71 | 1.9 |
| sr.pred[2] | 1.3 | 1.2 | 0.022 | -1.1 | 1.3 | 3.7 |
| sr.pred[3] | -0.27 | 1.1 | 0.019 | -2.4 | -0.27 | 1.8 |
| sr.pred[4] | -0.47 | 1.2 | 0.02 | -2.8 | -0.45 | 1.8 |
| sr.pred[5] | 0.13 | 1.3 | 0.023 | -2.3 | 0.14 | 2.6 |

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ*

**α) Πιθανότητα πιο ακραίας παρατήρησής**

(Chance of more extreme observation): min{P($Y_i$<$y_i$), P($Y_i$>$y_i$)}

```
Y.rep[i]<-dnorm(mu[i],tau)
p.smaller[i]<-step(y[i]-Y.rep[i])
```

Υπολογίζουμε τον εκ-των-υστερων μέσο του p.smaller {E(p.smaller|y)} και μετα παίρνουμε το PMEO= min { E(p.smaller|y), 1-E(p.smaller|y) }.

Αν αυτό είναι μικρό τότε σημαίνει ότι τα δεδομένα είναι συστηματικά μακριά από τις προβλεπόμενες τιμές του μοντέλου.

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ*

**α) Πιθανότητα πιο ακραίας παρατήρησής**

ΑΠΟΤΕΛΕΣΜΑΤΑ

| | DATA ΧΩΡΙΣ OUTLIER | | DATA ΜΕ OUTLIER | |
|---|---|---|---|---|
| **node** | **mean** | **PMEO** | **mean** | **PMEO** |
| p.smaller[1] | 0.36 | 0.36 | 0.30 | 0.30 |
| p.smaller[2] | 0.8 | 0.20 | 0.85 | 0.15 |
| p.smaller[3] | 0.5 | 0.50 | 0.40 | 0.40 |
| p.smaller[4] | 0.2 | 0.20 | 0.35 | 0.35 |
| p.smaller[5] | 0.65 | 0.35 | 0.54 | 0.44 |

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ*

**β) Εκ-των-υστέρων Επίπεδα Σημαντικότητας (Posterior p-values)**

Η λογική είναι η εξής:

- Φτιάχνουμε μια συνάρτηση των δεδομένων $T(\underline{y})$ που ελέγχει μια υπόθεση.
- Με τον ίδιο τρόπο μπορούμε να βρούμε και την κατανομή του $T(y)$ αν ισχύει το μοντέλο μας (δηλαδή να βασιστεί στις προβλεπόμενες τιμές $\underline{y}^{pred}$).
- Η σύγκριση των $T(\underline{y})$ και $T(\underline{y}^{pred})$ μας δίνει τα posterior p-values δηλαδή

$$\textbf{Posterior P-value} = P( T(\underline{y}) < T(\underline{y}^{pred}) )$$

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ*

**β) Εκ-των-υστέρων Επίπεδα Σημαντικότητας (Posterior p-values)**

- Οι συναρτήσεις ελέγχου μπόρουν να γενικευτούν και να περιλαμβάνουν και παραμέτρους δηλαδή

**Posterior P-value = P( $T(\underline{y}, \underline{\theta}) < T(\underline{y}^{pred}, \underline{\theta})$ )**

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ*

**β) Εκ-των-υστέρων Επίπεδα Σημαντικότητας (Posterior p-values)**

- **ΠΑΡΑΔΕΙΓΜΑ**: ΕΛΕΓΧΟΣ ΣΥΜΜΕΤΡΙΑΣ

- **$T(\underline{y}, \underline{\theta}) = \Sigma(y_i-\mu_i)^3$**

```
sresid.pred[i]<-(y.pred[i]-mu[i])*sqrt(tau)
sresid3[i]<-pow( sresid[i] , 3 )
sresid3.pred[i]<-pow( sresid.pred[i] , 3 )
skew.obs<-mean(sresid3[])
skew.pred<-mean(sresid3.pred[])
pval.pred<-step(skew.pred-skew.obs)
```

# 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

## 8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ

**β) Εκ-των-υστέρων Επίπεδα Σημαντικότητας (Posterior p-values)**

⌘ **ΑΠΟΤΕΛΕΣΜΑΤΑ**

$Y_2=2$

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| pval.pred | 0.5018 | 0.5 | 0.005355 | 0.0 | 1.0 | 1.0 |
| skew.obs | -0.01484 | 1.543 | 0.01706 | -3.252 | -0.011 | 3.296 |
| skew.pred | -0.01527 | 1.768 | 0.01759 | -3.918 | -0.01252 | 3.728 |

$Y_2=7$

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| pval.pred | 0.4222 | 0.4939 | 0.005451 | 0.0 | 0.0 | 1.0 |
| skew.obs | 0.4449 | 1.834 | 0.02173 | -2.883 | 0.2151 | 4.781 |
| skew.pred | -0.01527 | 1.768 | 0.01759 | -3.918 | -0.01252 | 3.728 |

$Y_2=10000$

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| pval.pred | 0.1577 | 0.3645 | 0.003941 | 0.0 | 0.0 | 1.0 |
| skew.obs | 2.089 | 2.119 | 0.01967 | 0.09692 | 1.439 | 7.821 |
| skew.pred | -0.01527 | 1.768 | 0.01759 | -3.918 | -0.01252 | 3.728 |

# 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

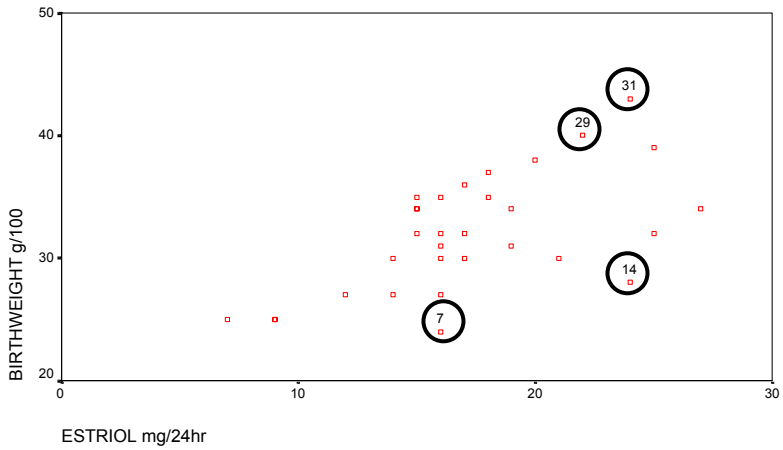
## 8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ

**ΑΠΟΤΕΛΕΣΜΑΤΑ ΑΠΟ ΤΟ estriol.dat**

| node | Mean p.smaller | PMOE | Mean st.res. |
|---|---|---|---|
| p.smaller[31] | 0.9509 | 0.0491 | 1.792 |
| p.smaller[29] | 0.9030 | 0.0970 | 1.327 |
| p.smaller[27] | 0.8720 | 0.1280 | 1.177 |
| p.smaller[22] | 0.8623 | 0.1377 | 1.130 |
| p.smaller[28] | 0.8576 | 0.1424 | 1.122 |
| | | | |
| p.smaller[13] | 0.1416 | 0.1416 | -1.115 |
| p.smaller[6] | 0.1388 | 0.1388 | -1.107 |
| p.smaller[18] | 0.1250 | 0.1250 | -1.226 |
| p.smaller[7] | 0.0358 | 0.0358 | -1.887 |
| p.smaller[14] | 0.0267 | 0.0267 | -2.108 |

# 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

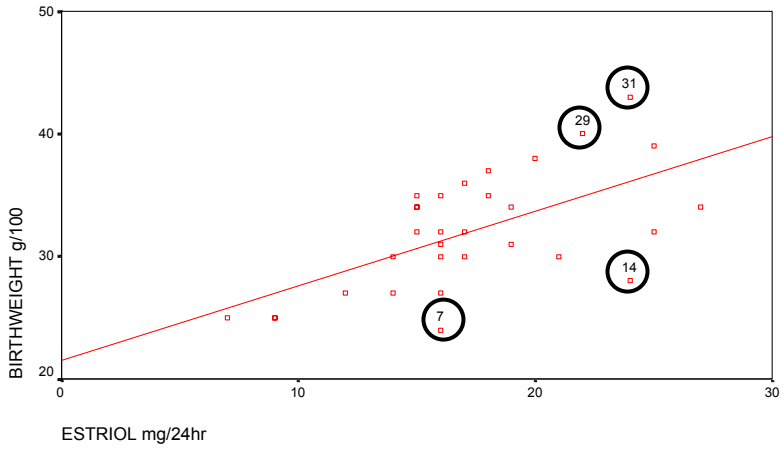
## *8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ*





# 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

## *8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ*

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ*

**ΑΠΟΤΕΛΕΣΜΑΤΑ ΑΠΟ ΤΟ estriol.dat**

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| pval.pred | 0.6041 | 0.489 | 0.004522 | 0.0 | 1.0 | 1.0 |
| skew.obs | -0.2509 | 0.6361 | 0.006642 | -1.59 | -0.2214 | 0.9583 |
| skew.pred | -0.003227 | 0.6939 | 0.007235 | -1.428 | -0.005572 | 1.413 |

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ*

**γ) ΔΙΑΓΝΩΣΤΙΚΑ ΤΩΝ IBRAHIM + LAUD**

- $L_m^2=\Sigma (y_i^{pred}- y_i)^2$
- $M_m = f(\underline{y}^{pred}|\underline{y},\underline{\theta})$ εκ-των-υστέρων πιθάνότητα εμφάνισης των $\underline{y}^{pred}$

  $E(M_m|\underline{y})$ = Posterior Bayes Factor (Aitkin, 1991)
- $M_m^{-1/n}$ = μετριέται σε ίδιες μονάδες με τα y

**ΜΕΙΟΝΕΚΤΗΜΑΤΑ**

- $M_m$ δεν μπορεί να υπολογιστεί εύκολα λόγω μεγάλων ή μικρών τιμών
- Δεν λαμβάνει υπόψη του τον αριθμό των παραμέτρων του κάθε μοντέλου.

# 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

## *8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ*

### γ) ΔΙΑΓΝΩΣΤΙΚΑ ΤΩΝ IBRAHIM + LAUD

```
# model 1
   birth.pred[i]~dnorm( mu[i], tau )
   loglike1.pred[i]<- -0.5*log(2*pi)+0.5*log(tau)-
        0.5*pow( birth.pred[i]-mu[i],2 )*tau
   like1[i]<- exp( loglike1[i] )
#  model 0
   birth0.pred[i]~dnorm( mu0[i], tau0 )
   loglike0.pred[i]<- -0.5*log(2*pi)+0.5*log(tau0)-
        0.5*pow( birth0.pred[i]-mu0[i],2 )*tau0
   like0[i]<- exp( loglike0[i] )
#  Lm criterion
     Lm1<- sum( ss1[] );  Lm0<- sum( ss0[] )
#
#  Mm criterion
#  Mm1<-exp( Lm1 ); Mm0<-exp( Lm0 )
#
   Mm1.star<-exp( -Lm1/n ); Mm0.star<-exp( -Lm0/n )
```

# 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

## *8.3. ΔΙΑΓΝΩΣΤΙΚΑ ΜΕΤΡΑ ΠΡΟΒΛΕΠΤΙΚΩΝ ΤΙΜΩΝ*

### ΑΠΟΤΕΛΕΣΜΑΤΑ(estriol.dat)

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| Lm0 | 1451.0 | 396.0 | 5.536 | 832.1 | 1401.0 | 2371.0 |
| Lm1 | 942.9 | 264.2 | 3.793 | 535.5 | 905.9 | 1576.0 |
| Mm0 | 1.035E-36 | 1.0E-10 | 1.414E-12 | 0.0 | 7.254E-41 | 1.415E-36 |
| Mm0.star | 20.28 | 3.906 | 0.05565 | 14.35 | 19.72 | 29.53 |
| Mm1 | 1.185E-33 | 1.0E-10 | 1.414E-12 | 2.382E-43 | 4.773E-38 | 1.606E-33 |
| Mm1.star | 16.39 | 3.128 | 0.04665 | 11.44 | 15.99 | 23.71 |

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.4. Προβλεπτικά Μέτρα Πάραλληλης Δειγματολειψίας*

*(Parallel Sampling Predictive Measures)*

- **Στα παραπάνω μέτρα τρέχουμε τη αλυσίδα του κάθε μοντέλου και συγκρίνουμε στο τέλους τους μέσους των μέτρων τους ($AIC_m$, $BIC_m$, $L_m$, $M_m$)**
- Στη σύγκριση με παράλληλες αλυσίδες τρέχουμε όλα τα μοντέλα μαζί και συγρκίνουμε τα μέτρα με διαφορές (π.χ. $\Delta AIC=AIC_1-AIC_0$) και πιθανότητες επικράτησης (π.χ. $P(AIC_1>AIC_0)$ ).

## 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

### *8.4. Προβλεπτικά Μέτρα Πάραλληλης Δειγματολειψίας*

*(Parallel Sampling Predictive Measures)* # parallel differences

```
  DBIC10<- BIC0-BIC1
  DAIC10<- AIC0-AIC1
  diff[1]<-DAIC10
  diff[2]<-DBIC10
  diff[3]<- Lm0-Lm1
  diff[4]<-Mm1-Mm0
  diff[5]<-Mm0.star-Mm1.star
  PBF<-Mm1/Mm0
  PBFn<-Mm0.star/Mm1.star
# parallel probabilities
  for (i in 1:5){ prob[i]<-step(diff[i]) }
```

# 8…ΠΡΟΒΛΕΠΤΙΚΟΙ ΔΙΑΓΝΩΣΤΙΚΟΙ ΕΛΕΓΧΟΙ ΤΩΝ ΜΟΝΤΕΛΩΝ

## *8.4. Προβλεπτικά Μέτρα Πάραλληλης Δειγματολειψίας*

***(Parallel Sampling Predictive Measures)***

**ΑΠΟΤΕΛΕΣΜΑΤΑ (estriol.dat)**

| node | | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|---|
| PBF | Post.BF | 1.067E+12 | 4.445E+13 | 6.202E+11 | 1.062E-4 | 772.0 | 5.358E+9 |
| PBFn | | 1.28 | 0.3432 | 0.005331 | 0.7444 | 1.239 | 2.06 |
| diff[1] | AIC | 11.29 | 3.277 | 0.04846 | 4.078 | 11.47 | 17.95 |
| diff[2] | BIC | 9.854 | 3.277 | 0.04846 | 2.644 | 10.03 | 16.52 |
| diff[3] | Lm | 508.0 | 477.7 | 6.617 | -364.8 | 483.3 | 1528.0 |
| diff[4] | Mm | 1.184E-33 | 1.0E-10 | 1.414E-12 | -8.809E-37 | 3.394E-38 | 1.606E-33 |
| diff[5] | Mm.star | 3.886 | 5.025 | 0.07427 | -5.609 | 3.785 | 14.31 |
| prob[1] | AIC | 0.9964 | 0.05989 | 8.406E-4 | 1.0 | 1.0 | 1.0 |
| prob[2] | BIC | 0.9922 | 0.08797 | 0.001298 | 1.0 | 1.0 | 1.0 |
| prob[3] | Lm | 0.8694 | 0.337 | 0.005005 | 0.0 | 1.0 | 1.0 |
| prob[4] | Mm | 0.794 | 0.4044 | 0.006368 | 0.0 | 1.0 | 1.0 |
| prob[5] | Mm.star | 0.794 | 0.4044 | 0.006368 | 0.0 | 1.0 | 1.0 |

# 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

## *9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ*

- Δεδομένα από το βιβλίο του Healy (1988).
- Μεταβλητή A = Κατάσταση Ασθενή (περισσότερο ή λιγότερο σοβαρή),
- Μεταβλητή B = Θεραπεία Αντιτοξίνης (Ναι/Όχι)
- Μεταβλητή C (μεταβλητή απόκρισης) = Επιβίωση Ασθενή (Ναι/Όχι).
- Χρησιμοποιούμε Λογιστική Παλινδρόμιση
- Λεπτομέρειες μπορείτε να βρείτε στις δημοσιεύσεις Dellaportas et al. (2000, BGLM).
- Επιπλέον παραδείγματα με επιλογή μεταβλητών στο BUGS μπορείτε να βρείτε στη δημοσίευση Ntzoufras (2002, JSS).
- Για ένα απλό έλεγχο υποθέσεων και σύγκριση κατανομών μπορείτε να δείτε τη δημοσίευση Katsis and Ntzoufras (2004, TR).

## 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

### *9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ*

| | | **ΕΠΙΒΙΩΣΗ(C)** | |
|---|---|---|---|
| **Κατάσταση (A)** | **Αντιτοξίνη(B)** | **Όχι** | **Ναι** |
| **Σοβαρή** | **Ναι** | 15 | 6 |
| | **Όχι** | 22 | 4 |
| **Λιγ.Σοβαρή** | **Ναι** | 5 | 15 |
| | **Όχι** | 7 | 5 |

## 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

### *9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ*

- Μεταβλητή Απόκρισης: C = Επιβίωση

Ανεξάρτητες Μεταβλητές

- Μεταβλητή A = Κατάσταση Ασθενή
- Μεταβλητή B = Θεραπεία Αντιτοξίνη
- Αλληλεπίδραση AB (interaction term)= Condition*Antitoxin

Μοντέλα ύπο διερεύνηση

- Μοντέλο 1: AB = 1+A+B+AB
- Μοντέλο 2: A+B = 1+A+B
- Μοντέλο 3: A = 1+A
- Μοντέλο 4: B = 1+B
- Μοντέλο 5: μηδενικό ή σταθερό (null/ constant)= 1

## 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

### 9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ

**Εκ-των-Προτέρων Κατανομές**

- Εκ-των-προτέρων διακύμανση= 4 X 2
- Εκ-των-προτέρων πιθανότητα κάθε μοντέλου $f(\gamma_A, \gamma_B, \gamma_{AB})=1/5$:

$$f(\gamma_A, \gamma_B, \gamma_{AB})= f(\gamma_{AB})\, f(\gamma_A \mid \gamma_{AB})\, f(\gamma_B \mid \gamma_{AB})$$

## 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

### 9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ

**Εκ-των-Προτέρων Κατανομές**

$$f(\gamma_A, \gamma_B, \gamma_{AB})= f(\gamma_{AB})\, f(\gamma_A \mid \gamma_{AB})\, f(\gamma_B \mid \gamma_{AB})$$

$\gamma_{AB} \sim$ Bernoulli(1/5)

$\gamma_A \mid \gamma_{AB} \sim$ Bernoulli($p_A$)
$p_A=0.5(1- \gamma_{AB}) + \gamma_{AB}$
δηλαδή $p_A=1$ αν $\gamma_{AB}=1$ και $p_A=0.5$ αν $\gamma_{AB}=0$

Όμοια για την $f(\gamma_B \mid \gamma_{AB})$
$\gamma_B \mid \gamma_{AB} \sim$ Bernoulli($p_B$)
$p_B=0.5(1- \gamma_{AB}) + \gamma_{AB}$

## 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

*9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ*

**DATA IN WINBUGS**

```
r[] n[] x[,1] x[,2] x[,3] x[,4]
 5 12 1 -1   -1   1
 4 26 1  1   -1 -1
15 20 1 -1    1 -1
 6 21 1  1    1  1
```

## 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

*9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ*

Κώδικα WINBUGS για την Επιλογή Μεταβλητών με τον Δειγματολείπτη Gibbs (Gibbs Variable Selection - GVS)

**Το μοντέλο**

```
for (i in 1:N) {
    r[i]~dbin(p[i],n[i]);
    logit(p[i])<-b[1] +  x[i,2]* g[2]* b[2]
                      +  x[i,3]* g[3]* b[3]
                      +  x[i,4]* g[4]* b[4];
  }
```

## 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

### *9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ*

### Η εκ-των-προτέρων κατανομές

```
b[1]~dnorm(0.0,0.0001); }
for (i in 2:N) {
  tau[i]<-g[i]/8+(1-g[i])/(se[i]*se[i]);
  bpriorm[i]<-mean[i]*(1-g[i]);
   b[i]~dnorm(bpriorm[i],tau[i]); }
```

| | PROPOSAL/ PSEUDOPRIOR | PRIOR |
|---|---|---|
| | g[i]=0 | g[i]=1 |
| bpriorm[i] | mean[i] | 0.0 |
| tau[i] | $1/se[i]^2$ | 1/8 |

## 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

### *9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ*

### Η εκ-των-προτέρων κατανομές

| | PROPOSAL/ PSEUDOPRIOR | PRIOR |
|---|---|---|
| | g[i]=0 | g[i]=1 |
| bpriorm[i] | mean[i] | 0.0 |
| tau[i] | $1/se[i]^2$ | 1/8 |

mean[i] και se[i] υπολογίζονται από την posterior του πλήρες μοντέλου AB.

## 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

### *9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ*

**Η εκ-των-προτέρων πιθανότητες των μοντέλων**

g[]: διάνυσμα με 4 στοιχεία (όσα και οι παράμετροι/όροι του μοντέλου

**ΚΩΔΙΚΑΣ**

```
for (i in 1:4){ g[i]~dbern(pi[i]) }
pi[1]<- 1.0
pi[2]<- 0.5*(1-g[4])+g[4]
pi[3]<- 0.5*(1-g[4])+g[4]
pi[4]<- 0.20
```

## 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

### *9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ*

**Εκτίμηση των εκ-των-υστέρων πιθανοτήτων των μοντέλων στο WINBUGS**

```
#     defining model code
#     0 for  constant, 1 for [A], 2 for [B], 3 for [A][B],
#     6 for [AB]
#
    mdl<-g[2]+2*g[3]+3*g[4];
    pmdl[1]<-equals(mdl,0)
    pmdl[2]<-equals(mdl,1)
    pmdl[3]<-equals(mdl,2)
    pmdl[4]<-equals(mdl,3)
    pmdl[5]<-equals(mdl,6)
```

# 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

## *9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ*

## 1… Τρέχουμε το πλήρες μοντέλο θέτοντας

| node | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|
| b[1] | -0.4889 | 0.2823 | 0.008722 | -1.039 | -0.4786 | 0.07779 |
| b[2] | -0.8919 | 0.2798 | 0.009499 | -1.446 | -0.8926 | -0.3501 |
| b[3] | 0.5866 | 0.2824 | 0.009441 | 0.06599 | 0.5809 | 1.15 |
| b[4] | -0.1773 | 0.272 | 0.008021 | -0.6896 | -0.1754 | 0.3716 |

θετουμε mean[i] και se[i] τις παραπάνω τιμές.

# 9…ΜΠΕΫΖΙΑΝΗ ΕΠΙΛΟΓΗ ΜΕΤΑΒΛΗΤΩΝ ΜΕ ΤΟ WINBUGS

## *9.1. ΠΑΡΑΔΕΙΓΜΑ ΣΕ 2X2X2 ΠΙΝΑΚΑ ΣΥΝΑΦΕΙΑΣ*

## 2… Τρέχουμε το GVS (5000+10000 iterations)

| node | | mean | sd | MC error | 2.5% | median | 97.5% |
|---|---|---|---|---|---|---|---|
| b[1] | | -0.4526 | 0.2656 | 0.002836 | -0.9756 | -0.4486 | 0.05737 |
| b[2] | | -0.9166 | 0.263 | 0.002535 | -1.44 | -0.9135 | -0.4159 |
| b[3] | | 0.5823 | 0.2759 | 0.002749 | 0.05192 | 0.5811 | 1.128 |
| b[4] | | -0.1748 | 0.2736 | 0.00251 | -0.7112 | -0.1759 | 0.369 |
| g[1] | | 1.0 | 0.0 | 1.0E-12 | 1.0 | 1.0 | 1.0 |
| g[2] | A | 0.9837 | 0.1266 | 0.001383 | 1.0 | 1.0 | 1.0 |
| g[3] | B | 0.501 | 0.5 | 0.004707 | 0.0 | 1.0 | 1.0 |
| g[4] | | 0.0496 | 0.2171 | 0.002251 | 0.0 | 0.0 | 1.0 |
| pmdl[1] | | 0.0045 | 0.06693 | 7.437E-4 | 0.0 | 0.0 | 0.0 |
| pmdl[2] | | 0.4945 | 0.5 | 0.004804 | 0.0 | 0.0 | 1.0 |
| pmdl[3] | | 0.0118 | 0.108 | 0.00114 | 0.0 | 0.0 | 0.0 |
| pmdl[4] | | 0.4396 | 0.4963 | 0.004209 | 0.0 | 0.0 | 1.0 |
| pmdl[5] | | 0.0496 | 0.2171 | 0.002251 | 0.0 | 0.0 | 1.0 |

Model A+B

Model A

## 10…ΕΠΙΛΟΓΗ ΜΟΝΤΕΛΩΝ

**Ανοικτό θέμα**

**Η Μπεϋζιανή προσέγγιση δίνει λύσεις αλλά έχει (ακόμα) προβλήματα**

**Υπάρχουν αρκετές άλλες προσεγγίσεις τις οποίες δεν καλύψαμε.**

# Bayesian Biostatistics Using BUGS

## ΤΕΛΟΣ ΤΕΤΑΡΤΟΥ ΜΑΘΗΜΑΤΟΣ ΜΑΘΗΜΑΤΟΣ

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Economics & Business

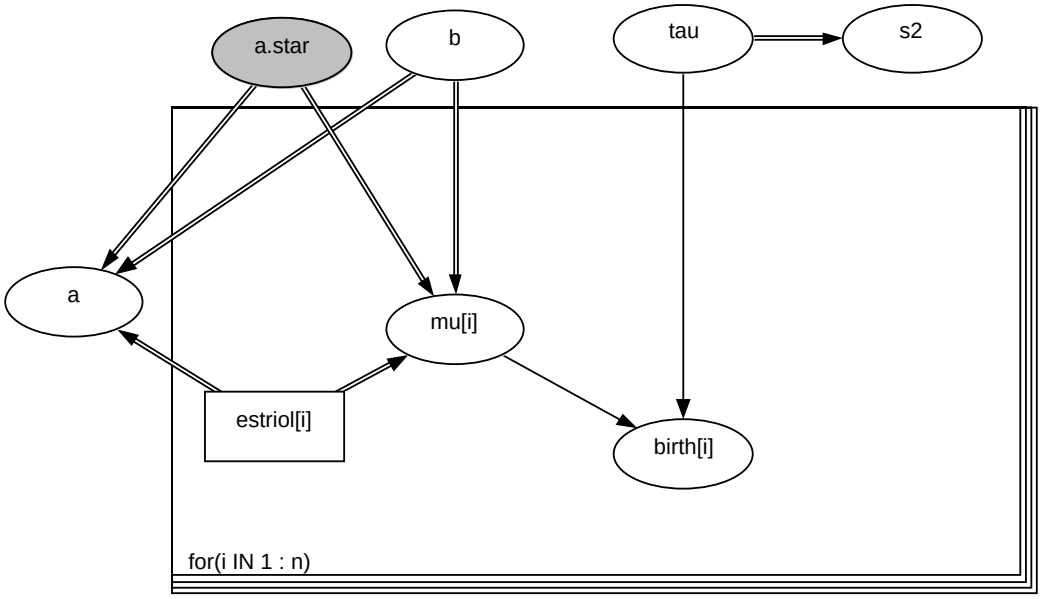
# ΠΑΡΑΡΤΗΜΑ Δ1 (4ου ΜΑΘΗΜΑΤΟΣ): ΠΑΡΑΔΕΙΓΜΑΤΑ ΕΛΕΓΧΩΝ ΥΠΟΘΕΣΕΩΝ, ΕΠΙΛΟΓΗΣ ΜΟΝΤΕΛΩΝ ΚΑΙ ΜΕΤΑΒΛΗΤΩΝ

## 1 ΠΑΡΑΔΕΙΓΜΑ WINBUGS 1: Ένας Απλός Έλεγχος Υπόθεσης (ESTRIOL DATASET)

```
model estriol;
{
#       definition of likelihood function
#
        for (i in 1:n) {
                birth[i]~dnorm( mu[i], tau ); # random component
                mu[i]<-a.star+gamma*b*(estriol[i]-mean(estriol[])); # systematic component
                                        #       & link function
        }
#       prior distributions
#
        a.star~dnorm( 0, 1.0E-04 ); # normal prior for a
        b~dnorm( 0, 1.575); # normal prior for b
                  gamma~dbern(0.5);
        tau~dgamma( 1.0E-04 , 1.0E-04 ); # gamma prior for precision
        s2<-1/tau;
        a<-a.star-b*mean(estriol[]);
}
list(a.star=0.0, b=0.0, tau=1.0,gamma=1)

list(n=31)
estriol[] birth[]
7               25
9               25
9               25
12              27
14              27
16              27
16              24
14              30
16              30
16              31
17              30
19              31
21              30
24              28
15              32
16              32
17              32
25              32
27              34
15              34
15              34
15              35
16              35
19              34
18              35
17              36
18              37
20              38
22              40
25              39
24              43
END
```

| name: | a.star | type: | stochastic | density: | dnorm | |
|---|---|---|---|---|---|---|
| mean | 0.0 | precision | 1.0E-6 | lower bound | | upper bound |



# 2 ΠΑΡΑΔΕΙΓΜΑ WINBUGS 2: Διαγνωστικά Τέστ και Συγκρίσεις μοντέλων (ESTRIOL DATASET)

```
model estriol_AIC_BIC;
{
#      definition of likelihood function
#
              pi<-3.14
      for (i in 1:n) {
            birth[i]~dnorm( mu[i], tau );                          # random component
            mu[i]<-a.star+b*(estriol[i]-mean(estriol[]));       # systematic component
                                                                  #      & link function
                                    birth.pred[i]~dnorm( mu[i], tau )
                                    loglike1[i]<- -0.5*log(2*pi)+0.5*log(tau)-0.5*pow( birth[i]-mu[i],2 )*tau
                                    loglike1.pred[i]<- -0.5*log(2*pi)+0.5*log(tau)-0.5*pow( birth.pred[i]-mu[i],2 )*tau
                                    like1[i]<- exp( loglike1[i] )
#
#                           model m_0
            birth0[i]<-birth[i]
                                     birth0[i]~dnorm( mu0[i], tau0 );                          # random component
            mu0[i]<-a0;                                              # systematic component
                                                                  #      & link function
                                    birth0.pred[i]~dnorm( mu0[i], tau0 )
                                    loglike0[i]<- -0.5*log(2*pi)+0.5*log(tau0)-0.5*pow( birth0[i]-mu0[i],2 )*tau0
                                    loglike0.pred[i]<- -0.5*log(2*pi)+0.5*log(tau0)-0.5*pow( birth0.pred[i]-mu0[i],2 )*tau0
                                    like0[i]<- exp( loglike0[i] )
#
#
                                    ss1[i] <- pow( birth.pred[i]-birth[i], 2 )
                                    ss0[i] <- pow( birth0.pred[i]-birth0[i], 2 )
      }
#      prior distributions for model m1
#
      a.star~dnorm( 0, 1.0E-04 ); # normal prior for a
      b~dnorm( 0, 1.0E-04 ); # normal prior for b
      tau~dgamma( 1.0E-04 , 1.0E-04 ); # gamma prior for precision
      s2<-1/tau;
      a<-a.star-b*mean(estriol[]);
#
#            prior distributions for model m0
      a0~dnorm( 0, 1.0E-04 ); # normal prior for a
      tau0~dgamma( 1.0E-04 , 1.0E-04 ); # gamma prior for precision
#
#            Bayesian versions of LogLikelihood
              L1<-sum( loglike1[] )
              L0<-sum( loglike0[] )
#
#            Bayesian versions of BIC
              BIC1<- -2*L1 + 3*log(n)
              BIC0<- -2*L0 + 2*log(n)
#
#            Bayesian versions of AIC
              AIC1<- -2*L1 + 3*2
              AIC0<- -2*L0 + 2*2
#
#            Lm criterion
              Lm1<- sum( ss1[] )
              Lm0<- sum( ss0[] )
#
#            Mm criterion
            Mm1<-exp( sum(loglike1.pred[]) )
            Mm0<-exp( sum(loglike0.pred[]) )
#
            Mm1.star<-exp( -sum(loglike1.pred[])/n )
            Mm0.star<-exp( -sum(loglike0.pred[])/n )
#
# parallel differences
              DBIC10<- BIC0-BIC1
              DAIC10<- AIC0-AIC1
              diff[1]<-DAIC10
              diff[2]<-DBIC10
              diff[3]<- Lm0-Lm1
              diff[4]<-Mm1-Mm0
```

```
            diff[5]<-Mm0.star-Mm1.star
            PBF<-Mm1/Mm0
            PBFn<-Mm0.star/Mm1.star
#
#           parallel probabilities
            for (i in 1:5){
                        prob[i]<-step(diff[i])
            }
}
```

# 3 ΠΑΡΑΔΕΙΓΜΑ WINBUGS 3: Διαγνωστικά Τέστ και Συγκρίσεις μοντέλων (LINE DATASET)

```
model{
            pi<-3.14
#
#           Likelihood
            for( i in 1 : N ) {
                        y[i] ~ dnorm(mu[i],tau)
                        mu[i] <- alpha + beta * (x[i] - mean(x[]))
#
#                       residuals
                          resid[i]<-y[i]-mu[i]
                          sresid[i]<-resid[i]*sqrt(tau)
#
#                       predicted values
                         y.pred[i]~dnorm(mu[i],tau)
#
#             predicted standardised residuals
                        sr.pred[i]<-(y[i]-y.pred[i])*sqrt(tau)
#
#           p.smaller
            p.smaller[i]<-step(y[i]-y.pred[i])
#
                        sresid.pred[i]<-(y.pred[i]-mu[i])*sqrt(tau)
                        sresid3[i]<-pow( sresid[i] , 3 )
                        sresid3.pred[i]<-pow( sresid.pred[i] , 3 )
                        }
#
#           Prior distributions
            tau ~ dgamma(0.001,0.001)
            sigma <- 1 / sqrt(tau)
            alpha ~ dnorm(0.0,1.0E-6)
            beta ~ dnorm(0.0,1.0E-6)
#
#
            skew.obs<-mean(sresid3[])
            skew.pred<-mean(sresid3.pred[])
            pval.pred<-step(skew.pred-skew.obs)
   }
```

**Data(WITHOUT OUTLIER)**: list(x = c(1, 2, 3, 4, 5), y= c(1, 3, 3, 3, 5), N = 5)

**Data(WITH OUTLIER)**: list(x = c(1, 2, 3, 4, 5), y= c(1, 10000, 3, 3, 5), N = 5)

**Inits**: list(alpha = 0, beta = 0, tau = 1)

# 4 ΠΑΡΑΔΕΙΓΜΑ WINBUGS 4: Πλήρες Μοντέλο για το Antitoxin dataset

```
model {
#
# model likelihood
for (i in 1:4) {
    r[i]~dbin(p[i],n[i]);
    logit(p[i])<-b[1] +  x[i,2]* b[2]
                      +  x[i,3]* b[3]
                      +  x[i,4]* b[4];  }
# priors and pseudopriors

b[1]~dnorm(0.0, 0.0001)
for (i in 2:4) {  b[i]~dnorm( 0.0 , 0.0001) ; }

}
```

**DATA**

```
r[] n[] x[,1] x[,2] x[,3] x[,4]
 5 12 1 -1  -1  1
 4 26 1  1  -1 -1
15 20 1 -1   1 -1
 6 21 1  1   1  1
END
```

**INITS**

```
list(  b=c(1,0,0,0) )
```

# 5 ΠΑΡΑΔΕΙΓΜΑ WINBUGS 5: Gibbs Variable Selection για το Antitoxin dataset

```
model {
#
#  model likelihood
for (i in 1:4) {
    r[i]~dbin(p[i],n[i]);
    logit(p[i])<-b[1] +  x[i,2]* g[2]* b[2]
                      +  x[i,3]* g[3]* b[3]
                      +  x[i,4]* g[4]* b[4];  }
# priors and pseudopriors
b[1]~dnorm( 0.0, 0.0001 )
for (i in 2:4) {
       tau[i]<-g[i]/8+(1-g[i])/(se[i]*se[i]);
       bpriorm[i]<-mean[i]*(1-g[i]);
  b[i]~dnorm(bpriorm[i],tau[i]); }

       mdl<-g[2]+2*g[3]+3*g[4];
    pmdl[1]<-equals(mdl,0)
    pmdl[2]<-equals(mdl,1)
    pmdl[3]<-equals(mdl,2)
    pmdl[4]<-equals(mdl,3)
    pmdl[5]<-equals(mdl,6)

for (i in 1:4) { g[i]~dbern( pi[i] ) }
pi[1]<-1.0
pi[2]<-0.5*(1-g[4])+g[4]
pi[3]<-0.5*(1-g[4])+g[4]
pi[4]<-0.20
}
```

**DATA**

```
r[] n[] x[,1] x[,2] x[,3] x[,4]
 5 12 1 -1  -1  1
 4 26 1  1  -1 -1
15 20 1 -1   1 -1
 6 21 1  1   1  1
END
```

**PROPOSAL / PSEUDOPRIOR VALUES**

```
 mean[]  se[]
-0.4889         0.2823
-0.8919         0.2798
 0.5866         0.2824
-0.1773         0.272
END
```

**INITS**

```
list( g=c(1,1,1,1),  b=c(1,0,0,0))
```

## ΠΑΡΑΡΤΗΜΑ Δ2: ΒΙΒΛΙΟΓΡΑΦΙΑ ΚΑΙ ΔΗΜΟΣΙΕΥΣΕΙΣ ΣΧΕΤΙΚΕΣ ΜΕ BAYESIAN MODEL AND VARIABLE SELECTION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# Gibbs Variable Selection Using BUGS

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**Abstract**

In this paper we discuss and present in detail the implementation of Gibbs variable selection as defined by Dellaportas *et al.* (2000, 2002) using the BUGS software (Spiegelhalter *et al.* , 1996a,b,c). The specification of the likelihood, prior and pseudo-prior distributions of the parameters as well as the prior term and model probabilities are described in detail. Guidance is also provided for the calculation of the posterior probabilities within BUGS environment when the number of models is limited. We illustrate the application of this methodology in a variety of problems including linear regression, log-linear and binomial response models.

*Keywords*: Logistic regression; Linear regression; MCMC; Model selection.

## 1 Introduction

In Bayesian model averaging or model selection we focus on the calculation of posterior model probabilities which involve integrals analytically tractable only in certain restricted cases. This obstacle has been overcomed via the construction of efficient MCMC algorithms for model and variable selection problems.

A variety of MCMC methods have been proposed for variable selection including the *Stochastic Search Variable Selection* (SSVS) of George and McCulloch (1993), the *reversible jump Metropolis* by Green (1995), the model selection approach of Carlin and Chib (1995) the variable selection sampler of Kuo and Mallick (1998) and the *Gibbs variable selection* (GVS) by Dellaportas *et al.* (2000, 2002).

The primary aim of this paper is to clearly illustrate how we can utilize BUGS (Spiegelhalter *et al.* , 1996a, see also `www.mrc-bsu.cam.ac.uk/bugs/welcome.shtml`) for the implementation of variable selection methods. We concentrate on Gibbs variable selection introduced by Dellaportas *et al.* (2000, 2002) with independent prior distributions. Extension to other Gibbs samplers such as George and McCullogh (1993) SSVS and Kuo and Mallick (1998) sampler is straightforward; see for example in Dellaportas *et al.* (2000). Finally, application of Carlin and Chib (1995) algorithm is also illustrated using BUGS by Spiegelhalter *et al.* (1996c).

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The paper is organised into three sections additional to this introductory one. Section 2 briefly describes the general Gibbs variable selection algorithm as introduced by Dellaportas *et al.* (2002), Section 3 provides detailed guidance for implementation in BUGS and finally Section 4 presents three illustrated examples.

## 2 Gibbs Variable Selection

Many statistical models may be represented naturally as $(s, \boldsymbol{\gamma}) \in \mathcal{S} \times \{0,1\}^p$, where the indicator vector $\boldsymbol{\gamma}$ identifies which of the $p$ possible sets of covariates are present in the model and $s$ denotes other structural properties of the model. For example, for a generalised linear model, $s$ may describe the distribution, link function and variance function, and the linear predictor may be written as

$$\boldsymbol{\eta} = \sum_{j=1}^{p} \gamma_j \boldsymbol{X}_j \boldsymbol{\beta}_j \tag{1}$$

where $\boldsymbol{X}_j$ is the design matrix and $\boldsymbol{\beta}_j$ the parameter vector related to the $j$th term. In the following, we restrict attention to variable selection aspects assuming that $s$ is known and we concentrate on the estimation of the posterior distribution of $\boldsymbol{\gamma}$.

We denote the likelihood of each model by $f(\boldsymbol{y}|\boldsymbol{\beta}, \boldsymbol{\gamma})$ and the prior by $f(\boldsymbol{\beta}, \boldsymbol{\gamma}) = f(\boldsymbol{\beta}|\boldsymbol{\gamma})f(\boldsymbol{\gamma})$, where $f(\boldsymbol{\beta}|\boldsymbol{\gamma})$ is the prior of the parameter vector $\boldsymbol{\beta}$ conditional on the model structure $\boldsymbol{\gamma}$ and $f(\boldsymbol{\gamma})$ is the prior of the corresponding model. Moreover, $\boldsymbol{\beta}$ can be partitioned into two vectors $\boldsymbol{\beta}_{\boldsymbol{\gamma}}$ and $\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}$ corresponding to parameters of variables included or excluded from the model. Under this approach the prior can be rewritten as

$$f(\boldsymbol{\beta}, \boldsymbol{\gamma}) = f(\boldsymbol{\beta}_{\boldsymbol{\gamma}}|\boldsymbol{\gamma}) f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}}, \boldsymbol{\gamma}) f(\boldsymbol{\gamma})$$

while, since we are using the linear predictor (1), the likelihood can be simplified to

$$f(\boldsymbol{y}|\boldsymbol{\beta}, \boldsymbol{\gamma}) = f(\boldsymbol{y}|\boldsymbol{\beta}_{\boldsymbol{\gamma}}, \boldsymbol{\gamma}).$$

From the above it is clear that the components of the vector $\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}$ do not affect the model likelihood and hence the posterior distribution within each model $\boldsymbol{\gamma}$ is given by

$$f(\boldsymbol{\beta}|\boldsymbol{\gamma}, \boldsymbol{y}) = f(\boldsymbol{\beta}_{\boldsymbol{\gamma}}|\boldsymbol{\gamma}, \boldsymbol{y}) \times f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}}, \boldsymbol{\gamma})$$

where $f(\boldsymbol{\beta}_{\boldsymbol{\gamma}}|\boldsymbol{\gamma}, \boldsymbol{y})$ is the actual posterior of the parameters of model $\boldsymbol{\gamma}$ and $f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}}, \boldsymbol{\gamma}, \boldsymbol{y})$ is the conditional prior distribution of the parameters not included in the model $\boldsymbol{\gamma}$. We may now interpret $f(\boldsymbol{\beta}_{\boldsymbol{\gamma}}|\boldsymbol{\gamma})$ as the actual prior of the model while the distribution $f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}}, \boldsymbol{\gamma})$ may be called as 'pseudoprior' since the parameter vector $\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}$ does not gain any information from the data and does not influence the actual posterior of the parameters of each model, $f(\boldsymbol{\beta}_{\boldsymbol{\gamma}}|\boldsymbol{\gamma}, \boldsymbol{y})$. Although this pseudoprior does not influence the posterior distributions of interest, it influences the performance of the MCMC algorithm and hence it should be specified with caution.

The sampling procedure is summarised by the following steps:

1. We sample the parameters included in the model by the posterior

$$f(\boldsymbol{\beta}_{\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}, \boldsymbol{\gamma}, \boldsymbol{y}) \propto f(\boldsymbol{y}|\boldsymbol{\beta}, \boldsymbol{\gamma}) f(\boldsymbol{\beta}_{\boldsymbol{\gamma}}|\boldsymbol{\gamma}) f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}}, \boldsymbol{\gamma}) \tag{2}$$

2. Sample the parameters excluded from the model from the pseudoprior

$$f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}},\boldsymbol{\gamma},\boldsymbol{y}) \propto f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}},\boldsymbol{\gamma}) \tag{3}$$

3. Sample each variable indicator $\gamma_j$ from a Bernoulli distribution with success probability $O_j/(1+O_j)$; where $O_j$ is given by

$$O_j = \frac{f(\boldsymbol{y}|\boldsymbol{\beta},\gamma_j=1,\boldsymbol{\gamma}_{\setminus j})}{f(\boldsymbol{y}|\boldsymbol{\beta},\gamma_j=0,\boldsymbol{\gamma}_{\setminus j})}\,\frac{f(\boldsymbol{\beta}|\gamma_j=1,\boldsymbol{\gamma}_{\setminus j})}{f(\boldsymbol{\beta}|\gamma_j=0,\boldsymbol{\gamma}_{\setminus j})}\,\frac{f(\gamma_j=1,\boldsymbol{\gamma}_{\setminus j})}{f(\gamma_j=0,\boldsymbol{\gamma}_{\setminus j})}. \tag{4}$$

The selection of priors and pseudopriors is a very important aspect in model selection. Here we briefly present the simplest approach where $f(\boldsymbol{\beta}|\boldsymbol{\gamma})$ is given a product of independent prior and pseudoprior densities: $f(\boldsymbol{\beta}|\boldsymbol{\gamma}) = \prod_{j=1}^{p} f(\boldsymbol{\beta}_j|\boldsymbol{\gamma}_j)$. In such case, a usual and simple choice of $f(\boldsymbol{\beta}_j|\boldsymbol{\gamma}_j)$ is given by

$$f(\boldsymbol{\beta}_j|\boldsymbol{\gamma}_j) = (1-\gamma_j)f(\boldsymbol{\beta}_j|\gamma_j=0) + \gamma_j f(\boldsymbol{\beta}_j|\gamma_j=1) \tag{5}$$

resulting to actual prior distribution $f(\boldsymbol{\beta}_{\boldsymbol{\gamma}}|\boldsymbol{\gamma}) = \prod_{\gamma_j=1} f(\boldsymbol{\beta}_j|\boldsymbol{\gamma}_j)$ and pseudoprior $f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}},\boldsymbol{\gamma}) = \prod_{\gamma_j=0} f(\boldsymbol{\beta}_j|\boldsymbol{\gamma}_j)$.

Note that the above prior can be efficiently used in any model selection problem if we orthogonalize the data matrix and then perform model choice using the new transformed data (see Clyde *et al.* , 1996). If orthogonalization is undesirable then we may need to construct more sophisticated and flexible algorithms such as reversible jump MCMC; see Green (1995) and Dellaportas *et al.* (2002).

The simplified prior (5) and model formulation such as (1), result in the following full conditional posterior

$$f(\boldsymbol{\beta}_j|\boldsymbol{\gamma},\boldsymbol{\beta}_{\setminus j},\boldsymbol{y}) \propto f(\boldsymbol{y}|\boldsymbol{\beta}_{\boldsymbol{\gamma}},\boldsymbol{\gamma}) \prod_{k=1}^{n} f(\beta_k|\gamma_k) \propto \begin{cases} f(\boldsymbol{y}|\boldsymbol{\gamma},\boldsymbol{\beta})f(\boldsymbol{\beta}_j|\gamma_j=1) & \gamma_j=1 \\ f(\boldsymbol{\beta}_j|\gamma_j=0) & \gamma_j=0 \end{cases} \tag{6}$$

indicating that the pseudoprior, $f(\boldsymbol{\beta}_j|\gamma_j=0)$ does not affect the posterior distribution of each model coefficient.

Similarly to George and McCulloch (1993), we use a mixture of Normal distribution for model parameters.

$$f(\boldsymbol{\beta_j}|\gamma_j=1) \equiv N(0,\Sigma_j) \;\text{ and }\; f(\boldsymbol{\beta_j}|\gamma_j=0) \equiv N(\bar{\mu}_j, S_j). \tag{7}$$

The hyperparameters $\bar{\mu}_j$ and $S_j$ are parameters of the pseudoprior distribution; therefore their choice is only relevant to the behaviour of the MCMC chain and do not affect the posterior distribution. Ideal choices of these parameters are the maximum likelihood or pilot run estimators of the full model (as, for example, in Dellaportas and Forster, 1999). However, in the experimental process, we noted that an automatic selection of $\bar{\mu}_j = 0$ and $S_j = \Sigma_j/k^2$ with $k = 10$ has also been proven an adequate choice; for more details see Ntzoufras (1999). This 'automatic selection' uses the properties of the prior distributions with 'large' and 'small' variance introduced in SSVS by George and McCulloch (1993). The parameter $k$ is now only a pseudoprior parameter and therefore it does not affect the posterior distribution. Suitable calibration of this parameter assists the chain to move better (or worse) between different models.



The prior proposed by Dellaportas and Forster (1999) for contingency tables, is also adopted here for logistic regression models with categorical explanatory variables (see Dellaportas *et al.* , 2000). Alternatively, for generalized linear models, Raftery (1996) has proposed to select the prior covariance matrix using elements from the data matrix multiplied by a hyperparameter. The latter was selected in such way that the effect of the prior distribution on the posterior odds becomes minimal.

When no restrictions on the model space are imposed then a common prior for the term indicators $\gamma_j$ is $f(\gamma_j) = Bernoulli\,(1/2)$, whereas in other cases (for example, hierarchical or graphical log-linear models) it is required that $f(\gamma_j|\boldsymbol{\gamma}_{\setminus j})$ depends on $\gamma_{\setminus j}$; for more details see Chipman (1996) and Section 3.4.

Other Gibbs samplers for model selection have also been proposed by George and McCulloch (1993), Carlin and Chib (1995) and Kuo and Mallick (1998). Detailed comparison and discussion of the above methods is given by Dellaportas *et al.* (2000, 2002). Implementation of Carlin and Chib methodology in BUGS is illustrated by Spiegelhater *et al.* (1996c, page 47) while an additional simple example of Gibbs variable selection methods is provided by Dellaportas *et al.* (2000).

# 3 Applying Gibbs Variable Selection Using BUGS

In this section we provide detailed guidance for implementing Gibbs variable selection using BUGS software. It is divided into four sub-sections involving the definition of the model likelihood $f(\boldsymbol{y}|\boldsymbol{\beta},\boldsymbol{\gamma})$, the specification of the prior distributions $f(\boldsymbol{\beta}|\boldsymbol{\gamma})$ and $f(\boldsymbol{\gamma})$, and, finally, the direct calculation of posterior model probabilities using BUGS.

## 3.1 Definition of likelihood

The linear predictor of type (1) used in Gibbs variable selection and Kuo and Mallick sampler can be easily incorporated in BUGS using the following code

```
for (i in 1:N) { for(j in 1:p) {z[i,j]<-x[i,j]*b[j]*g[j]}}
for (i in 1:N) {
            eta[i] <-sum(z[i,]) ;
            y[i]~distribution [ parameter1, parameter2 ] }
```

where

- `N` denotes the sample size,
- `p` the number of total variables under consideration,
- `x[i,j]` is the $i,j$ component of the data or design matrix $\boldsymbol{X}$,
- `y[i]` is $i$ element of the response vector $\boldsymbol{y}$,
- `b[j]` is the $j$ element of the parameter vector $\boldsymbol{\beta}$,

- `g[j]` is the inclusion indicator for $j$ element of $\boldsymbol{\gamma}$,
- `z[i,j]` is a matrix used to simplify calculations,
- `eta[i]` is the $i$ element of linear predictor vector $\boldsymbol{\eta}$ and should be substituted by the corresponding link function, for example `logit(p[i])` in binomial logistic regression,
- `distribution` should be substituted by appropriate BUGS command for the distribution that the user prefers (for example `dnorm` for normal distribution),
- `parameter1,parameter2` should be substituted according to distribution chosen, for example for the normal distribution with mean $\mu_i$ and variance $\tau^{-1}$ we may use `mu[i], tau`.

For the usual normal, binomial and Poisson models the model formulations are given by the following lines of BUGS code

**Normal:**
```
for (i in 1:N) { mu[i] <- sum(z[i,]) ;
                 y[i]~dnorm (mu[i], tau)  }
```
where `mu[i]` is the expected value for the $i$th observation and `tau` is the precision of the regression model.

**Poisson:**
```
for (i in 1:N) { log(lambda[i]) <- sum(z[i,]);
                 y[i] ~ dpois(lambda[i])}
```
where `lambda[i]` is the Poisson mean for the $i$th observation.

**Binomial:**
```
for (i in 1:N) { logit(p[i]) <- sum(z[i,]);
                  y[i] ~ dbin(p[i], n[i])}
```
where `p[i]` is the probability of success and `n[i]` is the total number of Bernoulli trials for the $i$th binomial experiment. Alternative link functions maybe used by substituting `logit(p[i])` by `probit(p[i])` or `cloglog(p[i])` for $\Phi^{-1}(p)$ and $log(-log(1-p))$; where $\Phi$ is the standardised normal cumulative distribution function.

### 3.2 Definition of Prior Distribution of Parameter Vector

When we use independent priors as given by (5) and each covariate parameter vector is univariate, the definition of the prior is straightforward. Our prior is a mixture of independent normal distributions

$$\beta_j \sim \gamma_j N(0, \Sigma_j) + (1-\gamma_j) N(\bar{\mu}_j, S_j), \quad j = 1, 2, \ldots, p \tag{8}$$

where $\bar{\mu}_j$, $S_j$ are the mean and variance respectively used in the corresponding pseudoprior distributions and $\Sigma_j$ is the prior variance, when the $j$ term is included in the model. In order to use (8) in BUGS we write

- `b[j]~dnorm( bpriorm[j], tprior[j])` denoting $\beta_j \sim N(m_j, \tau_j^{-1})$,
- `bpriorm[j] <- (1-g[j])*mean[j]` denoting $m_j = (1-\gamma_j)\bar{\mu}_j$,



- `tprior[j] <- g[j]*t[j]+(1-g[j])*pow(se[j],-2)` denoting $\tau_j = (1-\gamma_j)S_j^{-1} + \gamma_j \Sigma_j^{-1}$,

for $j = 1, 2, \ldots, p$; where $m_j$ and $\tau_j$ are the prior mean and precision for $\beta_j$ depending on $\gamma_j$ and `t[j], se[j], mean[j], bpriorm[j], tprior[j]` are the BUGS variables for $\Sigma_j^{-1}$, $\sqrt{S_j}$, $\bar{\mu}_j$, $m_j$ and $\tau_j$, respectively.

When we consider a categorical explanatory variable $j$ with $J > 2$ categories then the corresponding parameter vector $\boldsymbol{\beta}_j$ will be multivariate with dimension $d_j = J - 1$. In such cases we denote by $p$ and $d(> p)$ the dimensions of $\boldsymbol{\gamma}$ and the full parameter vector $\boldsymbol{\beta}$, respectively. Therefore, we need one variable to facilitate the association between these two vectors. This vector is denoted by the BUGS variable `pos`. The `pos` vector, which has dimension equal to the dimension of $\boldsymbol{\beta}$, takes values from $1, 2, ..., p$ and denotes that kth element of the parameter vector $\boldsymbol{\beta}$ is associated with the $\gamma_{pos_k}$ binary indicator for all $k = 1, 2, ..., d$.

For illustration, let us consider an ANOVA model with two categorical variables $X_1$ and $X_2$ with 3 and 4 categories respectively. Then, the terms under consideration are $X_0, X_1, X_2$ and $X_{12}$; where $X_0$ denotes the constant term and $X_{12}$ the interaction between the terms $X_1$ and $X_2$. The corresponding dimensions are $d_{X_0} = 1$, $d_{X_1} = 2$, $d_{X_2} = 3$ and $d_{X_{12}} = d_{X_1} \times d_{X_2} = 6$. Then, we set the `pos` vector equal to

```
pos <- c ( 1, 2,2, 3,3,3, 4,4,4,4,4,4 )
```

to state that the first parameter corresponds to the first term ($X_0$), parameters 2-3 correspond to the second term ($X_1$), parameters 4-6 correspond to the third term ($X_2$) and parameters 7-12 correspond to the fourth term ($X_{12}$). Finally, we use another vector called `gtemp` of dimension $d$ which is given by

```
gtemp[i] <- g[ pos[i] ]
```

for all $i = 1, \ldots, d$. The vector `gtemp` is used in the likelihood instead of the `g` vector. For details see example 1 and the associated BUGS code in the Appendix.

Moreover, the definition of the prior distribution when factors or terms with many parameters are considered is more complicated. For example a mixture of multivariate normal prior distributions as given by (5) can be expressed as a multivariate normal distribution on the 'full' parameter vector $\boldsymbol{\beta}$. Therefore we may write in BUGS

- `b[ ] ~ dmnorm( bpriorm[ ], Tau[,])` denoting $\boldsymbol{\beta} \sim N_d(\boldsymbol{m}, \boldsymbol{T}^{-1})$,
- `bpriorm[k]<-(1-g[pos[k]])*mean[k]` denoting $m_k = (1-\gamma_{pos_k})\bar{\mu}_k$,
- `Tau[k,l] <- g[pos[k]]*g[pos[l]]*t[k,l]+ +(1-g[pos[k]]*g[pos[l]])*equals(k,l)*pow(se[k],-2)` denoting that

$$T_{kl} = \begin{cases} [\boldsymbol{\Sigma}^{-1}]_{kl} & \text{when } \gamma_{pos_k} = \gamma_{pos_l} = 1 \\ se_k^{-2} & \text{when } k = l \ \& \ \gamma_{pos_k} = 0 \\ 0 & \text{otherwise} \end{cases} \quad \text{for } k, l = 1, 2, \ldots, d;$$

where $N_d$ is the d-dimensional normal distribution; $\mathbf{m}^T = (m_1, m_2, \ldots, m_d)$ and $\mathbf{T}$ are the prior mean vector and precision matrix depending on $\boldsymbol{\gamma}$; $\bar{\mu}_k$ is the corresponding pilot run estimate for $k$ element of model parameter vector $\boldsymbol{\beta}$; $\boldsymbol{\Sigma}$ is the constructed prior covariance matrix for the whole parameter vector $\boldsymbol{\beta}$ when we use for each $\boldsymbol{\beta}_j$ the multivariate extension of prior distribution (8); $T_{kl}$ and $[\boldsymbol{\Sigma}^{-1}]_{kl}$ is

the $k$ row and $l$ column elements of $\boldsymbol{T}$ and $\boldsymbol{\Sigma}^{-1}$ matrices respectively; and `Tau[,]`, `t[,]` are the BUGS matrices for $\boldsymbol{T}$ and $\boldsymbol{\Sigma}^{-1}$, respectively. An illustration of usage of such prior distribution is given in example 1.

### 3.3 Implementation of Other Gibbs Samplers for Variable Selection

SSVS and Kuo and Mallick sampler can easily be applied with minor modifications in the above code. In SSVS the prior (8) is used with $\bar{\mu}_j = 0$ and $S_j = \Sigma_j / k_j^2$, where $k_j^2$ should be large enough in order that $\beta_j$ will be close to zero when $\gamma_j = 0$. For selection of the prior parameters in SSVS see semiautomatic prior selection of George and McCulloch (1993). The above restriction can easily be applied in BUGS by

```
bpriorm[j] <- 0
tprior[j] <- t[j]*g[j]+(1-g[j])*t[j]*pow(k[j],2) .
```

Moreover, the likelihood in SSVS should be slightly modified by substituting the first line of the code in Section 3.1 with

```
for (i in 1:N) { for (j in 1:p) { z[i,j]<-x[i,j]*b[j]}}.
```

Kuo and Mallick sampler uses prior on $\boldsymbol{\beta}$ that does not depend on model indicator $\boldsymbol{\gamma}$. Therefore the specification of the prior is the same as in simple modelling using BUGS. Moreover, the likelihood definition is the same as in Gibbs variable selection described in Section 3.1.

### 3.4 Definition of Prior Term Probabilities

In order to apply any variable selection method in BUGS we need to define the prior probabilities $f(\boldsymbol{\gamma})$. When we are vague about models we may set $f(\boldsymbol{\gamma}) = 1/M$, where $M$ is the number of all models under consideration. When the explanatory variables do not involve interactions (for example in linear regression) then the number of models under consideration is $2^p$. In these situations the latent variables $\gamma_j$ can be treated as $a-priori$ independent and therefore set in BUGS

- `g[j]` $\sim$ `dbern(0.5)` denoting that $\gamma_j \sim Bernoulli(0.5)$.

for all $j = 1, 2, \ldots, p$. This prior results to $f(\boldsymbol{\gamma}) = 2^{-p}$ for all $\boldsymbol{\gamma} \in \{0,1\}^p$. When we are dealing with models using categorical explanatory variables with interaction terms, such as $ANOVA$ or log-linear models, we usually want to restrict attention to hierarchical models. The conditional distributions of $f(\gamma_j | \boldsymbol{\gamma}_{\setminus j})$ need to be specified in such way that $f(\boldsymbol{\gamma}) = 1/M$ when $\boldsymbol{\gamma}$ is referring to hierarchical model and $f(\boldsymbol{\gamma}) = 0$ otherwise.

For example, in a two way $ANOVA$ we have three terms under consideration; the main effects A,B and the interaction AB. All possible models are eight, while the hierarchical ones are only five ($constant, [A], [B], [A][B]$ and $[AB]$). Therefore, we wish to specify $f(\boldsymbol{\gamma}) = 0.20$ for the above five models and $f(\boldsymbol{\gamma}) = 0$ for the rest. This can be applied by setting in BUGS



- `g[3]` $\sim$ `dbern(0.2)` denoting that $\gamma_{AB} \sim Bernoulli(0.2)$.
- `pi` $<-$ `g[3]+0.5(1-g[3])` denoting that $\pi = \gamma_{AB} + 0.5 * (1 - \gamma_{AB})$,
- `for (i in 1:2) { g[j]` $\sim$ `dbern(pi) }` denoting that for all $i \in \{A, B\}$, $\gamma_j | \gamma_{AB} \sim Bernoulli(\pi)$.

From the above it is evident that

$$\begin{aligned} f([AB]) &= f(\gamma_{AB} = 1) f(\gamma_A = 1 | \gamma_{AB} = 1) f(\gamma_B = 1 | \gamma_{AB} = 1) \\ &= 0.2 \times 1 \times 1 = 0.2 \,, \end{aligned}$$

$$\begin{aligned} f([A][B]) &= f(\gamma_{AB} = 0) f(\gamma_A = 1 | \gamma_{AB} = 0) f(\gamma_B = 1 | \gamma_{AB} = 0) \\ &= 0.8 \times 0.5 \times 0.5 = 0.2 \,. \end{aligned}$$

Using similar calculations we find that $f(\boldsymbol{\gamma}) = 0.2$ for all five models under consideration. For further relevant discussion and application see Chipman (1996). For implementation in BUGS see examples 1 and 3.

### 3.5 Calculating Model Probabilities in Bugs

In order to directly calculate the posterior model probabilities in BUGS and avoid saving large MCMC output we may use matrix type variables with dimension equal to the number of models. Using a simple coding such as $1 + \sum_{j=1}^{p} \gamma_j 2^{j-1}$ we transform the vector $\boldsymbol{\gamma}$ in a unique, for each model index (noted by `mdl`) for which `pmdl[mdl]=1` and `pmdl[j]=0` for all `j` $\neq$ `mdl`. The above statements can be written in BUGS with the code

```
for (j in 1:p) { index[j] <- pow(2,j-1) }
mdl <- 1+inprod(g[ ], index[ ])
for (m in 1:mdl) { pmdl[m] <- equals(m,mdl) }
```

Then using the command `stats(pmdl)` in BUGS environment (or cmd file) we can monitor the posterior model probabilities. This is feasible only if the number of models is limited and therefore applicable only in some simple problems.

## 4 Examples

The implementation of three illustrated examples are briefly presented. The first example is a $3 \times 2 \times 4$ contingency table used to illustrate how to handle factors with more than two levels. Example 2 provides model selection details in a regression type problem involving many different error distributions while example 3 is a simple logistic regression problem with random effects. In all examples posterior probabilities are presented while the associated BUGS codes are provided in the appendix. Additional details (for example, convergence plots) are omitted since our aim is just to illustrate how to use BUGS for variable selection.

### 4.1 Example 1: $3 \times 2 \times 4$ Contingency Table

This example is a $3 \times 2 \times 4$ contingency table presented by Knuiman and Speed (1988) where 491 individuals are classified by three categorical variables: obesity (O: low,average,high), hypertension (H: yes,no) and alcohol consumption (A: 1,1–2,3–5,6+ drinks per day); see Table 1.

| | | Alcohol Intake | | | |
|---|---|---|---|---|---|
| **Obesity** | **High BP** | 0 | 1-2 | 3-5 | 6+ |
| Low | Yes | 5 | 9 | 8 | 10 |
| | No | 40 | 36 | 33 | 24 |
| Average | Yes | 6 | 9 | 11 | 14 |
| | No | 33 | 23 | 35 | 30 |
| High | Yes | 9 | 12 | 19 | 19 |
| | No | 24 | 25 | 28 | 29 |

Table 1: $3 \times 2 \times 4$ Contingency Table: Knuiman and Speed (1988) Dataset.

The full model is given by

$$n_{ilk} \sim Poisson(\lambda_{ilk}), \quad log(\lambda_{ilk}) = m + o_i + h_l + a_k + oh_{il} + oa_{ik} + ha_{lk} + oha_{ilk},$$

for $i = 1, 2, 3,\ l = 1, 2,\ k = 1, 2, 3, 4$. The above model can be rewritten with likelihood given by (1) where $\boldsymbol{\beta}$ can be divided to $\boldsymbol{\beta}_j$ sub-vectors with $j \in \{\emptyset, O, H, OH, A, OA, HA, OHA\}$; where $\beta_\emptyset = m$, $\boldsymbol{\beta}_O^T = [o_2, o_3]$, $\beta_H = h_2$, $\boldsymbol{\beta}_{OH}^T = [oh_{22}, oh_{32}]$, $\boldsymbol{\beta}_A^T = [a_2, a_3, a_4]$, $\boldsymbol{\beta}_{OA}^T = [oa_{22}, oa_{23}, oa_{32}, oa_{33}]$, $\boldsymbol{\beta}_{HA}^T = [ha_{22}, ha_{23}]$ and $\boldsymbol{\beta}_{OHA}^T = [oha_{222}, oha_{223}, oha_{322}, oha_{323}]$. Each $\boldsymbol{\beta}_j$ is a multivariate vector and therefore each prior distribution involves mixture multivariate normal distributions. We use sum-to-zero constraints and prior variance $\Sigma_j$ as in Dellaportas and Forster (1999). We restrict attention in hierarchical models including always the main effects since we are mainly interested for relationships between the categorical factors. Under these restrictions, the models under consideration are nine (9). In order to forbid moves to non hierarchical models we use the following BUGS code to define the prior model probabilities:

- `g[8] ~ dbern(0.1111)` for $\gamma_{OHA} \sim Bernoulli(1/9)$.
- `pi <- g[8]+0.5*(1-g[8])` for $\pi = \gamma_{OHA} + 0.5 * (1 - \gamma_{OHA})$,
- `for (i in 5:7) { g[j]~dbern(pi) }` for $\gamma_j | \gamma_{OHA} \sim Bernoulli(\pi)$ for all $i \in \{OH, OA, HA\}$,
- `for (j in 1:4) { g[j] ~ dbern(1) }` for $\gamma_j \sim Bernoulli(1)$ for all $i \in \{constant, O, H, A\}$.

These priors result to prior probability for all hierarchical models equal to 1/9 and zero otherwise.

Results using both pilot run pseudoprior and automatic pseudoprior with $k = 10$ are summarised in Table 2. The data give 'strong' evidence in favour of the model



| | Posterior Model Probabilities (%) | | | |
|---|---|---|---|---|
| Pseudopriors | k=10 | | Pilot Run | |
| Burn-in | 1,000 | 10,000 | 1,000 | 10,000 |
| Iterations | 1,000 | $10 \times 10,000$ | 1,000 | $10 \times 10,000$ |
| Models | | | | |
| $[O][H][A]$ | 62.80 | 68.87 | 65.20 | 67.80 |
| $[OH][A]$ | 36.90 | 30.53 | 34.40 | 31.63 |
| $[O][HA]$ | 0.20 | 0.40 | 0.10 | 0.43 |
| $[OH][HA]$ | 0.10 | 0.20 | 0.30 | 0.14 |
| Terms | | | | |
| $\gamma_{OH} = 1$ | 37.00 | 30.63 | 34.70 | 31.77 |
| $\gamma_{HA} = 1$ | 0.30 | 0.20 | 0.40 | 0.57 |

Table 2: $3 \times 2 \times 4$ Contingency Table: Posterior Model Probabilities Using BUGS.

of independence. Model [OH][A], in which obesity and hypertension are depending on each other given the level of alcohol consumption, is the model with the second highest posterior probability. All the other models have probability lower than 1%.

### 4.2 Example 2: Stacks Dataset

This example involves stack-loss data analysed by Spiegelhalter *et al.* (1996b, page 27) using the Gibbs sampling. The dataset features 21 daily responses of stack loss ($y$) which measures the amount of ammonia escaping with covariates the air flow ($x_1$), temperature ($x_2$) and acid concentration ($x_3$). Spiegelhalter *et al.* (1996b) consider regression models with four different error structures (normal, double exponential, logistic and Student's $t_4$ distributions). They also consider the cases of ridge and simple independent regression models. We extend their work by applying Gibbs variable selection on all these eight cases.

The full model will be

$$y_i \sim D(\mu_i, \tau),\ \mu_i = \beta_0 + \beta_1 z_{i1} + \beta_2 z_{i2} + \beta_3 z_{i3},\ i = 1, \ldots, 21$$

where $D_i(\mu_i, \tau)$ is the distribution of the errors with mean $\mu_i$ and variance $\tau^{-1}$ which here is assumed to be normal, or double exponential, or logistic or $t_4$; where $z_{ij} = (x_{ij} - \bar{x}_j)/sd(x_j)$ are the standardised covariates. The ridge regression approach assumes a further restriction that the $\beta_j$ for $j = 1, 2, 3$ are exchangable (Lindley and Smith, 1972) and therefore we have $\beta_j \sim N(0, \phi^{-1})$. We use 'non-informative' priors with prior precision equal to $10^{-3}$ for the independent regression and for $\phi$ in ridge regression we use gamma prior with parameters equal to $10^{-3}$. Since we do not wish to apply any restriction on the model space we use the prior probabilities $\gamma_j \sim Bernoulli(1/2)$ for $j = 1, 2, 3$ which results to prior probability of 1/8 for all possible models. For the pilot run pseudoprior parameters we use the posterior values as given Spiegelhalter *et al.* (1996b).

Tables 3 and 4 provide the results from all eight distinct cases using pilot run pseudopriors. In all cases flow of air ($z_1$) has posterior probability of inclusion higher than 99%. The temperature ($z_2$) seems to be also an important term with

posterior probability of inclusion varying from 39% to 96%. The last term ($z_3$) which measures the acid concentration in air has low posterior probabilities of inclusion which are less than 5% for simple independence models and less than 20% for 'ridge' regression models.

| | Independence Regression | | | |
|---|---|---|---|---|
| Models | Normal | D.Exp. | Logistic | $t_4$ |
| *Constant* | 0.00 | 0.00 | 0.00 | 0.00 |
| $z_1$ | 14.12 | 58.48 | 41.19 | 56.46 |
| $z_2$ | 0.56 | 0.01 | 0.02 | 0.00 |
| $z_1 + z_2$ | 81.25 | 38.64 | 55.25 | 40.46 |
| $z_3$ | 0.00 | 0.00 | 0.00 | 0.00 |
| $z_1 + z_3$ | 0.63 | 1.75 | 1.35 | 1.82 |
| $z_2 + z_3$ | 0.05 | 0.00 | 0.00 | 0.00 |
| $z_1 + z_2 + z_3$ | 3.39 | 1.11 | 2.18 | 1.26 |
| Terms | | | | |
| $\gamma_{z_1} = 1$ | 99.30 | 99.98 | 99.97 | 100.00 |
| $\gamma_{z_2} = 1$ | 84.90 | 39.76 | 57.45 | 41.72 |
| $\gamma_{z_3} = 1$ | 4.30 | 2.86 | 3.53 | 3.08 |

Table 3: Stacks Dataset: Posterior Model Probabilities in Independence Regression (burn-in 10,000, samples of $10 \times 10,000$, with pilot run pseudopriors).

| | Ridge Regression | | | |
|---|---|---|---|---|
| Models | Normal | D.Exp. | Logistic | $t_4$ |
| *Constant* | 0.00 | 0.00 | 0.00 | 0.00 |
| $z_1$ | 3.26 | 22.54 | 14.42 | 13.30 |
| $z_2$ | 0.05 | 0.00 | 0.00 | 0.00 |
| $z_1 + z_2$ | 79.79 | 65.00 | 73.32 | 70.92 |
| $z_3$ | 0.00 | 0.00 | 0.00 | 0.00 |
| $z_1 + z_3$ | 0.44 | 1.74 | 1.32 | 1.86 |
| $z_2 + z_3$ | 0.00 | 0.00 | 0.00 | 0.00 |
| $z_1 + z_2 + z_3$ | 16.46 | 10.72 | 11.01 | 13.92 |
| Terms | | | | |
| $\gamma_{z_1} = 1$ | 100.00 | 100.00 | 100.00 | 100.00 |
| $\gamma_{z_2} = 1$ | 96.50 | 75.72 | 84.33 | 84.84 |
| $\gamma_{z_3} = 1$ | 16.10 | 12.46 | 12.33 | 15.78 |

Table 4: Stacks Dataset: Posterior Model Probabilities in Ridge Regression (burn-in 10,000, samples of $10 \times 10,000$, with pilot run pseudopriors).

### 4.3 Example 3: Seeds Dataset, Logistic Regression with Random Effects

This example involves the examination of a proportion of seeds that germinated on 21 plates. For these 21 plates we have recorded the seed (bean or cucumber) and the type of root extract. This data set is analysed by Spiegelhalter *et al.* (1996b, page 10) using BUGS; for more details see references there in. The model



is a logistic regression with 2 categorical explanatory variables and random effects. The full model will be written

$$y_{ilk} \sim Bin(n_{ilk}, p_{ilk}),\ log\left(\frac{p_{ilk}}{1-p_{ilk}}\right) = m + a_i + b_l + ab_{il} + w_k,$$

for $i, l = 1, 2$ and $k = 1, \ldots, 21$; where $y_{ilk}$ and $n_{ilk}$ is the number of seeds germinated and total number of seeds respectively for $i$ seed, $l$ type of root extract and $k$ plate; $w_k$ is the random effect for the $k$ plate.

We use sum-to-zero constraints for both fixed and random effects. Following Dellaportas and Forster (1999) we use prior variance for the fixed effects $\Sigma = 4 \times 2$. The prior for the precision of the random effects is considered to be a gamma distribution with parameters equal to $10^{-3}$. The pseudoprior parameters were taken from a pilot chain of the saturated model. The models under consideration are ten. The prior term probabilities for the fixed effects are assigned similarly as in the example for two-way ANOVA models. For the random effects term indicator we have that $\gamma_w \sim Bernoulli(0.5)$.

| | Fixed Effects | | Random Effects | |
|---|---|---|---|---|
| Models | k=10 | Pilot | k=10 | Pilot |
| *Constant* | 0.00 | 0.00 | 1.21 | 0.99 |
| $[A]$ | 0.00 | 0.00 | 0.22 | 0.07 |
| $[B]$ | 32.34 | 32.07 | 50.61 | 50.75 |
| $[A][B]$ | 3.78 | 3.84 | 7.24 | 7.60 |
| $[AB]$ | 2.80 | 2.83 | 1.80 | 1.85 |
| Total | 38.92 | 38.74 | 61.08 | 61.26 |

Table 5: Seeds Dataset: Posterior Model Probabilities Using BUGS (burn-in 10,000, samples of $10 \times 10,000$).

Table 5 provides the calculated posterior model probabilities. We used both pilot run proposals and automatic pseudoprior with $k = 10$. Both chains gave the same results as expected and the type of root extract ($B$) is the only factor that influences the proportion of germinated gems. The corresponding models with random and fixed effects have posterior probability equal to 51% and 32%, respectively. The marginal posterior probability of random effects is 61% which is about 56% higher than the posterior probability of fixed effects models.

# 5 Appendix: BUGS Codes

Bugs code and all associated data files are freely available in electronic form at the *Journal of Statistical Software* web site `www.jstatsoft.org/v07/i07/` or by electronic mail request.

## 5.1 Example 1

```
model log-linear;
#
#       3x2x4 LOG-LINEAR MODEL SELECTION WITH BUGS (GVS)
#       (c) OCTOBER 1996
#       (c) REVISED OCTOBER 1997
#
const
   terms=8, # number of terms
   N = 24;  # number of Poisson cells
var
        include,    # conditional prior probability for gi
        pmdl[9],    # model indicator vector
        mdl,        # code of model
        b[N],       # model coefficients
        mean[N],    # proposal mean used in pseudoprior
        se[N],      # proposal standard deviation used in
                    # pseudoprior
        bpriorm[N], # prior mean for b depending on g
        Tau[N,N],   # model coefficients precision
        tprior[N,N],# prior value for Tau when all terms
                    # are included in model
        x[N,N],     # design matrix
        z[N,N],     # matrix with z_ij=x_ij b_j g_j, used in
                    # likelihood
        n[N],       # Poisson cells
        pos[N],     # position of each parameter
        lambda[N],  # Poisson mean for each cell
        gtemp[N],   # temporary term indicator vector
        g[terms];   # term indicator vector
data pos,n in "ex2.dat", x in 'ex2des.dat',
     mean, se in 'prop2.dat', tprior in 'cov.dat';
inits in "ex2.in";
{
#
#       associate g[i] with coefficients.
#
        for (i in 1:N) {
                gtemp[i]<-g[pos[i]];
                }
#
#       calculation of the z matrix used in likelihood
#
        for (i in 1:N) {
                for (j in 1:N) {
                        z[i,j]<-x[i,j]*b[j]*gtemp[j]
                }
        }
#
#       model configuration
        for (i in 1:N) {
                log(lambda[i])<-sum(z[i,])
                n[i]~dpois(lambda[i]);
                }
#       defining model code
#       0 for independence model [A][B][C], 1 for [AB][C],
```



```
#       2 for [AC][B],  3 for [AB][AC], 4 for [BC][A],
#       5 for [AB][BC], 6 for [AC][BC], 7 for [AB][BC],
#       15 for [ABC].
#
        mdl<-g[5]+2*g[6]+4*g[7]+8*g[8];
        for (i in 0:7) {
                pmdl[i+1]<-equals(mdl,i)
                }
        pmdl[9]<-equals(mdl,15)
#
#       Prior for b model coefficient
#       Mixture normal depending on current status of g[i]
#
        for (i in 1:N) { for (j in 1:N) {
#
#               GVS using se,mean from pilot run
#               *******************************
#
                Tau[i,j]<-0+tprior[i,j]*(gtemp[i]*gtemp[j])+
                (1-gtemp[i]*gtemp[j])*equals(i,j)/(se[i]*se[i]);
#
#           Automatic proposal using prior similar to SSVS
#                           with k=10
#           ************************************************
#           Tau[i,j]<-tprior[i,j]*pow(100,1-gtemp[i]*gtemp[j]);
#
#            Kuo and Mallick proposal is independent of g[i]
#                      [tau[i]=1/2   and bpriorm[i]=0]
#            ********************************************
#
#
#             Tau[i,j]<-tprior[i,j];
#
        }
#
#               GVS PRIOR M FROM PILOT RUN
#               **************************
#               bpriorm[i]<-mean[i]*(1-gtemp[i]);
#
#               PRIOR M FOR THAT DOES NOT DEPEND ON G.
#               **************************************
#                 bpriorm[i]<-0.0;
        }
        b[]~dmnorm(bpriorm[],Tau[,]);
#
#       defining prior information for gi to
#       allow only hierarchical models with equal probability.
#       We also ignore models nested to the model of
#       independence [A][B][C] since we are interested in
#       associations between factors.
        g[8]~dbern(0.1111111);
        include<-(1-g[8])*0.5+g[8]*1.0;
        g[7]~dbern(include);
        g[6]~dbern(include);
        g[5]~dbern(include);
        for (i in 1:4) {
                g[i]~dbern(1.0);
        }
}
```

## 5.2 Example 2

```
model stacks;
#
#       LINEAR REGRESSION VARIABLE SELECTION WITH BUGS (GVS)
#          BUGS EXAMPLE: STACKS, see BUGS examples vol.1
#
#       (c) OCTOBER 1997
#
const
   p = 3,          # number of covariates
   N = 21,         # number of observations
   models=8,       # number of models under consideration 2^8
   PI = 3.141593;
var
   x[N,p],         # raw covariates
   z[N,p] ,        # standardised covariates
   Y[N],mu[N],     # data and expectations
   stres[N],       # standardised residuals
   outlier[N],     # indicator if |stan res|  > 2.5
   beta0,beta[p], # standardised intercept, coefficients
   b0,b[p],        # unstandardised intercept, coefficients
   phi,            # prior precision of standardised coef.
   tau,sigma,d,    # precision, sd and d.f. of t distribution
   g[p],           # variable indicators
   mdl,            # Model index
   pmdl[models],  # Vector with model indicators
   mean[p],se[p], # pseudoprior mean and se error
   bprior[p],      # Conditional to model Prior prior mean
   tprior[p];      # Conditional to model Prior prior precision
data Y,x in  "STACKS.DAT",
# files with proposed values
mean,se in 'pnorm.dat';   # Normal distribution
#mean,se in 'pdexp.dat';  # Double exponential distribution
#mean,se in 'plogist.dat';# Logistic distribution
#mean,se in 'pt4.dat';    # Student(4) distribution
inits in "STACKS.IN";
{
# Standardise x's and coefficients
  for (j in 1:p) {
      b[j] <- beta[j]/sd(x[,j]) ;
      for (i in 1:N) {
          z[i,j] <- (x[i,j] -  mean(x[,j]))/sd(x[,j]) ;
      }
  }
  b0<-beta0-b[1]*mean(x[,1])-b[2]*mean(x[,2])-b[3]*mean(x[,3]);

# Model
  d <- 4;  # degrees of freedom for t
  for (i in 1:N) {
#
#     Normal Distribution
#     -------------------
      Y[i] ~ dnorm(mu[i],tau);
#
#     Double Exponential Distribution
#     -------------------------------
#     Y[i] ~ ddexp(mu[i],tau);
#
#     Logistic Distribution
#     ---------------------
#     Y[i] ~ dlogis(mu[i],tau);
#
#     Student t4 Distribution
#     -----------------------
```



```
#     Y[i] ~ dt(mu[i],tau,d);
#
      mu[i] <- beta0 + g[1]*beta[1]*z[i,1]+g[2]*beta[2]*z[i,2]
                     + g[3]*beta[3]*z[i,3];
      stres[i] <- (Y[i] - mu[i])/sigma;
#
#     if standardised residual is greater than 2.5 then outlier
      outlier[i]<-step(stres[i] -2.5) + step(-(stres[i]+2.5) );
  }
#
#       Defining Model Code
        mdl<- 1+g[1]*1+g[2]*2+g[3]*4
#
#       defining vector with model indicators
        for (j in 1:models){
        pmdl[j]<-equals(mdl,j);}
# Priors
  beta0 ~  dnorm(0,.00001);
  for (j in 1:p) {
#
#      ******** GVS PRIORS FOR INDEPENDENCE REGRESSION ********
#
#      GVS priors with proposals from pilot run
#       bprior[j]<-(1-g[j])*mean[j];
#       tprior[j] <-g[j]*0.001+(1-g[j])/(se[j]*se[j]);
#
#      GVS priors with proposals a mixture of Normals(0,c^2t^2)
       bprior[j]<-0.0;
       tprior[j] <-pow(100,1-g[j])*0.001;
#
#      ******** GVS PRIORS FOR RIDGE REGRESSION ********
#
#      GVS priors with proposals from pilot run
#       bprior[j]<-(1-g[j])*mean[j];
#       tprior[j] <-g[j]*phi+(1-g[j])/(se[j]*se[j]);
#
#      GVS priors with proposals a mixture of Normals(0,c^2t^2)
#       bprior[j]<-0.0;
#       tprior[j] <-pow(100,1-g[j])*phi;
       beta[j] ~ dnorm(bprior[j],tprior[j]); # coefs independent

  }
  tau ~ dgamma(1.0E-3,1.0E-3);
#
#  phi ~ dgamma(1.0E-3,1.0E-3);
#
#  when we use pilot run based pseudopriors bugs was unable
#  to select update method. Therefore we use an upper limit
#  which makes bugs work with Metropolis instead Gibbs
#
#  phi ~ dgamma(1.0E-3,1.0E-3)I(0,10000);
# standard deviation of error distribution
  sigma <- sqrt(1/tau);             # normal errors
# sigma <- sqrt(2)/tau;             # double exponential errors
# sigma <- sqrt(pow(PI,2)/3)/tau ;  # logistic errors
# sigma <- sqrt(d/(tau*(d-2)));     # errors of t with d d.f.
#
#
# Priors for variable indicators
  for (j in 1:p) { g[j]~ dbern(0.5);}
}
```

### 5.3 Example 3

```
model seedszrogvs;
#
#               LOGISTIC REGRESSION VARIABLE AND
#            RANDOM EFFECTS SELECTION WITH BUGS (GVS)
#
#          BUGS EXAMPLE: SEEDS, see BUGS examples vol.1
#
#       (c) OCTOBER 1997
#

const
   terms=4,  # Number of terms under consideration
   models=16,# number of models under consideration 2^4
   N = 21;   # number of samples
var
   alpha0, alpha1, alpha2, alpha12,  # model coefficients
   tau, sigma,     # variance of random effects (tau=1/sigma)
   x1[N], x2[N],   # Design Column for factor a1 and a2
                   # here we used the STZ constraints
   p[N],           # Success probability for Binomial
   n[N],           # Total number of trials for Binomial
   r[N],           # Binomial data
   b[N],           # Random effects  (standardised)
   c[N],           # Random effects c[i] (unstandardised)
   include,        # conditional model probability for
                   # main effects
   g[terms],       # terms indicator vector
   mdl,            # model index
   pmdl[models],   # model indicator
   mean[terms-1],  # proposal mean
   se[terms-1],    # proposal se
   bprior[terms-1],# prior mean for model coefficients
   tprior[terms-1];# prior precision for model coefficients
data r,n,x1,x2 in "seeds.dat", mean,se in 'prop6.dat';
inits in "seeds.in";

{
   alpha0 ~ dnorm(0.0,1.0E-6);  # intercept

        for (j in 1:(terms-1))  {
#      ******** GVS PRIORS ***********
#
#      GVS priors with proposals from pilot run
       bprior[j]<-(1-g[j])*mean[j];
       tprior[j] <-g[j]/8+(1-g[j])/(se[j]*se[j]);
#
#      GVS priors with proposals a mixture of Normals(0,c^2t^2)
#      bprior[j]<-0.0;
#      tprior[j] <-pow(100,1-g[j])/8;
      }
#
#
   alpha1 ~  dnorm(bprior[1],tprior[1]);  # seed coeff
   alpha2 ~  dnorm(bprior[2],tprior[2]);  # extract coeff
   alpha12 ~ dnorm(bprior[3],tprior[3]);
   tau ~ dgamma(1.0E-3,1.0E-3);           # 1/sigma^2
   for (i in 1:N) {
      c[i] ~ dnorm(0.0,tau);
      b[i] <- c[i] - mean(c[]);    #  make sure b's add to zero
      logit(p[i]) <-alpha0+g[1]*alpha1*x1[i]+g[2]*alpha2*x2[i]
                          +g[3]*alpha12*x1[i]*x2[i]+g[4]*b[i];
      r[i] ~ dbin(p[i],n[i]);
   }
```



```
   sigma <- 1.0/sqrt(tau);
#
#       Defining Model Code
        mdl<- 1+g[1]*1+g[2]*2+g[3]*4+g[4]*8
#
#       defining vector with model indicators
        for (j in 1:models){
        pmdl[j]<-equals(mdl,j);}
# Priors for variable indicators
        g[4]~ dbern(0.50);
        g[3]~ dbern(0.20);
        include<-g[3]+(1-g[3])*0.5
        g[2]~ dbern(include);
        g[1]~ dbern(include);
                    }
```

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# Bayesian Variable Selection Using the Gibbs Sampler

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ABSTRACT Specification of the linear predictor for a generalised linear model requires determining which variables to include. We consider Bayesian strategies for performing this variable selection. In particular we focus on approaches based on the Gibbs sampler. Such approaches may be implemented using the publically available software BUGS. We illustrate the methods using a simple example. BUGS code is provided in an appendix.

## 1 Introduction

In a Bayesian analysis of a generalised linear model, model uncertainty may be incorporated coherently by specifying prior probabilities for plausible models and calculating posterior probabilities using

$$f(m|\boldsymbol{y}) \;=\; \frac{f(m)f(\boldsymbol{y}|m)}{\sum_{m\in\mathcal{M}} f(m)f(\boldsymbol{y}|m)}, \qquad m\in\mathcal{M} \tag{1.1}$$

where $m$ denotes the model, $\mathcal{M}$ is the set of all models under consideration, $f(m)$ is the prior probability of model $m$. The observed data $\boldsymbol{y}$ contribute to the posterior model probabilities through $f(\boldsymbol{y}|m)$, the marginal likelihood calculated using $f(\boldsymbol{y}|m) = \int f(\boldsymbol{y}|m,\boldsymbol{\beta}_m)f(\boldsymbol{\beta}_m|m)d\boldsymbol{\beta}_m$ where $f(\boldsymbol{\beta}_m|m)$ is the conditional prior distribution of $\boldsymbol{\beta}_m$, the model parameters for model $m$ and $f(\boldsymbol{y}|m,\boldsymbol{\beta}_m)$ is the likelihood of the data $\boldsymbol{y}$ under model $m$.

In particular, the relative probability of two competing models $m_1$ and $m_2$ reduces to

$$\frac{f(m_1|\boldsymbol{y})}{f(m_2|\boldsymbol{y})} \;=\; \frac{f(m_1)}{f(m_2)} \;\; \frac{\int f(\boldsymbol{y}|m_1,\boldsymbol{\beta}_{m_1})f(\boldsymbol{\beta}_{m_1}|m_1)\,d\boldsymbol{\beta}_{m_1}}{\int f(\boldsymbol{y}|m_2,\boldsymbol{\beta}_{m_2})f(\boldsymbol{\beta}_{m_2}|m_2)\,d\boldsymbol{\beta}_{m_2}} \tag{1.2}$$

which is the familiar expression relating the posterior and prior odds of two models in terms of the Bayes factor, the second ratio on the right hand side of (1.2).

The principal attractions of this approach are that (1.1) allows the calculation of posterior probabilities of all competing models, regardless of their relative size or structure, and this model uncertainty can be incorporated into any decisions or predictions required (Draper, 1995, gives examples of this).

Generalised linear models are specified by three components, distribution, link and linear predictor. Model uncertainty may concern any of these, and the approach outlined above is flexible enough to deal with this. In this chapter, we shall restrict attention to variable selection problems, where the models concerned differ only in the form of the linear predictor. Suppose that there are $p$ possible covariates which are candidates for inclusion in the linear predictor. Then each $m\in\mathcal{M}$ can be naturally represented by a $p$-vector $\boldsymbol{\gamma}$ of binary indicator variables determining whether or not a covariate is included in the model, and $\mathcal{M}\subset\{0,1\}^p$. The linear predictor for the generalised linear model determined by $\boldsymbol{\gamma}$ may be written as

$$\boldsymbol{\eta} = \sum_{i=1}^{p} \gamma_i \boldsymbol{X}_i\boldsymbol{\beta}_i \tag{1.3}$$

where $\boldsymbol{\beta}$ is the 'full' parameter vector with dimension $p$, and $\boldsymbol{X}_i$ and $\boldsymbol{\beta}_i$ are the design sub-matrix and parameter vector, corresponding to the $i$th covariate. This specification allows for covariates of dimension greater than 1, for example terms in factorial models.

There has been a great deal of recent interest in Bayesian approaches for identifying promising sets of predictor variables. See for example Brown *et al.*(1998) and Chipman (1996, 1997), Clyde *et al.*(1996), Clyde and DeSimone-Sasinowska (1997), George *et al.*(1996), George and McCulloch (1993, 1996, 1997), Geweke (1996), Hoeting *et al.*(1996), Kuo and Mallick (1998), Mitchell and Beauchamp (1988), Ntzoufras *et al.*(1997), Smith and Kohn (1996) and Wakefield and Bennet (1996).

Most approaches require some kind of analytic, numerical or Monte Carlo approximation because the integrals involved in (1.2) are only analytically tractable in certain restricted examples. A further problem is that the size of the set of possible models $\mathcal{M}$ may be extremely large, so that calculation or approximation of $f(\boldsymbol{y}|m)$ for all $m \in \mathcal{M}$ is very time consuming. One of the most promising approaches has been Markov chain Monte Carlo (MCMC). MCMC methods enable one, in principle, to obtain observations from the joint posterior distribution of $(m, \boldsymbol{\beta}_m)$ and consequently estimate $f(m|\boldsymbol{y})$ and $f(\boldsymbol{\beta}_m|m, \boldsymbol{y})$.

In this chapter we restrict attention to model determination approaches which can be implemented by using one particular MCMC method, the Gibbs sampler. The Gibbs samper is particularly convenient for Bayesian computation in generalised linear models, due to the fact that posterior distributions are generally log-concave (Dellaportas and Smith, 1992). Furthermore, the Gibbs sampler can be implemented in a straightforward manner using the BUGS software (Spiegelhalter *et al.*, 1996a). To facilitate this, we provide BUGS code for various approaches in Appendix A.

The rest of the chapter is organised as follows. Section 2 describes several variable selection strategies that can be implemented using the Gibbs sampler Section 3 contains an illustrative example analysed using BUGS code. We conclude this chapter with a brief discussion in Section 4.

# 2 Gibbs Sampler Based Variable Selection Strategies

As we are assuming that model uncertainty is restricted to variable selection, $m$ is determined by $\boldsymbol{\gamma}$. We require a MCMC approach for obtaining observations from the joint posterior distribution of $f(m, \boldsymbol{\beta}_m)$. The Gibbs sampler achieves this by generating successively from univariate conditional distributions, so, in principle, the Gibbs sampler is determined by $f(m, \boldsymbol{\beta}_m)$. However, flexibility in the choice of parameter space, likelihood and prior has led to a number of different Gibbs sampler variable selection approaches being proposed.

The first method we shall discuss is a general Gibbs sampler based model



determination strategy. The others have been developed more specifically for variable selection problems.

## *2.1 Carlin and Chib's Method*

This method, introduced by Carlin and Chib (1995) is a flexible Gibbs sampling strategy for any situation involving model uncertainty. It proceeds by considering the extended parameter vector $(m, \boldsymbol{\beta}_k; k \in \mathcal{M})$. If a sample can be generated from the joint posterior density for this extended parameter, a sample from the required posterior distribution $f(m, \boldsymbol{\beta}_m)$ can be extracted easily.

A joint prior distribution for $m$ and $(\boldsymbol{\beta}_k; k \in \mathcal{M})$ is required. Here, $(\boldsymbol{\beta}_k; k \in \mathcal{M})$ contains the model parameters for every model in $\mathcal{M}$. Carlin and Chib (1995) specify the joint prior distribution through the marginal prior model probability $f(m)$ and prior density $f(\boldsymbol{\beta}_m|m)$ for each model, as above, together with independent 'pseudoprior' or linking densities $f(\boldsymbol{\beta}_{m'}|m \neq m')$ for each model.

The conditional posterior distributions required for the Gibbs sampler are

$$f(\boldsymbol{\beta}_{m'}|m,\ \{\boldsymbol{\beta}_k : k \in \mathcal{M} \setminus \{m'\}\}, \boldsymbol{y},) \propto \begin{cases} f(\boldsymbol{y}|m, \boldsymbol{\beta}_m) f(\boldsymbol{\beta}_m|m) & m' = m \\ f(\boldsymbol{\beta}_{m'}|m) & m' \neq m \end{cases} \tag{1.4}$$

$$f(m|\{\boldsymbol{\beta}_k : k \in \mathcal{M}\}, \boldsymbol{y}) = \frac{A_m}{\sum\limits_{k \in \mathcal{M}} A_k}. \tag{1.5}$$

where

$$A_m = f(\boldsymbol{y}|m, \boldsymbol{\beta}_m) \prod_{s \in \mathcal{M}} [f(\boldsymbol{\beta}_s|m)] f(m), \quad \forall \ \ m \in \mathcal{M}.$$

Therefore, when $m' = m$, we generate from the usual conditional posterior for model $m$, and when $m' \neq m$ we generate from the corresponding pseudoprior, $f(\boldsymbol{\beta}_{m'}|m)$. The model indicator $m$ is generated as a discrete random variable using (1.5).

The pseudopriors have no influence on $f(\boldsymbol{\beta}_m|m)$, the marginal posterior distribution of interest. They act as a linking density, and careful choice of pseudoprior is essential, if the Gibbs sampler is to be sufficiently mobile.

Ideally, $f(\boldsymbol{\beta}_{m'}|m \neq m')$ should resemble the marginal posterior distribution $f(\boldsymbol{\beta}_{m'}|m', \boldsymbol{y})$, and Carlin and Chib suggest strategies to achieve this.

The flexibility of this method lies in the facility to specify pseudopriors which help the sampler run efficiently. This may also be perceived as a drawback in problems where there are a large number of models under consideration, such as variable selection involving a moderate number of potential variables. Then, specification of efficient pseudopriors may become too time-consuming. A further drawback of the method is the requirement to generate every $\boldsymbol{\beta}_{m'}$ at each stage of the sampler. (This may be avoided by using a 'Metropolis-Hastings' step to generate $m$, but is outside the scope of the current chapter; see Dellaportas *et al.*, 1997, for details).

Examples which show how BUGS can be used to perform this method can be found in Spiegelhalter *et al.*(1996b).

## *2.2 Stochastic Search Variable Selection*

Stochastic Search Variable Selection (SSVS) was introduced by George and McCulloch (1993) for linear regression models and has been adapted for more complex models such as pharmacokinetic models (Wakefield and Bennett, 1996), construction of stock portfolios in finance (George and McCulloch, 1996), generalised linear models (George *et al.*, 1996, George and McCulloch, 1997), log-linear models (Ntzoufras *et al.*, 1997) and multivariate regression models (Brown *et al.*, 1998).

The difference between SSVS and other variable selection approaches is that the parameter vector $\boldsymbol{\beta}$ is specified to be of full dimension $p$ under all models, so the linear predictor is

$$\boldsymbol{\eta} = \sum_{i=1}^{p} \boldsymbol{X}_i \boldsymbol{\beta}_i. \tag{1.6}$$

Therefore $\boldsymbol{\eta} = \boldsymbol{X}\boldsymbol{\beta}$ for all models, where $\boldsymbol{X}$ contains all the potential explanatory variables. The indicator variables $\gamma_i$ are involved in the modelling process through the prior

$$\boldsymbol{\beta}_i|\gamma_i \sim \gamma_i N(0, c_i^2\Sigma_i) + (1-\gamma_i)N(0, \Sigma_i) \tag{1.7}$$

for specified $c_i$ and $\Sigma_i$. The prior parameters $c_i$ and $\Sigma_i$ in (1.7) are chosen so that when $\gamma_i = 0$ (covariate is 'absent' from the linear predictor) the



prior distribution for $\boldsymbol{\beta}_i$ ensures that $\boldsymbol{\beta}_i$ is constrained to be 'close to $\mathbf{0}$'. When $\gamma_i = 1$ the prior is diffuse, assuming that little prior information is available about $\boldsymbol{\beta}_i$.

The full conditional posterior distributions of $\boldsymbol{\beta}_i$ and $\gamma_i$ are given by

$$f(\boldsymbol{\beta}_i|\boldsymbol{y}, \boldsymbol{\gamma}, \boldsymbol{\beta}_{\setminus i}) \propto f(\boldsymbol{y}|\boldsymbol{\gamma}, \boldsymbol{\beta}) f(\boldsymbol{\beta}_i|\gamma_i)$$

and

$$\frac{f(\gamma_i = 1|\boldsymbol{y}, \boldsymbol{\gamma}_{\setminus i}, \boldsymbol{\beta})}{f(\gamma_i = 0|\boldsymbol{y}, \boldsymbol{\gamma}_{\setminus i}, \boldsymbol{\beta})} = \frac{f(\boldsymbol{\beta}|\gamma_i = 1, \boldsymbol{\gamma}_{\setminus i})}{f(\boldsymbol{\beta}|\gamma_i = 0, \boldsymbol{\gamma}_{\setminus i})} \frac{f(\gamma_i = 1, \boldsymbol{\gamma}_{\setminus i})}{f(\gamma_i = 0, \boldsymbol{\gamma}_{\setminus i})} \tag{1.8}$$

where $\boldsymbol{\gamma}_{\setminus i}$ denotes all terms of $\boldsymbol{\gamma}$ except $\gamma_i$.

If we use the prior distributions for $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ defined by (1.7) and assume that $f(\gamma_i = 0, \boldsymbol{\gamma}_{\setminus i}) = f(\gamma_i = 1, \boldsymbol{\gamma}_{\setminus i})$ for all $i$, then

$$\frac{f(\gamma_i = 1|\boldsymbol{y}, \boldsymbol{\gamma}_{\setminus i}, \boldsymbol{\beta})}{f(\gamma_i = 0|\boldsymbol{y}, \boldsymbol{\gamma}_{\setminus i}, \boldsymbol{\beta})} = c_i^{-d_i} exp\left(0.5 \frac{c_i^2 - 1}{c_i^2} \boldsymbol{\beta}_i^T \boldsymbol{\Sigma}_i^{-1} \boldsymbol{\beta}_i\right) \tag{1.9}$$

where $d_i$ is the dimension of $\boldsymbol{\beta}_i$.

The prior for $\boldsymbol{\gamma}$ with each term present or absent independently with probability $1/2$ may be considered non-informative in the sense that it gives the same weight to all possible models. George and Foster (1997) argue that this prior can be considered as informative because it puts more weight on models of size close to $p/2$. However, posterior model probabilities are most heavily dependent on the choice of the prior parameters $c_i^2$ and $\Sigma_i$. One way of specifying these is by setting $c_i^2\Sigma_i$ as a diffuse prior (for $\gamma_i = 1$) and then choosing $c_i^2$ by considering the the value of $|\boldsymbol{\beta}_i|$ at which the densities of the two components of the prior distribution are equal. This can be considered to be the smallest value of $|\boldsymbol{\beta}_i|$ at which the term is considered of practical significance. George and McCulloch (1993) applied this approach. Ntzoufras *et al.*(1997) considered log-linear interaction models where $\boldsymbol{\beta}_i$ terms are multidimensional.

## *2.3 Unconditional Priors for Variable Selection*

Kuo and Mallick (1998) advocated the use of the linear predictor $\boldsymbol{\eta} = \sum_{i=1}^{p} \gamma_i \boldsymbol{X}_i \boldsymbol{\beta}_i$ introduced in (1.3) for variable selection. They considered a prior distribution $f(\boldsymbol{\beta})$ which is independent of $\boldsymbol{\gamma}$ (and therefore $\mathcal{M}$) so that $f(\boldsymbol{\beta}_i|\boldsymbol{\beta}_{\setminus i}, \boldsymbol{\gamma}) = f(\boldsymbol{\beta}_i|\boldsymbol{\beta}_{\setminus i})$

Therefore, the full conditional posterior distributions are given by

$$f(\boldsymbol{\beta}_i|\boldsymbol{y},\boldsymbol{\gamma},\boldsymbol{\beta}_{\setminus i}) \propto \begin{cases} f(\boldsymbol{y}|\boldsymbol{\gamma},\boldsymbol{\beta})f(\boldsymbol{\beta}_i|,\boldsymbol{\beta}_{\setminus i}) & \gamma_i = 1 \\ f(\boldsymbol{\beta}_i|\boldsymbol{\beta}_{\setminus i}) & \gamma_i = 0 \end{cases} \tag{1.10}$$

and

$$\frac{f(\gamma_i = 1|\boldsymbol{y},\boldsymbol{\gamma}_{\setminus i},\boldsymbol{\beta})}{f(\gamma_i = 0|\boldsymbol{y},\boldsymbol{\gamma}_{\setminus i},\boldsymbol{\beta})} = \frac{f(\boldsymbol{y}|\gamma_i = 1,\boldsymbol{\gamma}_{\setminus i},\boldsymbol{\beta})}{f(\boldsymbol{y}|\gamma_i = 0,\boldsymbol{\gamma}_{\setminus i},\boldsymbol{\beta})}\frac{f(\gamma_i = 1,\boldsymbol{\gamma}_{\setminus i})}{f(\gamma_i = 0,\boldsymbol{\gamma}_{\setminus i})}. \tag{1.11}$$

The advantage of the above approach is that it is extremely straightforward. It is only required to specify the usual prior on $\boldsymbol{\beta}$ (for the full model) and the conditional prior distributions $f(\boldsymbol{\beta}_i|\boldsymbol{\beta}_{\setminus i})$ replace the pseudopriors required by Carlin and Chib's method. However, this simplicity may also be a drawback, as there is no flexibility here to alter the method to improve efficiency. In practice, if, for any $\boldsymbol{\beta}_i$, the prior is diffuse compared with the posterior, the method may be inefficient.

### *2.4 Gibbs Variable Selection*

Dellaportas *et al.*(1997) considered a natural hybrid of SSVS and the 'Unconditional Priors' approach of Kuo and Mallick (1998). The linear predictor is assumed to be of the form of (1.3) where , unlike SSVS, variables corresponding to $\gamma_i = 0$ are genuinely excluded from the model. The prior for $(\boldsymbol{\gamma},\boldsymbol{\beta})$ is specified as $f(\boldsymbol{\gamma},\boldsymbol{\beta}) = f(\boldsymbol{\gamma})f(\boldsymbol{\beta}|\boldsymbol{\gamma})$. Consider the partition of $\boldsymbol{\beta}$ into $(\boldsymbol{\beta}_{\boldsymbol{\gamma}},\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}})$ corresponding to those components of $\boldsymbol{\beta}$ which are included $(\gamma_i = 1)$ or not included $(\gamma_i = 0)$ in the model, then the prior $f(\boldsymbol{\beta}|\boldsymbol{\gamma})$ may be partitioned into model prior $f(\boldsymbol{\beta}_{\boldsymbol{\gamma}}|\boldsymbol{\gamma})$ and pseudoprior $f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}},\boldsymbol{\gamma})$.

The full conditional posterior distributions are given by

$$f(\boldsymbol{\beta}_{\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}},\boldsymbol{\gamma},\boldsymbol{y}) \propto f(\boldsymbol{y}|\boldsymbol{\beta},\boldsymbol{\gamma})f(\boldsymbol{\beta}_{\boldsymbol{\gamma}}|\boldsymbol{\gamma})f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}},\boldsymbol{\gamma}) \tag{1.12}$$

$$f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}},\boldsymbol{\gamma},\boldsymbol{y}) \propto f(\boldsymbol{\beta}_{\setminus\boldsymbol{\gamma}}|\boldsymbol{\beta}_{\boldsymbol{\gamma}},\boldsymbol{\gamma}) \tag{1.13}$$

and

$$\frac{f(\gamma_i = 1|\boldsymbol{\gamma}_{\setminus i},\boldsymbol{\beta},\boldsymbol{y})}{f(\gamma_i = 0|\boldsymbol{\gamma}_{\setminus i},\boldsymbol{\beta},\boldsymbol{y})} = \frac{f(\boldsymbol{y}|\boldsymbol{\beta},\gamma_i = 1,\boldsymbol{\gamma}_{\setminus i})}{f(\boldsymbol{y}|\boldsymbol{\beta},\gamma_i = 0,\boldsymbol{\gamma}_{\setminus i})}\frac{f(\boldsymbol{\beta}|\gamma_i = 1,\boldsymbol{\gamma}_{\setminus i})}{f(\boldsymbol{\beta}|\gamma_i = 0,\boldsymbol{\gamma}_{\setminus i})}\frac{f(\gamma_i = 1,\boldsymbol{\gamma}_{\setminus i})}{f(\gamma_i = 0,\boldsymbol{\gamma}_{\setminus i})}. \tag{1.14}$$



This approach is simplified if it is assumed that the prior for $\boldsymbol{\beta}_i$ depends only on $\gamma_i$ and is given by

$$f(\boldsymbol{\beta}_i|\boldsymbol{\gamma}_i) = \gamma_i N(0,\Sigma_i) + (1-\gamma_i)N(\tilde{\mu}_i,S_i). \tag{1.15}$$

This prior, where $f(\boldsymbol{\beta}_i|\boldsymbol{\gamma}) = f(\boldsymbol{\beta}_i|\gamma_i)$ potentially makes the method less efficient and is most appropriate in examples where $\boldsymbol{X}$ is orthogonal. In prediction, rather than inference about the variables themselves is of primary interest, then $\boldsymbol{X}$ may always be chosen to be orthogonal (see Clyde *et al.*, 1996).

There is a similarity between this prior and the prior used in SSVS. However, here the full conditional posterior distribution is given by

$$f(\boldsymbol{\beta}_i|\boldsymbol{\gamma},\boldsymbol{\beta}_{\setminus i},\boldsymbol{y}) \propto \begin{cases} f(\boldsymbol{y}|\boldsymbol{\gamma},\boldsymbol{\beta})N(0,\Sigma_i) & \gamma_i = 1 \\ N(\tilde{\mu}_i,S_i) & \gamma_i = 0 \end{cases}$$

and a clear difference between this and SSVS is that the pseudoprior $f(\boldsymbol{\beta}_i|\gamma_i = 0)$ does not affect the posterior distribution and may be chosen as a 'linking density' to increase the efficiency of the sampler, in the same way as the pseudopriors of Carlin and Chib's method. Possible choices of $\tilde{\mu}_i$ and $S_i$ may be obtained from a pilot run of the full model; see, for example Dellaportas and Forster (1999).

### *2.5 Summary of Variable Selection Strategies*

The similarities and differences between the three Gibbs sampling variable selection methods presented in sections 2.2, 2.3 and 2.4 may easily be summarised by inspecting the conditional probabilities (1.8), (1.11) and, in particular, (1.14).

In SSVS, $f(\boldsymbol{y}|\boldsymbol{\beta},\boldsymbol{\gamma})$ is independent of $\boldsymbol{\gamma}$ and so the first ratio on the right hand side of (1.14) is absent in (1.8). For the 'Unconditional Priors' approach of Kuo and Mallick (1998), the second term on the right hand side of (1.14) is absent in (1.11) as $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ are *a priori* independent. For Gibbs Variable Selection, both likelihood and prior appear in the variable selection step. These differences are also evident by looking at the graphical representations of the three methods in Figure 1.

The key differences between the methods (including Carlin and Chib's method) are in their requirements in terms of prior and/or linking densities.

Carlin and Chib's method and GVS both require linking densities whose sole function is to aid the efficiency of the sampler. GVS is less expensive in requirement of pseudopriors, but correspondingly less flexible. The prior parameters in SSVS all have an impact on the posterior, and therefore the densities cannot really be thought of linking densities. The simplest method that described by Kuo and Mallick (1988) does not require one to specify anything other than the usual priors for the model parameters.

## 3 Illustrative Example: $2 \times 2 \times 2$ Contingency Table

We present an analysis of the data in table 1.1, taken from Healy (1988). This is a three-way table with factors A,B and C. Factor A denotes the condition of the patient (more or less severe), factor B denotes if the patient was accepting antitoxin medication and the (response) factor C denotes whether the patient survived or not.

| | | Survival(C) | |
|---|---|---|---|
| Condition (A) | Antitoxin (B) | No | Yes |
| More Severe | Yes | 15 | 6 |
| | No | 22 | 4 |
| Less Severe | Yes | 5 | 15 |
| | No | 7 | 5 |

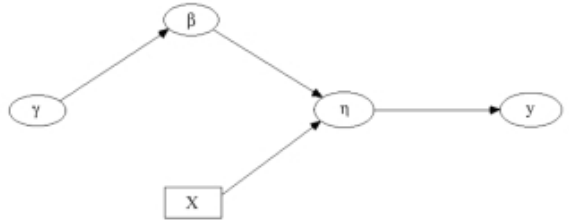
TABLE 1.1. Example Dataset.

Purely for illustration purposes, and to present the BUGS code in Appendix A, we model the above data using both log-linear and logistic regression models.

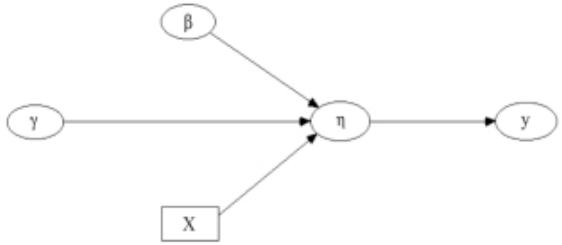
### *3.1 Log-linear models*

We focus attention on hierarchical models including the main effects focussing our interest on associations between model factors and the corresponding interaction terms in the models. Here, $i \in \{1, A, B, C, AB, AC,$

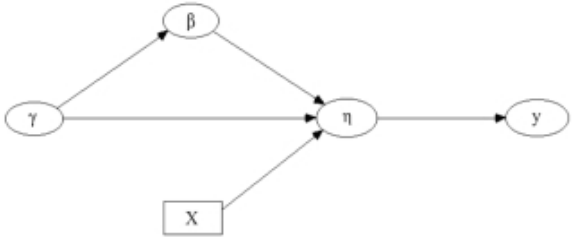





***SSVS Graphical Model***




***Kuo and Mallick Graphical Model***




***Gibbs Variable Selection Graphical Model***

FIGURE 1. Graphical Model Representation for Stochastic Search Variable Selection, Kuo and Mallick Sampler and Gibbs Variable Selection [Squares denote Constants; Circles denote Stochastic Nodes].

$BC, ABC\}$ so $p = 8$. The prior specification for model vector $\boldsymbol{\gamma}$ is $\gamma_i \sim Bernoulli(\pi)$ with $\pi = 1/9$ if $i = ABC$, $\pi = 1$ if $i \in \{1, A, B, C\}$ and $\gamma_i|\gamma_{ABC} \sim Bernoulli(\pi)$ with $\pi = 0.5(1-\gamma_{ABC})+\gamma_{ABC}$ for the two factor interactions ($i \in \{AB, AC, BC\}$). This specification implies that the prior probability of including a two factor interaction in the model is 0.5 if the three factor interaction is excluded from the model and 1 if it is included in the model. Hence the prior probabilities for all 9 possible hierarchical models are 1/9 and and non-hierarchical models are not considered.

For the model coefficients we used the prior specification suggested by Dellaportas and Forster (1999) for log linear models which results in $\Sigma_i = 2$ in (1.15) when the $\beta_i$ are considered to be the usual 'sum-to-zero' constrained model parameters For SSVS we used $c_i^2\Sigma_i = 2$ and $c_i = 10^3$ in (1.7), as suggested by Ntzoufras *et al.*(1997).

| | | SSVS | KM | GVS |
|---|---|---|---|---|
| Models | $A+B+C$ | 0.1 | 0.2 | 0.2 |
| | $AB+C$ | 0.0 | 0.1 | 0.1 |
| | $AC+B$ | 25.1 | 25.7 | 25.6 |
| | $BC+A$ | 0.3 | 0.6 | 0.6 |
| | $AB+AC$ | 7.9 | 7.5 | 7.3 |
| | $AB+BC$ | 0.1 | 0.2 | 0.2 |
| | $AC+BC$ | 58.9 | 58.4 | 58.9 |
| | $AB+BC+CA$ | 6.4 | 6.6 | 6.4 |
| | $ABC$ | 1.0 | 0.8 | 0.6 |

TABLE 1.2. Posterior model probabilities (%) for log-linear models. SSVS: Stochastic Search Variable Selection; KM: Kuo and Mallick's Unconditional Priors approach; GVS: Gibbs Variable Selection.

The results are based on 100,000 iterations for Gibbs variable selection and Kuo and Mallick's method, and 400,000 iterations for SSVS which seemed to be less efficient. For all methods we discarded 10,000 iterations as a burn-in period. The pseudoprior densities for Gibbs variable selection were constructed from the sample moments of a pilot run of the full model of size 1,000 iterations. All three methods give similar results supporting the same models with very similar posterior probabilities.



### *3.2 Logistic regression models*

When we consider binomial logistic regression models for response variable $C$ and explanatory factors $A$ and $B$, there are 5 possible nested models, 1, $A$, $B$, $A+B$ and $AB$. Priors are specified by setting $c_i^2\Sigma_i = 4 \times 2$ in (1.7) and $\Sigma_i = 4 \times 2$ in (1.15) which is equivalent to the prior used above for log-linear model selection. The pseudoprior parameters were specified as before, through a pilot chain, and finally we set $\gamma_{ABC} \sim Bernoulli(1/5)$ and $\gamma_i|\gamma_{AB} \sim Bernoulli(\pi)$, with $\pi = 0.5(1-\gamma_{AB})+\gamma_{AB}$ for $i \in \{A, B\}$. The resulting prior probabilities for all models are 1/5. The results in table (1.3) are based on 500,000 iterations for SSVS and Kuo and Mallick's method and 100,000 iterations for Gibbs variable selection, with burn-in period of 10,000 iterations. Again, the results are very similar, although Gibbs variable selection seemed to be most efficient.

The equivalent log-linear models in Table 1.2 are those which include the $AB$ term, so the results can be seen to be in good agreement.

| | | SSVS | KM | GVS |
|---|---|---|---|---|
| Models | 1 | 0.2 | 0.5 | 0.5 |
| | $A$ | 48.0 | 49.2 | 49.3 |
| | $B$ | 1.0 | 1.2 | 1.2 |
| | $A+B$ | 45.3 | 44.0 | 43.9 |
| | $AB$ | 5.5 | 5.2 | 5.1 |

TABLE 1.3. Posterior model probabilities (%) for logistic regression. SSVS: Stochastic Search Variable Selection; KM: Kuo and Mallick's Unconditional Priors approach; GVS: Gibbs Variable Selection.

## 4 Discussion

We have reviewed a number of Bayesian variable selection strategies based on the Gibbs sampler. Their major practical advantage is that they can be easily applied with a Gibbs sampling software such as BUGS.

It is impossible to provide a general recommendation for a method of computation for a class of problems as large as variable selection in gener-

alised linear models. The methods we have discussed range from the 'Unconditional Priors approach' which is extremely easy to implement, but may be insufficiently flexible for many practical problems, to the approach of Carlin and Chib, which is very flexible, but requires a lot of careful specification.

We have only discussed methods based on the Gibbs sampler. Of course other extremely flexible MCMC methods exist, such the reversible jump approach introduced by Green (1996). All MCMC methods require careful implementation and monitoring, and other approaches should also be considered. For many model selection problems involving generalised linear models, an alternative approach is through asymptotic approximation. Raftery (1996) has provided a series of Splus routines for this kind of calculation. Such methods can be used in conjunction with the Gibbs sampler approaches discussed here.

Any Bayesian model selection requires careful attention to prior specification. For discussion of elicitation of prior distributions for variable selection, see Garthwaite and Dickey (1992) and Ibrahim and Chen (1998).

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# 6 Appendix: BUGS CODES

Code and data files are freely available in the web adress *http://www.stat-athens.aueb.gr/~jbn/* or by electronic mail request.

## *6.1 Code for Log-linear Models for $2^3$ Contingency Table*

```
model loglinear;
#
#       2x2x2 LOG-LINEAR VARIABLE SELECTION WITH BUGS
#       (c) OCTOBER 1996 FIRST VERSION
#       (c) OCTOBER 1997 FINAL VERSION
#           WRITTEN BY IOANNIS NTZOUFRAS
#       ATHENS UNIVERSITY OF ECONOMICS AND BUSINESS
#
#           SSVS: Stochastic Search Variable Selection
#           KM  : Kuo and Mallick Gibbs sampler
#           GVS : Gibbs Variable Selection
#
const
   N = 8;  # number of Poisson cells
```

```
var
        include,    # conditional prior probabability for gi
        pmdl[9],    # model indicator vector
        mdl,        # code of model
        b[N],       # model coefficients
        mean[N],    # mean used in pseudoprior   (GVS only)
        se[N],      # st.dev. used in pseudoprior(GVS only)
        bpriorm[N], # prior mean for b depanding on g
        tau[N],     # model coefficients precision
#       c,          # precision multiplicator    (SSVS only)
        x[N,N],     # design matrix
        z[N,N],     # matrix used in likelihood
        n[N],       # Poisson cells
        lambda[N],  # Poisson mean for each cell
        g[N];       # term indicator vector
data n,x in "ex1log.dat", mean, se in 'prop1ll.dat';
inits in "ex1ll.in";
{
#       c<-1000.0 # SSVS only
#
#       calculation of the z matrix used in likelihood
        for (i in 1:N) { for (j in 1:N) {
               z[i,j]<-x[i,j]*b[j]*g[j]   # For GVS/KM
#               z[i,j]<-x[i,j]*b[j];      # For SSVS
               }}
#
#       model configuration
        for (i in 1:N) {
                log(lambda[i])<-sum(z[i,]);
                n[i]~dpois(lambda[i])    }
#       defining model code
#       0 for [A][B][C], 1 for [AB][C],      2 for [AC][B],
#       3 for [AB][AC],  4 for [BC][A],      5 for [AB][BC],
#       6 for [AC][BC],  7 for [AB][BC][CA],15 for [ABC].
#
        mdl<-g[5]+2*g[6]+4*g[7]+8*g[8];
        for (i in 0:7) { pmdl[i+1]<-equals(mdl,i) }
        pmdl[9]<-equals(mdl,15)
#
#       Prior for b model coefficient
        tau[1]<-0.1;
        bpriorm[1]<-0.0;
        b[1]~dnorm(bpriorm[1],tau[1]);
        for (i in 2:N) {
#
#                   GVS using se,mean from pilot run
#               ----------------------------------------
                tau[i]<-g[i]/2+(1-g[i])/(se[i]*se[i]);
                bpriorm[i]<-mean[i]*(1-g[i]);
#
#               Kuo and Mallick (prior indepedent of g[i])
#               ----------------------------------------
#                tau[i]<-1/2;
#                bpriorm[i]<-0.0;
#
#                            SSVS PRIOR SET-UP
#               ----------------------------------------
#                tau[i]<-pow(c,2-2*g[i])/2;
```



```
#                bpriorm[i]<-0.0;
#
                b[i]~dnorm(bpriorm[i],tau[i]);
        }
#
#       defining prior information for gi in such way that
#       allow only hierarhical models with equal probability.
#
        include<-(1-g[8])*0.5+g[8]*1.0;
        g[8]~dbern(0.1111111);
        g[7]~dbern(include);
        g[6]~dbern(include);
        g[5]~dbern(include);
        for (i in 1:4) { g[i]~dbern(1.0)}}
```

### 6.2 *Code for Logistic Models with 2 Binary Explanatory Factors*

```
model Binomial;
#
#       LOGISTIC REGRESSION VARIABLE SELECTION WITH BUGS
#       (c) OCTOBER 1996 FIRST VERSION
#       (c) OCTOBER 1997 FINAL VERSION
#           WRITTEN BY IOANNIS NTZOUFRAS
#       ATHENS UNIVERSITY OF ECONOMICS AND BUSINESS
#
#           SSVS: Stochastic Search Variable Selection
#           KM  : Kuo and Mallick Gibbs sampler
#           GVS : Gibbs Variable Selection
#
const
   N = 4;  # number of binomial experiments
var
      include,   # conditional prior probabability for gi
      pmdl[5],   # model indicator vector
      mdl,       # code of model
      b[N],      # model coefficients
      mean[N],   # mean used in pseudoprior    (GVS only)
      se[N],     # st.dev, used in pseudoprior (GVS only)
      bpriorm[N],# prior mean for b depanding on g
      tau[N],    # model coefficients precision
#     c,         # precision multiplicator    (SSVS only)
      x[N,N],    # design matrix
      z[N,N],    # matrix used in likelhood
      r[N],      # number of successes in binomial
      n[N],      # total number of observations for binomial
      p[N],      # probability of success for binomial model
      g[N];      # term indicator vector
data r,n,x in "ex1logit.dat", mean, se in 'prop1.dat';
inits in "ex1.in";
{
#       c<-1000 # SSVS only
#
#       calculation of the z matrix used in likelihood
        for (i in 1:N) { for (j in 1:N) {
               z[i,j]<-x[i,j]*b[j]*g[j]  # for GVS
#              z[i,j]<-x[i,j]*b[j];      # for SSVS
               }}
#
#       model configuration
```

```
        for (i in 1:N) {
                r[i]~dbin(p[i],n[i]);
                logit(p[i])<-sum(z[i,]) }
#       defining model code
#       0 constant, 1 for [A], 2 for [B],
#       3 for [A][B], and 6 for [AB]
#
        mdl<-g[2]+2*g[3]+3*g[4];
        pmdl[1]<-equals(mdl,0)
        pmdl[2]<-equals(mdl,1)
        pmdl[3]<-equals(mdl,2)
        pmdl[4]<-equals(mdl,3)
        pmdl[5]<-equals(mdl,6)
#
#       Prior for b model coefficient
        tau[1]<-0.1;
        bpriorm[1]<-0.0;
        b[1]~dnorm(bpriorm[1],tau[1]);
        for (i in 2:N) {
#
#               GVS using se,mean from pilot run
#               --------------------------------
#
                tau[i]<-g[i]/8+(1-g[i])/(se[i]*se[i]);
                bpriorm[i]<-mean[i]*(1-g[i]);
#
#               Kuo and Mallick proposal is indedent of g[i]
#               --------------------------------------------
#
#                tau[i]<-1/8;
#                bpriorm[i]<-0.0;
#
#                           SSVS PRIOR SET-UP
#               ----------------------------------------
#                tau[i]<-pow(c,2-2*g[i])/8;
#                bpriorm[i]<-0.0;
#
                b[i]~dnorm(bpriorm[i],tau[i]);
        }
#
#       defining prior information for gi in such way that
#       allow only hierarhical models with 0.2 probability.
#
        g[4]~dbern(0.2);
        include<-(1-g[4])*0.5+g[4]*1.0
        g[2]~dbern(include);
        g[3]~dbern(include);
        g[1]~dbern(1.0)               }
```

# Bayesian Hypothesis Testing for the Distribution of Insurance Claim Counts Using the Gibbs Sampler

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**Abstract**

We construct and present a Markov Chain Monte Carlo (MCMC) algorithm for the estimation of posterior odds and probabilities of alternative models used to evaluate competing hypotheses regarding three common discrete distributions involved in the modeling of the outstanding claim counts in actuarial science. The proposed methodology involves advanced statistical techniques of Bayesian modeling which make use of the Gibbs sampling variable selection algorithm. One of the main advantages of this approach over the popular reversible jump algorithm (Green, 1995) is its straightforward implementation using the MCMC language tool of WINBUGS software (Spiegelhalter et al. 2003). The methodology is applied to a real data set. Directions regarding the implementation in WINBUGS are provided at the Appendix. It is worth noting that although the context of the problem is actuarial, the methodology can be applied to any field of science where the aim is the comparison or selection of discrete distributions of counts.

*Keywords*: Bayesian point of view, Gibbs Sampling, Hypothesis Tests, Markov Chain Monte Carlo, Reversible Jump, WINBUGS.

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## 1 Introduction

Modeling random events has always generated a great deal of research interest in Science, Economics and Engineering. Relevant topics range from the level of rainfall and car traffic to market penetration of a certain commodity and the pricing of an option. However, the researcher is often uncertain about the appropriate statistical representation of the phenomenon under study. Initially, the most pressing statistical question she/he faces is

*Which is the best statistical distribution to use?*

which usually leads to the more specific one:

*How do we evaluate the available 'candidate' distributions and choose the best one(s)?*

To this end, Bayesian Statistics seems like a natural approach since any prior beliefs about the unknown parameters may affect the final decision. Therefore, the researcher must incorporate these beliefs while conducting the analysis of the experiment. However, most of the Bayesian algorithms on the topic of Bayesian model comparison are so computationally intensive that effectively forbid most practitioners from applying them to their work. Hence, the need for a simpler and software-friendlier approach is apparent.

In actuarial science particularly, the choice of the distribution for the modeling and prediction of outstanding claims incurred in an insurance company has been extremely important to both practitioners and academics. It is common practice for these companies not to pay the outstanding claims immediately but with some delay. Hence, an accurate representation of the number of outstanding claims is of important practical significance. In addition to that, the Bayesian paradigm has become an integral research tool in the actuarial discipline (see Makov, 2001 for a review). However, in the outstanding claims problem, the Bayesian approach has been mostly confined to parameter estimation (see Verrall 1990, de Alba 2002, Ntzoufras and Dellaportas 2002) rather than to testing hypotheses about distributions.

The contribution of this paper is twofold. Firstly, we develop a new algorithm for the estimation of posterior model odds based on the idea of Gibbs variable selection algorithm of Dellaportas et al. (2002). The algorithm is used to evaluate and compare three discrete statistical distributions for the modeling of the outstanding claim counts in actuarial science

using the Bayesian approach. The proposed methodology is computationally simpler and can be generalized to a larger number of candidate distributions as well as to any other similar research problem in another field (e.g. compare the distributions of arrivals in a queue). Secondly, we implement our algorithm on the popular, freely available, software WINBUGS (Spiegelhalter et al. , 2003). Competing methods such as RJMCMC can not be implemented via WINBUGS. This is an important advantage since many researchers favoring the Bayesian approach are familiar with WINBUGS. Hence, they can now implement our proposed methodology directly following the detailed description provided at the Appendix of this paper.

The paper is organized into five further sections. Section 2 reviews the basic formulation of Bayesian model comparison. A description of the distributions for the modeling of the outstanding claims is provided in Section 3. In Section 4 we describe in detail the Gibbs sampling algorithm constructed for our hypothesis tests and its advantages over the existing techniques. Section 5 analyzes the implementation of the method in a specific example of insurance claims data using WINBUGS. Finally, conclusions and closing remarks are presented in Section 6.

## 2 Bayesian Inference

Generally, Bayesian inference is based on constructing a model $m$, its likelihood $f(\boldsymbol{y}|\boldsymbol{\theta}_m, m)$ and the corresponding prior distribution $f(\boldsymbol{\theta}_m|m)$, where $\boldsymbol{\theta}_m$ is a parameter vector and $\boldsymbol{y}$ is the data vector. Although, inference is primarily based on the posterior distribution $f(\boldsymbol{\theta}_m|\boldsymbol{y}, m)$, we may also be interested in quantifying model uncertainty by estimating the posterior model probability $f(m|\boldsymbol{y})$.

Let us consider two competing models $m_0$ and $m_1$. If $f(m)$ is the prior probability of model $m$, then, using the Bayes theorem, the posterior odds $PO_{01}$ of model $m_0$ versus model $m_1$ are given by

$$PO_{01} = \frac{f(m_0|\boldsymbol{y})}{f(m_1|\boldsymbol{y})} = \frac{f(\boldsymbol{y}|m_0)}{f(\boldsymbol{y}|m_1)} \times \frac{f(m_0)}{f(m_1)} = B_{01} \times \frac{f(m_0)}{f(m_1)} \tag{1}$$

where $B_{01}$ and $\frac{f(m_0)}{f(m_1)}$ are the 'Bayes factor' and the 'prior model odds' of model $m_0$ against



model $m_1$, respectively. The quantity $f(\boldsymbol{y}|m)$ involved in the Bayes Factor is defined as the marginal likelihood of model $m$ and is given by $f(\boldsymbol{y}|m) = \int f(\boldsymbol{y}|\boldsymbol{\theta}_m, m) f(\boldsymbol{\theta}_m|m) d\boldsymbol{\theta}_m$. The Bayes factor $B_{10}$, of model $m_1$ against $m_0$, evaluates the evidence *against* the null hypothesis which is a familiar concept to classical significance tests. Thus, large values of, say, $B_{01}$ (usually greater than 12) indicate strong posterior support of model $m_0$ against model $m_1$ For more details on Bayes factors see Kass and Raftery (1995). Alternatively, when we consider a set of competing models $\mathcal{M} = \{m_1, m_2, \cdots, m_{|\mathcal{M}|}\}$, then we focus our interest on the posterior probability of model $m \in \mathcal{M}$, defined as

$$f(m|\boldsymbol{y}) = \frac{f(\boldsymbol{y}|m) f(m)}{\sum\limits_{m_l \in \mathcal{M}} f(\boldsymbol{y}|m_l) f(m_l)} = \left( \sum_{m_l \in \mathcal{M}} PO_{m_l,m} \right)^{-1}$$

where $\mathcal{M}$ and $|\mathcal{M}|$ denote the set and the number of models under consideration respectively.

The integrals involved in the computation of the posterior model probabilities are mostly analytically intractable. Therefore asymptotic approximations or alternative computational methods must be frequently employed. One of the most popular techniques for calculation of these quantities is the Markov Chain Monte Carlo (MCMC) methodology (see Gilks et al. , 1996) and its recent extensions (reversible jump MCMC algorithm or RJMCMC) in varying dimension models (Green, 1995). Moreover, RJMCMC methodology helps us to account for model uncertainty using Bayesian model averaging techniques (see Draper, 1995, Chatfield, 1995, Kass and Raftery, 1995, Cairns, 2000). However, this methodology is demanding in both the design stage and the implementation.

## 3 Distributions for claim counts

In this section we focus on three popular distributions for modeling the marginal claim counts, more specifically the simple Poisson distribution (Ter Berg, 1980), the negative binomial (Verrall, 2000) and the Generalized Poisson distribution (see Consul, 1989) denoted by $m_1, m_2$ and $m_3$ respectively. The Generalized Poisson distribution is also known as Lagrangian Poisson distribution. Consequently, the simple Poisson model can be regarded as a special case of either the negative binomial or the Generalized Poisson distribution.

Let us assume data $y_i$, $i = 1, \ldots, n$. Consequently, the simple Poisson model is given by

$$f(y_i|\lambda, m_1) = \frac{\lambda^{y_i} exp(-\lambda)}{y_i!}.$$

It is well known that for the Poison distribution the mean equals the variance. This property is not common in real data sets where the sample variance usually exceeds the sample mean. For this reason alternative models that allow for over-dispersion relative to the simple Poisson model have been considered. The variance to the mean ratio, called Dispersion Index (DI), is usually calculated as a measure for data dispersion; see for example Douglas (1980). For the Poisson random variable the Dispersion Index is equal to one.

An alternative model for this type of data is the negative binomial distribution given by

$$f(y_i|\lambda, \vartheta, m_2) = \frac{\Gamma(y_i + \vartheta)}{\Gamma(y_i + 1)\Gamma(\vartheta)} \left(\frac{\lambda}{\lambda + \vartheta}\right)^{y_i} \left(\frac{\vartheta}{\lambda + \vartheta}\right)^{\vartheta} \tag{2}$$

where $\vartheta > 0$. Although the mean of the negative binomial model is the same as in the Poisson model, $E(y_i) = \lambda$, the variance now also depends on the parameter $\vartheta$ since $V(y_i) = \lambda + \lambda^2/\vartheta$. The Poisson model is a limiting distribution of (2) for $\vartheta \to \infty$. We may adopt the parameterization $\vartheta = \lambda/\phi$. For the negative binomial distribution, the Dispersion Index is equal to $DI = 1 + \phi$. For $\phi \to 0$ the above distribution reduces to the simple Poisson distribution.

Finally, the Generalized Poisson model with parameters $\lambda$ and $\omega$, is defined in the following way:

$$f(y_i|\lambda, \omega, m_3) = (1 - \omega)\lambda_i \frac{\{(1 - \omega)\lambda_i + \omega y_i\}^{y_i - 1}}{y_i!} e^{-\{(1-\omega)\lambda_i + \omega y_i\}}. \tag{3}$$

According to Ter Berg (1996), valid values for $\omega$ are within the interval $[0, 1)$. Typically, the distribution can be defined for $|\omega| < 1$ but negative values lead to under-dispersion which is not a common property of claim count data. For this reason we will not consider this case in the present paper. For $\omega = 0$, the above distribution reduces also to the simple Poisson model with mean $\lambda$. The mean of $y_i$ is given by $E(y_i) = \lambda$ while the variance and the dispersion index are obtained by $V(y_i) = \lambda(1 - \omega)^{-2}$ and $DI = (1 - \omega)^{-2}$ respectively. This parameterization is beneficial for the interpretation of the parameters of the three models and also simplifies the implementation of the MCMC algorithm described below.



# 4 Gibbs Sampling for Testing Hypotheses.

Gibbs sampling has been widely used for Bayesian model, variable selection and hypothesis tests; see George and McCullogh (1993), Carlin and Chib (1995), Kuo and Mallick (1998) and Dellaportas et al. (2002). The Gibbs sampling approach presented here is mainly based on the approach of Gibbs variable selection of Dellaportas et al. (2002) and although some concepts are common with the algorithm of Carlin and Chib (1995), it is more flexible since it allows common parameters among different models avoiding over-parameterization and generation of nuisance parameters.

Without loss of generality, we describe the methodology for a general setup of comparing two nested models $m_1$ and $m_0$. We wish to test that a parameter sub-vector of the super-model $m_1$ is constrained to a sub-model $m_0$. Incorporation of more models (or even non-nested models) is possible in a similar manner.

Let us denote the parameter vectors of models $m_0$ and $m_1$ by $\boldsymbol{\theta}_{m_0}$ and $\boldsymbol{\theta}_{m_1}$ respectively. Then we have the parameter vector $\boldsymbol{\theta}_{m_1}^T = (\boldsymbol{\theta}_{m_0}^T, \boldsymbol{\theta}_{\setminus m_0}^T)$; where $\boldsymbol{\theta}_{\setminus m_0}$ denotes the parameters of model $m_1$ that do not appear in the sub-model $m_0$. We should further note that common parameters should have similar interpretation otherwise posterior distributions will be different and the algorithm will fail (for example in our distributions the parameter $\lambda$ has exactly the same interpretation since it is the mean of $y_i$ in all models).

The hypothesis we wish to test takes the form $H_0 : \boldsymbol{\theta}_{\setminus m_0} = \boldsymbol{\mu}_0$ (model $m_0$) versus $H_1 : \boldsymbol{\theta}_{\setminus m_0} \neq \boldsymbol{\mu}_0$ (model $m_1$). Model $m_0$ is exactly the same (in terms of likelihood) with model $m_1$ with parameter vector $(\boldsymbol{\theta}_{m_0}^T,\ \boldsymbol{\theta}_{\setminus m_0}^T = \boldsymbol{\mu}_0^T)$.

In order to construct our algorithm we employ a latent binary indicator $\gamma$ taking values zero and one when supporting the null or the alternative hypothesis. The posterior distribution of this indicator will give us the posterior probability of each model (or hypothesis) and/or the posterior odds for each model (or hypothesis) comparison. When no prior information concerning the prior model weights $f(m_i)$ is provided then we use $f(\gamma) = 1/2$ for $\gamma = 0, 1$.

For $\gamma = 0, 1$ the model likelihood is now rewritten as

$$f(\boldsymbol{y}|\boldsymbol{\theta}_{m_\gamma}, m_\gamma) = f(\boldsymbol{y}|\boldsymbol{\theta}_{m_0}, m_0)^{1-\gamma} f(\boldsymbol{y}|\boldsymbol{\theta}_{m_1}, m_1)^{\gamma}$$

while the prior distributions are given by $f(\boldsymbol{\theta}_{m_i}, m_\gamma, \gamma)$ for $i = 0, 1$. If $\gamma = i$ then we have the usual prior distributions

$$f(\boldsymbol{\theta}_{m_\gamma}, m_\gamma, \gamma) = f(\boldsymbol{\theta}_{m_\gamma}|m_\gamma) f(\gamma).$$

If $\gamma \neq i$, the resulting distributions are called pseudo-prior distributions since they do not affect the posterior distributions; for details see Carlin and Chib (1995) and Dellaportas et al. (2002). More specifically,

$$\begin{aligned} f(\boldsymbol{\theta}_{m_1}, m_0, \gamma = 0) &= f(\boldsymbol{\theta}_{m_1}|m_0) f(\gamma = 0) \\ &= f(\boldsymbol{\theta}_{m_0}, \boldsymbol{\theta}_{\setminus m_0}|m_0) f(\gamma = 0) \\ &= f(\boldsymbol{\theta}_{m_0}|m_0) f(\boldsymbol{\theta}_{\setminus m_0}|\boldsymbol{\theta}_{m_0}, m_0) f(\gamma = 0). \end{aligned} \tag{4}$$

Thus, the pseudo-prior distribution in (4) can be rewritten as a product of an actual prior distribution of simpler model $m_0$ given by $f(\boldsymbol{\theta}_{m_0}|m_0)$ and an additional pseudo-prior distribution $f(\boldsymbol{\theta}_{\setminus m_0}|\boldsymbol{\theta}_{m_0}, m_0)$ for the non-common parameters. This distribution is specified via a pilot run of model $m_1$. Similarly, the pseudo-prior

$$f(\boldsymbol{\theta}_{m_0}, m_1, \gamma = 1) = f(\boldsymbol{\theta}_{m_0}|m_1) f(\gamma = 1)$$

is the prior of model $m_1$ for the common parameters $\boldsymbol{\theta}_{m_0}$. Using this setup, the resulting Gibbs Sampler is given by

1. Sample model parameters:
   - If $\gamma = 0$ then
     (a) Sample $\boldsymbol{\beta}_{m_0}$ from the conditional posterior distribution
     $$f(\boldsymbol{\beta}_{m_0}|m_0, \boldsymbol{y}) \propto f(\boldsymbol{y}|\boldsymbol{\beta}_{m_0}, m_0, ) f(\boldsymbol{\beta}_{m_0}|m_0).$$
     (b) Sample $\boldsymbol{\beta}_{\setminus m_0}$ from the pseudo-prior distribution $f(\boldsymbol{\beta}_{\setminus m_0}|\boldsymbol{\beta}_{m_0}, m_1)$.
   - If $\gamma = 1$ then sample $\boldsymbol{\beta}_{m_1} = (\boldsymbol{\beta}_{m_0}^T, \boldsymbol{\beta}_{\setminus m_0}^T)$ from the conditional posterior distribution $f(\boldsymbol{\beta}_{m_1}|m_1, \boldsymbol{y}) \propto f(\boldsymbol{y}|\boldsymbol{\beta}_{m_1}, m_1, ) f(\boldsymbol{\beta}_{m_1}|m_1)$.



2. Sample $\gamma$ from the posterior distribution $f(\gamma|\boldsymbol{\theta}_{m_0}, \boldsymbol{\theta}_{\setminus m_0}, \boldsymbol{y}) = Bernoulli\left(\frac{\Omega}{1+\Omega}\right)$; where $\Omega$ is given by
   $$\Omega = LR \times PR_0 \times PR_{\setminus 0} \times \frac{f(m_1)}{f(m_0)}$$
   where $LR$, $PR_0$ and $PR_{\setminus 0}$ denote the likelihood ratio, and the prior ratios given by
   $$LR = \frac{f(\boldsymbol{y}|\boldsymbol{\theta}_{m_1}, m_1)}{f(\boldsymbol{y}|\boldsymbol{\theta}_{m_0}, m_0)}, \quad PR_0 = \frac{f(\boldsymbol{\theta}_{m_0}|m_1)}{f(\boldsymbol{\theta}_{m_0}|m_0)} \quad \text{and} \quad PR_{\setminus 0} = \frac{f(\boldsymbol{\theta}_{\setminus m_0}|\boldsymbol{\theta}_{m_0}, m_1)}{f(\boldsymbol{\theta}_{\setminus m_0}|\boldsymbol{\theta}_{m_0}, m_0)}.$$
   Note that common parameters are assumed to have the same interpretation hence the prior distributions for the two models can be set equal resulting to $PR_0 = 1$.

The approach described above can be easily extended for non-nested models say, $m_1$ and $m_2$ much like our comparison between the negative binomial and generalized Poisson models. Let us assume a model $m_0$ with parameter vector $\boldsymbol{\theta}_{m_0}$ including all parameters common in both model $m_1$ and $m_2$ (if no common parameters can be identified, then $m_0$ can be set to the null model with no parameters). Then we may rewrite the parameters $\boldsymbol{\theta}_{m_i} = (\boldsymbol{\theta}_{m_0}, \boldsymbol{\theta}_{m_i \setminus m_0})$ for $i = 1, 2$ and follow the same approach as in the previous section. In limiting cases, we may identify links between parameters and use suitable transformations in order to automatically specify the pseudo-priors and avoid having to use pilot-run estimates (the approach is analogous to setting suitable transformations in reversible jump MCMC algorithm). Such a case is here where $\boldsymbol{\theta}_{m_1} = (\lambda, \vartheta)$ and $\boldsymbol{\theta}_{m_2} = (\lambda, \omega)$. The non-common parameters $\vartheta$ and $\omega$ can be efficiently linked by equating the dispersion indexes of the two models.

Unlike reversible jump MCMC, the proposed algorithm is simpler because it is based on Gibbs sampler rather than Metropolis Hastings algorithm. Since it is a Gibbs sampling based algorithm it can be implemented in a straightforward manner using the freely available MCMC software of WINBUGS. It is flexible enough to handle nested models or models with common and non-common parameters. For this reason, it can be used in a wide variety of similar problems and can be easily extended to accommodate a larger number of distributions. An application of the aforementioned methodology is presented in Section 5.

# 5 Implementation in Insurance Claims Data

In this section we demonstrate the proposed model formulation in the insurance claim data of Belgium for the year 1993 (Denuit, 1997). The determination of the prior distributions, algorithm specifications and the results are presented below. Details for the implementation on the WINBUGS software are given at the Appendix. The full code is available from the authors upon request.

## 5.1 Prior Distributions

The specification of the prior distributions is very important in Bayesian model comparison. As we have already mentioned, we examine three models: $m_1$ (Poisson), $m_2$ (negative binomial) and $m_3$ (generalized Poisson) with parameter vectors $\boldsymbol{\theta}_{m_1} = (\lambda)$, $\boldsymbol{\theta}_{m_2} = (\lambda, \vartheta)^T$ and $\boldsymbol{\theta}_{m_3} = (\lambda, \omega)^T$ respectively.

In order to be consistent across models we must specify the same prior distributions over the common parameter $\lambda$. Hence, we consider a Gamma distribution, that is,

$$f(\lambda|m_i) = Gamma(0.01,\ 0.01) \text{ for } i = 1, 2, 3.$$

The effect of this choice on the model comparisons will be minimal since $\lambda$ is a common parameter in all models.

The prior distributions $f(\vartheta|\lambda, m_2)$ and $f(\omega|\lambda, m_3)$ will be determined in a way such that the Dispersion Index will induce the same a priori information for both models. Hence, for the prior of $\omega$ we use the Uniform non-informative prior distribution which gives the equal probability to any interval of the same range, that is,

$$f(\omega|m_3) = Uniform(0,\ 1)$$

while the prior $f(\vartheta|m_2)$ is constructed by setting the dispersion indexes equal for the two distributions resulting to

$$\vartheta = \lambda\frac{(1-\omega)^2}{\omega(2-\omega)}. \tag{5}$$

Assuming uniform prior for $\omega$, the resulting distribution for $\vartheta$ is a scaled Beta type II prior distribution given by

$$f(\vartheta|\lambda, m_2) = \frac{1}{2}\lambda\vartheta^{-2}(1+\lambda/\vartheta)^{-3/2}$$



## 5.2 Algorithm specifications: the pseudo-prior distributions

The pseudo-prior distributions are defined by pilot runs estimates. Hence for model $m_3$ we use a Beta distribution, that is,

$$f(\omega|m_1) = Beta(\bar{a}, \bar{b})$$

where the parameters $\bar{a}$, $\bar{b}$ of the Beta distribution are matched with the posterior mean and variance of a pilot run of model $m_2$. Hence $\bar{a}$ and $\bar{b}$ are obtained by

$$\bar{\omega} = \frac{\bar{a}}{\bar{a}+\bar{b}}, \quad \bar{\sigma}^2_\omega = \frac{\bar{a}\bar{b}}{(\bar{a}+\bar{b})^2(\bar{a}+\bar{b}+1)}$$

which leads to

$$\bar{a} = \bar{\omega}\left(\frac{\bar{\omega}(1-\bar{\omega})}{\bar{\sigma}^2_\omega} - 1\right), \quad \bar{b} = \bar{a}\ \frac{1-\bar{\omega}}{\bar{\omega}}.$$

where $\bar{\omega}$ and $\bar{\sigma}^2$ are the posterior mean and variance of $\omega$ estimated by a pilot run. The efficiency of the chain can be improved by suitably increasing or decreasing the variance of the pseudo-prior distribution in order to achieve high acceptance rates. In our example the pseudo-priors where estimated from a pilot run of 1000 iterations and were found $\bar{\omega} = 0.039$ and $\bar{\sigma} = 0.0036$ resulting to $f(\omega|m_1) = Beta(112.7, 2778.1)$.

The pseudo-prior $f(\vartheta|m_1)$ is defined indirectly by specifying a pseudo-prior for $\omega$ and using equation (5). When comparing negative binomial and generalized Poisson models then pseudo-priors are indirectly defined using (5). This results to pseudo-priors which take values directly from the posterior distribution of the competing model and transforming it appropriately.

Finally, if we wish to estimate the log-Bayes posterior odds or the Bayes factor with increased precision, we may use initial model probabilities $f^{(0)}(m_i)$ which will result to posterior weights in the interval (0.40 - 0.60) and then recalculate the desired posterior model odds using the following equation:

$$\log PO_{ij} = \log PO^{(0)}_{ij} - \log\left(\frac{f^{(0)}(m_i)}{f^{(0)}(m_j)}\right) + \log\left(\frac{f(m_i)}{f(m_j)}\right) \tag{6}$$

where $f^{(0)}(m_i)$ are the initial model probabilities only used to estimate posterior odds with precision, $PO^{(0)}_{ij}$ are the posterior model odds estimated using the initial model probabilities while $f(m_i)$ and $\log PO_{ij}$ are the desired prior probabilities and posterior model odds

respectively. When there is no prior information concerning the model space, the log Bayes factor is estimated by the above equation eliminating the log-ratio of the actual prior model probabilities which is equal zero. In our example we have used $\log f^{(0)}(m_2)/f^{(0)}(m_1) = 81$, $\log f^{(0)}(m_3)/f^{(0)}(m_1) = 82$ and $\log f^{(0)}(m_3)/f^{(0)}(m_2) = 0$. Initial values of $f^{(0)}(m)$ can be obtained using simple estimators of the marginal likelihood (for example using Laplace approximation; for details see Kass and Raftery, 1995).

### 5.3 Results

Results for the Belgium 1993 dataset are provided in Table 1. Trace, density and probability plots of the dispersion index and the model indicator for each pairwise comparison are also provided in Figures 1-3. All results have been generated using 1,000 iterations as an initial burn-in period while keeping additional 10,000 iterations for the estimation of the posterior distribution.

Regarding Table 1, the first two columns provide details of the compared models. In the third column we present the initial model odds used to make the chain mobile (i.e. 'jump' from one model to the other) while the next two columns display the MCMC results directly from the WINBUGS output. The last column presents the final estimate of the logarithm of the Bayes Factor for each model comparison using equation (6), the initial model odds (third column) and the MCMC results. For example, the second line of the Table depicts the comparison of the Generalised Poisson versus the Poisson model (model $m_3$ vs. model $m_2$). The initial model odds was set equal to 82 in favor of the Poisson model while the Gibbs sampling algorithm yielded the posterior model probability for the Generalised Poisson model equal to 0.533. Furthermore, the logarithm of the posterior model odds, $\log PO_{31}^{(0)}$, is equal 0.134. Using (6), we derive the final estimate for the logarithm of the posterior model odds equal to 82.134 which strongly supports the Generalised Poisson model.

Figures 1-3 are produced directly from WINBUGS software and are provided to give some insight for the results and the convergence of the algorithm. In all figures, plot (a) depicts the marginal posterior distribution of the Dispersion index for each comparison using the corresponding initial model odds. In Figures 1 and 2 we clearly see a spike at the value of one. This is natural since the Poisson distribution is compared with the Negative Binomial



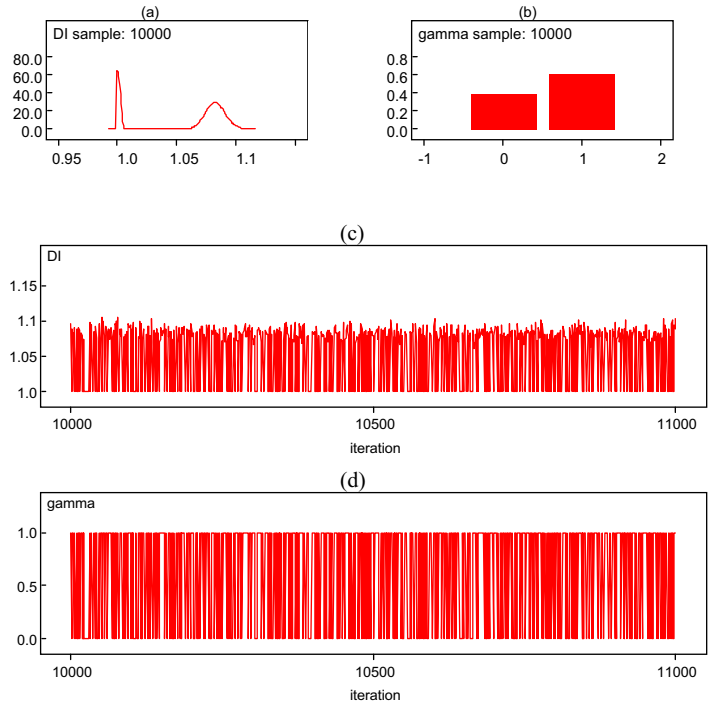


Figure 1: Plots from MCMC Output for Comparison of Negative Binomial vs. Poisson model: (a) Histrogram of the Margingal Posterior Distribution of DI; (b) Posterior Model Weights (0=Poisson, 1=Neg.Binomial); (c) Trace Plot of DI; (d) Trace Plot of Model Indicator $\gamma$.

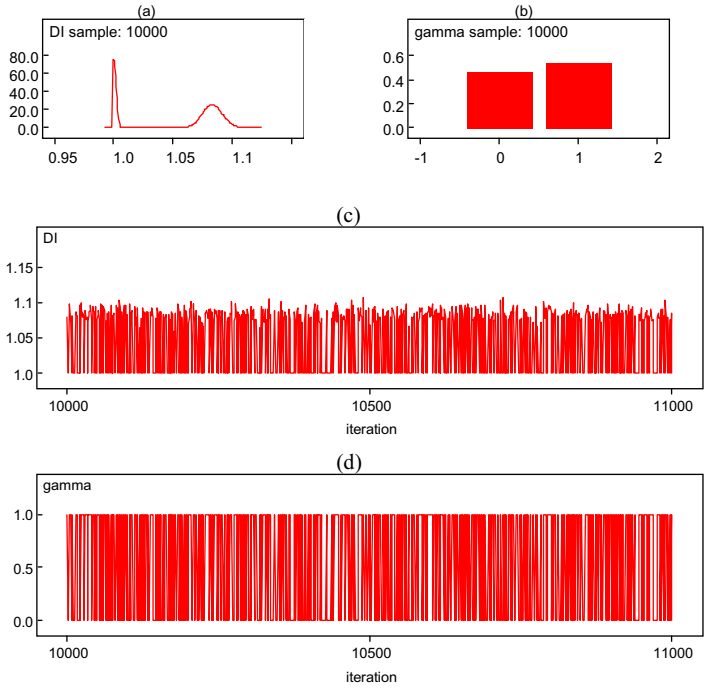


Figure 2: Plots from MCMC Output for Comparison of Generalized Poisson vs. Poisson model: (a) Histrogram of the Margingal Posterior Distribution of DI; (b) Posterior Model Weights (0=Poisson, 1=Gen.Poisson); (c) Trace Plot of DI; (d) Trace Plot of Model Indicator $\gamma$.



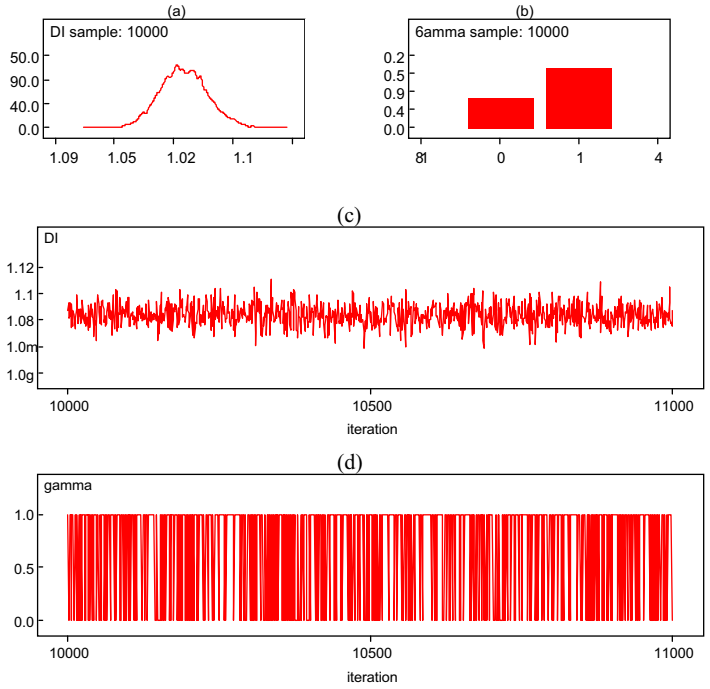


Figure 3: Plots from MCMC Output for Comparison of Generalized Poisson vs. Negative Binomial model: (a) Histogram of the Margingal Posterior Distribution of DI; (b) Posterior Model Weights (0=Neg.Binomial, 1=Gen.Poisson); (c) Trace Plot of DI; (d) Trace Plot of Model Indicator $\gamma$.

and Generalised Poisson, respectively. When the chain supports the Poisson model (in both cases) then the produced DI is equal to one. In most cases, when two models are compared using MCMC, the marginal posterior distribution of a parameter of interest will produce two modes (one for each model) unless the parameters have similar behavior in both models (this is the case in Figure 3a) or one model is not supported at all (i.e. has low posterior probability). Figures 1b-3b present a graph of the posterior distribution of $\gamma$, $f(\gamma|\boldsymbol{y})$, that is the posterior model weights for each comparison (also provided in the fourth column of Table 1). Figures 1c-3c are Trace plots of the DI for each comparison. In common MCMC (when only parameter estimation in a single model is considered) we use such graphs to monitor the convergence of the chain. Plots similar to 3c indicate convergence. In MCMC constructed for model comparison, it is natural to expect violent jumps from the posterior distribution of one model to the other as in plots 1c and 2c. Such jumps are not observed in the comparison of Generalised Poisson and Negative Binomial model because in both models the distributions of the dispersion index are quite close (as plot 3a also indicated). Finally, Figures 1d-3d are also trace plots of the model indicator $\gamma$. These plots are used to monitor the convergence of $\gamma$. A large number of jumps (changes from one model to the other) indicates that the algorithm works efficiently. When the chain remains in one model for many iterations then the graph presents a gap of white area. In all comparisons, the chains were highly mobile and this is also depicted in the corresponding graphs with few short white sequences.

As a conclusion, we observe that the data strongly support the negative binomial and the generalized Poisson models in favor of the simple Poisson model (log-Bayes factors equal to 81.45 and 82.13 respectively). For the comparison between generalized Poisson and negative binomial models we may calculate the corresponding log-Bayes factor directly by the difference of the above log-Bayes factors (equal to 0.69 in favor of the generalized Poisson model) or by generating results from an MCMC directly sampling from these two models (log Bayes factor equal to 0.71). This leads to a slight advantage of the Generalized Poisson Model over the Negative binomial one ($B_{32} \approx 2$ and posterior probability $f(m_3|\boldsymbol{y}) = 0.671$).



| Compared Models | | MCMC Results | | | Estimates |
|---|---|---|---|---|---|
| | $i,j$ | $\log PrM_{ji}^{(0)}$ | $f^{(0)}(m_i\|\boldsymbol{y})$ | $\log PO_{ij}^{(0)}$ | $\log B_{ij}$ |
| Neg.Bin. vs. Poisson | 2,1 | 81 | 0.610 | 0.447 | 81.447 |
| Gen.Poisson vs. Poisson | 3,1 | 82 | 0.533 | 0.134 | 82.134 |
| Gen.Poisson vs. Neg.Bin. | 3,2 | 0 | 0.671 | 0.714 | 0.714 |

Table 1: Posterior Odds and Probabilities for the Belgium 1993 dataset; 1=Poisson, 2=Negative Binomial, 3=Generalized Poisson Model; [$PrM_{ji}^{(0)} = f^{(0)}(m_j)/f^{(0)}(m_i)$, $f^{(0)}(m_i|\boldsymbol{y})$ posterior weights obtained from MCMC using $PrM_{ji}^{(0)}$].

# 6 Conclusions

In this paper, we have developed an advanced MCMC algorithm based on the idea of Gibbs variable selection in order to compare three statistical distributions that model the marginal claim counts in actuarial science. The proposed algorithm is simpler than the existing ones such as RJMCMC and can be implemented in the software-friendly environment of WINBUGS. Furthermore, it can be extended to a wide variety of applications that include model comparisons. A larger number of distributions may be examined as well.

The results from our case study demonstrate the superiority of the Negative Binomial and the Generalized Lagrangian Poisson distributions over the simpler Poisson. Between the first two distributions, the Generalized Langrangian distribution seems to be slightly supported a-posteriori. Further research may include covariates on $\lambda$ in order to treat more sophisticated cases such as the prediction of outstanding claim reserves. Another important issue is the possible extension of our proposed methodology to a larger variety of claim distributions. Using this approach, we may compare different models involved in the claim counts and amounts literature. Implementing Gibbs sampling in a wider variety of actuarial models and problems will enable us to use Bayesian model averaging techniques which increase the predictive ability of any quantity of interest.

# A Appendix: Implementation Using WINBUGS

**Data:** Data are in the form of two vectors: `y[ ]` for the values of $y$ and `w[ ]` the frequency of each value of $y$.

**Likelihood:** The likelihood is defined using the method of zeros and ones (see Spiegelhalter et al. 2003, in section: Tricks: Advanced Use of the BUGS Language). This allows us to use any form likelihood and does not restrict us in the limited number of distributions available in WINBUGS. If `K` is the number of observed values of $y$ then the likelihood is defined as:

```
for (i in 1:K) {
ones[i]<-w[i];
ones[i]~dbin( p[i], w[i] );
p[i]<-gamma*exp(loglike1[i])+(1-gamma)*exp(loglike0[i])
}
```

where `likelihood1[i]` and `likelihood0[i]` are the densities of the distribution models $m_1$ and $m_0$, respectively, evaluated at $y_i$. In our examples `likelihood0[i]` is set equal to the Poisson log-density while `likelihood1[i]` is set equal to the negative binomial or generalized Poisson log-density depending on the comparison we wish to implement. The WINBUGS code for setting the distribution used in this paper follows:

```
# likelihood of poisson
loglike0[i] <-  -lambda + y[i] * log( lambda ) - logfact( y[i] );
#likelihood of negative binomial
loglike1[i] <-  loggam( y[i] + theta ) - loggam( y[i]+1 ) - loggam( theta )
                  + y[i]*log( lambda ) + theta* log( theta )
                  -(y[i]+theta)*log(lambda+theta);
#likelihood of generalized  poisson
loglike1[i] <-   log(1-omega)+log(lambda)
                   +(y[i]-1)*log( (1-omega)*lambda+omega*y[i] )
                   -( (1-omega)*lambda+omega*y[i] ) -logfact(y[i]) ;
```



**Prior Distribution of $\lambda$:** The prior distribution on $\lambda$ is common for all models. Since no information is available we use a $Gamma(0.01, 0.01)$ prior distribution defined in WINBUGS by

```
lambda~dgamma(0.01,0.01);
```

**Prior and Pseudo-prior Distributions on $\vartheta$ :** Here we set $\vartheta$ indirectly as a function of $\omega$ which follows $Uniform(0,1)$ - or equivalently $Beta(1,1)$ - prior distribution when $\gamma = 1$. When $\gamma = 0$ then we have the pseudo-prior for $\omega$ which is set as a beta distribution with parameters specified by a pilot run. The WINBUGS variables `wmean` and `s2` are the posterior mean and variance of $\omega$ when we run the negative binomial model. Then the parameters `abar` and `bbar` of the beta pseudo-prior are matched using the moments estimates. The parameter `c2` is used to adjust the variance of the pseudo-prior. The relevant code for the Belgium 1993 example is the following:

```
theta<-lambda*(1-omega)*(1-omega)/(omega*(2-omega))
omega~dbeta(a,b);
a<-gamma*1 +(1-gamma)*abar;
b<-gamma*1 +(1-gamma)*bbar;
abar<-wmean*(  wmean*(1-wmean)/(c2*s2)-1);
bbar<-abar*(1-wmean)/wmean;
wmean<-0.039;
s2<-pow(0.0036,2);
c2<-0.20;
```

**Prior and Pseudo-prior Distributions on $\omega$:** The approach similar as above with the difference now we directly estimate $\omega$. The WINBUGS code for example one is given by

```
omega~dbeta(a,b);
a<-gamma*1 +(1-gamma)*abar;
b<-gamma*1 +(1-gamma)*bbar;
abar<-wmean*(  wmean*(1-wmean)/(c2*s2)-1);
```

```
bbar<-abar*(1-wmean)/wmean;
wmean<-0.039;
s2<-pow(0.036,2);
c2<-1.0;
```

**Prior on Model Indicator $\gamma$:** When no prior information is available and we wish to roughly estimate the posterior model probabilities then we simply set that $\gamma$ to follow a Bernoulli distribution with probability 1/2 defined by

```
gamma~dbern( 0.5 );
```

When we wish to estimate the posterior model odds with higher precision then we may use a prior such that the posterior model weights are close to 0.5 (this can be achieved by repeated pilot runs) and then calculate backwards the Bayes factor using equation (6). In such case we use the code for example one are given by

```
gamma~dbern( pmp );
#  values for the comparison Poisson vs. Negative Binomial
pmp2<- -81;
pmp<-exp(pmp2)/(1+exp(pmp2))
#  values for the comparison Poisson vs. Generalized Poisson
pmp2<- -82;
pmp<-exp(pmp2)/(1+exp(pmp2));
```

**Comparison of Negative Binomial and Generalized Poisson:** The approach is similar as above but no pseudo-prior is needed since we link the parameters by equating the dispersion indexes of the two models. Hence the WINBUGS code for $\vartheta$ and $\omega$ is simply given by

```
theta<-lambda*(1-omega)*(1-omega)/(omega*(2-omega))
omega~dbeta(1,1);
```



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# Bayesian measures of model complexity and fit

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**Summary.** We consider the problem of comparing complex hierarchical models in which the number of parameters is not clearly defined. Using an information theoretic argument we derive a measure $p_D$ for the effective number of parameters in a model as the difference between the posterior mean of the deviance and the deviance at the posterior means of the parameters of interest. In general $p_D$ approximately corresponds to the trace of the product of Fisher's information and the posterior covariance, which in normal models is the trace of the 'hat' matrix projecting observations onto fitted values. Its properties in exponential families are explored. The posterior mean deviance is suggested as a Bayesian measure of fit or adequacy, and the contributions of individual observations to the fit and complexity can give rise to a diagnostic plot of deviance residuals against leverages. Adding $p_D$ to the posterior mean deviance gives a *deviance information criterion* for comparing models, which is related to other information criteria and has an approximate decision theoretic justification. The procedure is illustrated in some examples, and comparisons are drawn with alternative Bayesian and classical proposals. Throughout it is emphasized that the quantities required are trivial to compute in a Markov chain Monte Carlo analysis.

*Keywords*: Bayesian model comparison; Decision theory; Deviance information criterion; Effective number of parameters; Hierarchical models; Information theory; Leverage; Markov chain Monte Carlo methods; Model dimension

## 1. Introduction

The development of Markov chain Monte Carlo (MCMC) methods has made it possible to fit increasingly large classes of models with the aim of exploring real world complexities of data (Gilks *et al.*, 1996). This ability naturally leads us to wish to compare alternative model formulations with the aim of identifying a class of succinct models which appear to describe the information in the data adequately: for example, we might ask whether we need to incorporate a random effect to allow for overdispersion, what distributional forms to assume for responses and random effects, and so on.

Within the classical modelling framework, model comparison generally takes place by defining a measure of *fit*, typically a deviance statistic, and *complexity*, the number of free parameters in the model. Since increasing complexity is accompanied by a better fit, models are compared by trading off these two quantities and, following early work of Akaike (1973), proposals are often formally based on minimizing a measure of expected loss on a future replicate data set: see, for example, Efron (1986), Ripley (1996) and Burnham and Anderson (1998). A model comparison using the Bayesian information criterion also requires the specification of the number of parameters in each model (Kass and Raftery, 1995), but in complex hierarchical models parameters may outnumber observations and these methods clearly cannot be directly applied (Gelfand and Dey, 1994). The most ambitious attempts to tackle this problem appear in the smoothing and neural network literature (Wahba, 1990; Moody, 1992; MacKay, 1995; Ripley, 1996). This paper suggests Bayesian measures of complexity and fit that can be combined to compare models of arbitrary structure.

In the next section we use an information theoretic argument to motivate a complexity measure $p_D$ for the effective number of parameters in a model, as the difference between the posterior mean of the deviance and the deviance at the posterior estimates of the parameters of interest. This quantity can be trivially obtained from an MCMC analysis and algebraic forms and approximations are unnecessary for its use. We nevertheless investigate some of its formal properties in the following three sections: Section 3 shows that $p_D$ is approximately the trace of the product of Fisher's information and the posterior covariance matrix, whereas in Section 4 we show that for normal models $p_D$ corresponds to the trace of the 'hat' matrix projecting observations onto fitted values and we illustrate its form for various hierarchical models. Its properties in exponential families are explored in Section 5.

The posterior mean deviance $\bar{D}$ can be taken as a Bayesian measure of fit or 'adequacy', and Section 6 shows how in exponential family models an observation's contributions to $\bar{D}$ and $p_D$ can be used as residual and leverage diagnostics respectively. In Section 7 we tentatively suggest that the adequacy $\bar{D}$ and complexity $p_D$ may be added to form a *deviance information criterion* DIC which may be used for comparing models. We describe how this parallels the development of non-Bayesian information criteria and provide a somewhat heuristic decision theoretic justification. In Section 8 we illustrate the use of this technique on some reasonably complex examples. Finally, Section 9 draws some conclusions concerning these proposed techniques.

## 2. The complexity of a Bayesian model

### 2.1. 'Focused' full probability models

Parametric statistical modelling of data $y$ involves the specification of a probability model $p(y|\theta)$, $\theta \in \Theta$. For a Bayesian 'full' probability model, we also specify a prior distribution $p(\theta)$ which may give rise to a marginal distribution

$$p(y) = \int_{\Theta} p(y|\theta)\, p(\theta)\, \mathrm{d}\theta. \tag{1}$$

Particular choices of $p(y|\theta)$ and $p(\theta)$ will be termed a model 'focused' on $\Theta$. Note that we might further parameterize our prior with unknown 'hyperparameters' $\psi$ to create a hierarchical model, so that the full probability model factorizes as

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$$p(y, \theta, \psi) = p(y, \theta)\, p(\theta|\psi)\, p(\psi).$$

Then, depending on the parameters in focus, the model may compose the likelihood $p(y|\theta)$ and prior

$$p(\theta) = \int_{\Psi} p(\theta|\psi)\, p(\psi)\, \mathrm{d}\psi,$$

or the likelihood

$$p(y|\psi) = \int_{\Theta} p(y|\theta)\, p(\theta|\psi)\, \mathrm{d}\theta$$

and prior $p(\psi)$. Both these models lead to the same marginal distribution (1) but can be considered as having different numbers of parameters. A consequence is that in hierarchical modelling we cannot uniquely define a 'likelihood' or 'model complexity' without specifying the level of the hierarchy that is the focus of the modelling exercise (Gelfand and Trevisani, 2002). In fact, by focusing our models on a particular set of parameters $\Theta$, we essentially reduce all models to non-hierarchical structures.

For example, consider an unbalanced random-effects one-way analysis of variance (ANOVA) focused on the group means:

$$y_i|\theta_i \sim N(\theta_i, \tau_i^{-1}), \qquad \theta_i \sim N(\psi, \lambda^{-1}), \qquad i = 1, \ldots, p. \tag{2}$$

This model could also be focused on the overall mean $\psi$ to give

$$y_i|\psi \sim N(\psi, \tau_i^{-1} + \lambda^{-1}),$$

in which case it could reasonably be considered as having a different complexity.

It is natural to wish to measure the complexity of a focused model, both in its own right, say to assess the degrees of freedom of estimators, and as a contribution to model choice: for example, criteria such as BIC (Schwarz, 1978), AIC (Akaike, 1973), TIC (Takeuchi, 1976) and NIC (Murata *et al.*, 1994) all trade off model fit against a measure of the effective number of parameters in the model. However, the foregoing discussion suggests that such measures of complexity may not be unique and will depend on the number of parameters in focus. Furthermore, the inclusion of a prior distribution induces a dependence between parameters that is likely to reduce the effective dimensionality, although the degree of reduction may depend on the data that are available. Heuristically, complexity reflects the 'difficulty in estimation' and hence it seems reasonable that a measure of complexity may depend on both the prior information concerning the parameters in focus and the specific data that are observed.

### 2.2. Is there a true model?

We follow Box (1976) in believing that 'all models are wrong, but some are useful'. However, it can be useful to posit a 'true' distribution $p^{\mathrm{t}}(Y)$ of unobserved future data $Y$ since, for any focused model, this defines a 'pseudotrue' parameter value $\theta^{\mathrm{t}}$ (Sawa, 1978) which specifies a likelihood $p(Y|\theta^{\mathrm{t}})$ that minimizes the Kullback–Leibler distance $E^{\mathrm{t}}[\log\{p^{\mathrm{t}}(Y)\}/p(Y|\theta^{\mathrm{t}})]$ from $p^{\mathrm{t}}(Y)$. Having observed data $y$, under reasonably broad conditions (Berk, 1966; Bunke and Milhaud, 1998) $p(\theta|y)$ converges to $\theta^{\mathrm{t}}$ as information on the components of $\theta$ increases. Thus Bayesian analysis implicitly relies on $p(Y|\theta^{\mathrm{t}})$ being a reasonable approximation to $p^{\mathrm{t}}(Y)$, and we shall indicate where we make use of this 'good model' assumption.



### 2.3. True and estimated residual information

The residual information in data $y$ conditional on $\theta$ may be defined (up to a multiplicative constant) as $-2\log\{p(y|\theta)\}$ (Kullback and Leibler, 1951; Burnham and Anderson, 1998) and can be interpreted as a measure of 'surprise' (Good, 1956), logarithmic penalty (Bernardo, 1979) or uncertainty. Suppose that we have an estimator $\tilde{\theta}(y)$ of the pseudotrue parameter $\theta^{\mathrm{t}}$. Then the excess of the true over the estimated residual information will be denoted

$$d_{\Theta}\{y, \theta^{\mathrm{t}}, \tilde{\theta}(y)\} = -2\log\{p(y|\theta^{\mathrm{t}})\} + 2\log[p\{y|\tilde{\theta}(y)\}]. \tag{3}$$

This can be thought of as the reduction in surprise or uncertainty due to estimation, or alternatively the degree of 'overfitting' due to $\tilde{\theta}(y)$ adapting to the data $y$. We now argue that $d_{\Theta}$ may form the basis for both classical and Bayesian measures of model dimensionality, with each approach differing in how it deals with the unknown true parameters in $d_{\Theta}$.

### 2.4. Classical measures of model dimensionality

In a non-Bayesian likelihood-based context, we may take $\tilde{\theta}(y)$ to be the maximum likelihood estimator $\hat{\theta}(y)$, expand $2\log\{p(y|\theta^{\mathrm{t}})\}$ around $2\log[p\{y|\hat{\theta}(y)\}]$, take expectations with respect to the unknown true sampling distribution $p^{\mathrm{t}}(Y)$ and hence show (Ripley, 1996) (page 34) that

$$E^{\mathrm{t}}[d_{\Theta}\{Y, \theta^{\mathrm{t}}, \tilde{\theta}(Y)\}] \approx p^* = \mathrm{tr}(KJ^{-1}), \tag{4}$$

where

$$\begin{aligned} J &= -E^{\mathrm{t}}\left[\frac{\partial^2 \log\{p(Y|\theta^{\mathrm{t}})\}}{\partial\theta^2}\right], \\ K &= \mathrm{var}^{\mathrm{t}}\left[\frac{\partial \log\{p(Y|\theta^{\mathrm{t}})\}}{\partial\theta}\right]. \end{aligned} \tag{5}$$

This is the measure of complexity that is used in TIC (Takeuchi, 1976). Burnham and Anderson (1998) (page 244) pointed out that

$$p^* = \mathrm{tr}(J\Sigma), \tag{6}$$

where $\Sigma = J^{-1}KJ^{-1}$ is the familiar 'sandwich' approximation to the variance–covariance matrix of the $\hat{\theta}(y)$ (Huber, 1967). If $p^{\mathrm{t}}(y) = p(y|\theta^{\mathrm{t}})$, i.e. one of the models is true, then $K = J$ and $p^* = p$, the number of independent parameters in $\Theta$.

For example, in a fixed effect ANOVA model

$$y_i|\theta_i \sim N(\theta_i, \tau_i^{-1}), \qquad i = 1, \ldots, p,$$

with $\tau_i^{-1}$s known,

$$d_{\Theta}\{y, \theta^{\mathrm{t}}, \hat{\theta}(y)\} = \sum_i \tau_i (y_i - \theta_i^{\mathrm{t}})^2,$$

whose expectation under $p^{\mathrm{t}}(Y)$ is $p^* = \Sigma_i \tau_i\, E^{\mathrm{t}}(Y_i - \theta^{\mathrm{t}})^2$. If the model is true, $E^{\mathrm{t}}(Y_i - \theta^{\mathrm{t}})^2 = \tau_i^{-1}$ and so $p^* = p$.

Ripley (1996) (page 140) showed how this procedure may be extended to 'regularized' models in which a specified prior term $p(\theta)$ is introduced to form a penalized log-likelihood. Replacing $\log(p)$ by $\log\{p(y|\theta)\} + \log\{p(\theta)\}$ in equations (5) yields a more general definition of $p^*$ that

was derived by Moody (1992) and termed the 'effective number of parameters'. This is the measure of dimensionality that is used in NIC (Murata *et al.*, 1994): the estimation of $p^*$ is generally not straightforward (Ripley, 1996).

In the random-effects ANOVA example with $\theta_i \sim N(\psi, \lambda^{-1})$, $\psi$ and $\lambda$ known, let $\rho_i = \tau_i/(\tau_i + \lambda)$ be the intraclass correlation coefficient in the $i$th group. We then obtain

$$p^* = \sum_i \rho_i \tau_i \, E^{\mathrm{t}}(Y_i - \theta^{\mathrm{t}})^2, \tag{7}$$

which becomes

$$p^* = \sum_i \rho_i \tag{8}$$

if the likelihood is true.

### 2.5. A Bayesian measure of model complexity

From a Bayesian perspective, the unknown $\theta^{\mathrm{t}}$ may be replaced by a random variable $\theta$. Then $d_\Theta\{y, \theta, \tilde{\theta}(y)\}$ can be estimated by its posterior expectation with respect to $p(\theta|y)$, denoted

$$\begin{aligned} p_D\{y, \Theta, \tilde{\theta}(y)\} &= E_{\theta|y}[d_\Theta\{y, \theta, \tilde{\theta}(y)\}] \\ &= E_{\theta|y}[-2 \log\{p(y|\theta)\}] + 2 \log[p\{y|\tilde{\theta}(y)\}]. \end{aligned} \tag{9}$$

$p_D\{y, \Theta, \tilde{\theta}(y)\}$ is our proposal as the effective number of parameters with respect to a model with focus $\Theta$: we shall usually drop the arguments $\{y, \Theta, \tilde{\theta}(y)\}$ from the notation. In our examples we shall generally take $\tilde{\theta}(y) = E(\theta|y) = \bar{\theta}$, the posterior mean of the parameters. However, we note that it is not strictly necessary to use the posterior mean as an estimator of either $d_\Theta$ or $\theta$, and the mode or median could be justified (Section 2.6).

Taking $f(y)$ to be some fully specified standardizing term that is a function of the data alone, $p_D$ may be written as

$$p_D = \overline{D(\theta)} - D(\bar{\theta}) \tag{10}$$

where

$$D(\theta) = -2 \log\{p(y|\theta)\} + 2 \log\{f(y)\}.$$

We shall term $D(\theta)$ the 'Bayesian deviance' in general and, more specifically, for members of the exponential family with $E(Y) = \mu(\theta)$ we shall use the saturated deviance $D(\theta)$ obtained by setting $f(y) = p\{y|\mu(\theta) = y\}$: see Section 8.1.

Equation (10) shows that $p_D$ can be considered as a 'mean deviance minus the deviance of the means'. A referee has pointed out the related argument used by Meng and Rubin (1992), who showed that such a difference, between the average of log-likelihood ratios and the likelihood ratio evaluated at the average (over multiple imputations) of the parameters, is the key quantity in estimating the degrees of freedom of a test.

For example, in the random-effects ANOVA (2) with $\psi$ and $\lambda$ known,

$$D(\theta) = \sum_i \tau_i (y_i - \theta_i)^2,$$



which is $-2$ log(likelihood) standardized by the term $-2 \log\{f(y)\} = \Sigma_i \log(2\pi/\tau_i)$ obtained from setting $\theta_i = y_i$. Now $\theta_i|y \sim N\{\rho_i y_i + (1 - \rho_i)\psi, \rho_i \tau_i^{-1}\}$ and hence it can be shown that the posterior distribution of $D(\theta)$ has the form

$$D(\theta) \sim \sum \rho_i \, \chi^2\{1, (y_i - \psi)^2(1 - \rho_i)\lambda\},$$

where $\chi^2(a, b)$ is a non-central $\chi^2$-distribution with mean $a + b$. Thus, since $\rho_i \lambda = (1 - \rho_i)\tau_i$, we have

$$\begin{aligned} \overline{D(\theta)} &= \sum \rho_i + \sum \tau_i (1 - \rho_i)^2 (y_i - \psi)^2, \\ D(\bar{\theta}) &= \sum \tau_i (1 - \rho_i)^2 (y_i - \psi)^2, \end{aligned}$$

and so

$$p_D = \sum_i \rho_i = \sum_i \frac{\tau_i}{\tau_i + \lambda}. \tag{11}$$

The effective number of parameters is therefore the sum of the intraclass correlation coefficients, which essentially measures the sum of the ratios of the precision in the likelihood to the precision in the posterior. This exactly matches Moody's approach (8) when the model is true.

If $\psi$ is unknown and given a uniform hyperprior we obtain a posterior distribution $\psi \sim N\{\bar{y}, (\lambda \Sigma \rho_i)^{-1}\}$, where $\bar{y} = \Sigma \rho_i y_i / \Sigma \rho_i$. It is straightforward to show that

$$\begin{aligned} \overline{D(\theta)} &= \sum \rho_i + \lambda \sum \rho_i (1 - \rho_i)(y_i - \bar{y})^2 + \sum \rho_i (1 - \rho_i) / \sum \rho_i, \\ D(\bar{\theta}) &= \lambda \sum \rho_i (1 - \rho_i)(y_i - \bar{y})^2, \end{aligned}$$

and so $p_D = \Sigma \rho_i + \Sigma \rho_i (1 - \rho_i)/\Sigma \rho_i$. If the groups are independent, $\lambda = 0$, $\rho_i = 1$ and $p_D = p$. If the groups all have the same mean, $\lambda \to \infty$, $\rho_i \to 0$ and $p_D \to 1$. If all group precisions are equal, $p_D = 1 + (p - 1)\rho$, as obtained by Hodges and Sargent (2001).

### 2.6. Some observations on $p_D$

(a) Equation (10) may be rewritten as

$$\overline{D(\theta)} = D(\bar{\theta}) + p_D, \tag{12}$$

which can be interpreted as a classical 'plug-in' measure of fit plus a measure of complexity. Thus our Bayesian measure of fit, $\overline{D(\theta)}$, could perhaps be better considered as a measure of 'adequacy', and we shall use these terms interchangeably. However, in Section 7.3 we shall suggest that an additional penalty for complexity may be reasonable when making model comparisons.

(b) Simple use of the Bayes theorem reveals the expression

$$p_D = E_{\theta|y}\left[-2 \log\left\{\frac{p(\theta|y)}{p(\theta)}\right\}\right] + 2 \log\left\{\frac{p(\tilde{\theta}|y)}{p(\tilde{\theta})}\right\},$$

which can be interpreted as (minus twice) the posterior estimate of the gain in information provided by the data about $\theta$, minus the plug-in estimate of the gain in information.

(c) It is reasonable that the effective number of parameters in a model might depend on the data, the choice of focus $\Theta$ and the prior information (Section 2.1). Less attractive, perhaps, is that $p_D$ may also depend on the choice of estimator $\tilde{\theta}(y)$, since this can produce a lack of invariance of $p_D$ to apparently innocuous transformations, such as making inferences on logits instead of probabilities in Bernoulli trials. Our usual choice of the posterior mean is largely based on the subsequent ability to investigate approximate forms for $p_D$ (Section 3), and the positivity properties described below. A choice of, say, posterior medians would produce a measure of model complexity that was invariant to univariate 1–1 transformations, and we explore this possibility in Section 5.

(d) It follows from equation (10) and Jensen's inequality that, when using the posterior mean as an estimator $\tilde{\theta}(y)$, $p_D \geqslant 0$ for any likelihood that is log-concave in $\theta$, with 0 being approached for a degenerate prior on $\theta$. Non-log-concave likelihoods can, however, give rise to a negative $p_D$ in certain circumstances. For example, consider a single observation from a Cauchy distribution with deviance $D(\theta) = 2\log\{1 + (y - \theta)^2\}$, with a discrete prior assigning probability 1/11 to $\theta = 0$ and 10/11 to $\theta = 3$. If we observe $y = 0$, then the posterior probabilities are changed to 0.5 and 0.5, and so $\bar{\theta} = 1.5$. Thus $p_D = \overline{D(\theta)} - D(\bar{\theta}) = \log(10) - 2\log(13/4) = \log(160/169) < 0$. Our experience has been that negative $p_D$s indicate substantial conflict between the prior and data, or where the posterior mean is a poor estimator (such as a symmetric bimodal distribution).

(e) The posterior distribution that is used in obtaining $p_D$ conditions on the truth of the model, and hence $p_D$ may only be considered an appropriate measure of the complexity of a model that reasonably describes the data. This is reflected in the finding that $p_D$ in the simple ANOVA example (11) will not necessarily be approximately equivalent to the classical $p^*$ (7) if the assumptions of the model are substantially inaccurate. This good model assumption (Section 2.2) is further considered when we come to comparisons of models (Section 7.3).

(f) Provided that $D(\theta)$ is available in closed form, $p_D$ may be easily calculated after an MCMC run by taking the sample mean of the simulated values of $D(\theta)$, minus the plug-in estimate of the deviance using the sample means of the simulated values of $\theta$. No 'small sample' adjustment is necessary. This ease of computation should be contrasted with the frequent difficulty within the classical framework with deriving the functional form of the measure of dimensionality and its subsequent estimation.

(g) Since the complexity depends on the focus, a decision must be made whether nuisance parameters, e.g. variances, are to be included in $\Theta$ or integrated out before specifying the model $p(y|\theta)$. However, such a removal of nuisance parameters may create computational difficulties.

$p_D$ has been defined and is trivially computable by using MCMC methods, and so strictly speaking there is no need to explore exact forms or approximations. However, to provide insight into the behaviour of $p_D$, the following three sections consider the form of $p_D$ in different situations and draw parallels with alternative suggestions: note that we are primarily concerned with the 'preasymptotic' situation in which prior opinion is still influential and the likelihood has not overwhelmed the prior.

## 3. Forms for $p_D$ based on normal approximations

In Section 2.1 we argued that focused models are essentially non-hierarchical with a likelihood $p(y|\theta)$ and prior $p(\theta)$. Before considering particular assumptions for these we examine the form



of $p_D$ under two general conditions: approximately normal likelihoods and negligible prior information.

### 3.1. $p_D$ assuming a normal approximation to the likelihood

We may expand $D(\theta)$ around $E_{\theta|y}(\theta) = \bar{\theta}$ to give, to second order,

$$D(\theta) \approx D(\bar{\theta}) + (\theta - \bar{\theta})^{\mathrm{T}} \frac{\partial D}{\partial \theta}\bigg|_{\bar{\theta}} + \frac{1}{2}(\theta - \bar{\theta})^{\mathrm{T}} \frac{\partial^2 D}{\partial \theta^2}\bigg|_{\bar{\theta}} (\theta - \bar{\theta}), \tag{13}$$

$$= D(\bar{\theta}) - 2(\theta - \bar{\theta})^{\mathrm{T}} L'_{\bar{\theta}} - (\theta - \bar{\theta})^{\mathrm{T}} L''_{\bar{\theta}} (\theta - \bar{\theta}) \tag{14}$$

where $L = \log\{p(y|\theta)\}$ and $L'$ and $L''$ represent first and second derivatives with respect to $\theta$. This corresponds to a normal approximation to the likelihood.

Taking expectations of equation (14) with respect to the posterior distribution of $\theta$ gives

$$\begin{aligned} E_{\theta|y}\{D(\theta)\} &\approx D(\bar{\theta}) - E[\mathrm{tr}\{(\theta - \bar{\theta})^{\mathrm{T}} L''_{\bar{\theta}} (\theta - \bar{\theta})\}] \\ &= D(\bar{\theta}) - E[\mathrm{tr}\{L''_{\bar{\theta}} (\theta - \bar{\theta})(\theta - \bar{\theta})^{\mathrm{T}}\}] \\ &= D(\bar{\theta}) - \mathrm{tr}[L''_{\bar{\theta}} E\{(\theta - \bar{\theta})(\theta - \bar{\theta})^{\mathrm{T}}\}] \\ &= D(\bar{\theta}) + \mathrm{tr}(-L''_{\bar{\theta}} V) \end{aligned}$$

where $V = E\{(\theta - \bar{\theta})(\theta - \bar{\theta})^{\mathrm{T}}\}$ is the posterior covariance matrix of $\theta$, and $-L''_{\bar{\theta}}$ is the observed Fisher information evaluated at the posterior mean of $\theta$. Thus

$$p_D \approx \mathrm{tr}(-L''_{\bar{\theta}} V), \tag{15}$$

which can be thought of as a measure of the ratio of the information in the likelihood about the parameters as a fraction of the total information in the likelihood and the prior. We note the parallel with the classical $p^*$ in equation (6).

We also note that

$$L''_{\bar{\theta}} = Q''_{\bar{\theta}} - P''_{\bar{\theta}}$$

where $Q'' = \partial^2 \log\{p(\theta|y)\}/\partial\theta^2$ and $P'' = \partial^2 \log\{p(\theta)\}/\partial\theta^2$, and hence approximation (15) can be written

$$p_D \approx \mathrm{tr}(-Q''_{\bar{\theta}} V) - \mathrm{tr}(-P''_{\bar{\theta}} V).$$

Under approximate posterior normality $V^{-1} \approx -Q''_{\bar{\theta}}$ and hence

$$p_D \approx p - \mathrm{tr}(-P''_{\bar{\theta}} V) \tag{16}$$

where $p$ is the cardinality of $\Theta$.

### 3.2. $p_D$ for approximately normal likelihoods and negligible prior information

Consider a focused model in which $p(\theta)$ is assumed to be dominated by the likelihood, either because of assuming a 'flat' prior or by increasing the sample size. Assume that the approximation

$$\theta|y \sim N(\hat{\theta},\ -L''_{\hat{\theta}}) \tag{17}$$

holds, where $\bar{\theta} = \hat{\theta}$ are the maximum likelihood estimates such that $L'_{\hat{\theta}} = 0$ (Bernardo and Smith (1994), section 5.3). From equation (14)

$$\begin{aligned} D(\theta) &\approx D(\hat{\theta}) - (\theta - \hat{\theta})^{\mathrm{T}} L''_{\hat{\theta}} (\theta - \hat{\theta}) \\ &\approx D(\hat{\theta}) + \chi^2_p, \end{aligned} \tag{18}$$

since, by approximation (17), $-(\theta - \hat{\theta})^{\mathrm{T}} L''_{\hat{\theta}} (\theta - \hat{\theta})$ has an approximate $\chi^2$-distribution with $p$ degrees of freedom.

Rearranging approximation (18) and taking expectations with respect to the posterior distribution of $\theta$ reveals that

$$p_D = E_{\theta|y}\{D(\theta)\} - D(\hat{\theta}) \approx p,$$

i.e. $p_D$ will be approximately the true number of parameters: this approximation could also be derived by letting $P''_{\hat{\theta}} \to 0$ in approximation (16). This approximate identity is illustrated in Section 8.1.

We note in passing that we might use MCMC output to estimate the classical deviance $D(\hat{\theta})$ of any likelihood-based model by

$$\hat{D}(\hat{\theta}) = E_{\theta|y}\{D(\theta)\} - p. \tag{19}$$

Although the maximum likelihood deviance is theoretically the minimum of $D$ over all feasible values of $\theta$, $D(\hat{\theta})$ will generally be very badly estimated by the sample minimum over an MCMC run, and so the estimator given by equation (19) may be preferable.

## 4. $p_D$ for normal likelihoods

In this section we illustrate the formal behaviour of $p_D$ for normal likelihoods by using exact and approximate identities. However, it is important to keep in mind that in practice such forms are unnecessary for computation and that $p_D$ should automatically allow for fixed effects, random effects and unknown precisions.

### 4.1. The normal linear model

We consider the general hierarchical normal model described by Lindley and Smith (1972). Suppose that

$$\begin{aligned} y &\sim N(A_1\theta, C_1), \\ \theta &\sim N(A_2\psi, C_2) \end{aligned} \tag{20}$$

where all matrices and vectors are of appropriate dimension, and $C_1$ and $C_2$ are assumed known and $\theta$ is the focus: unknown precisions are considered in Section 4.5. Then the standardized deviance is $D(\theta) = (y - A_1\theta)^{\mathrm{T}} C_1^{-1} (y - A_1\theta)$, and the posterior distribution for $\theta$ is normal with



mean $\bar{\theta} = Vb$ and covariance $V$: $V$ and $b$ will be left unspecified for the moment. Expressing $y - A_1\theta$ as $y - A_1\bar{\theta} + A_1\bar{\theta} - A_1\theta$ reveals that

$$D(\theta) = D(\bar{\theta}) - 2(y - A_1\bar{\theta})^{\mathrm{T}} C_1^{-1} A_1 (\theta - \bar{\theta}) + (\theta - \bar{\theta})^{\mathrm{T}} A_1^{\mathrm{T}} C_1^{-1} A_1 (\theta - \bar{\theta}).$$

Taking expectations with respect to the posterior distribution of $\theta$ eliminates the middle term and gives

$$\bar{D} = D(\bar{\theta}) + \mathrm{tr}(A_1^{\mathrm{T}} C_1^{-1} A_1 V),$$

and thus $p_D = \mathrm{tr}(A_1^{\mathrm{T}} C_1^{-1} A_1 V)$. We note that $A_1^{\mathrm{T}} C_1^{-1} A_1$ is the Fisher information $-L''$, $V$ is the posterior covariance matrix and hence

$$p_D = \mathrm{tr}(-L''V): \tag{21}$$

an exact version of approximation (15). It is also clear that in this context $p_D$ is invariant to affine transformations of $\theta$.

If $\psi$ is assumed known, then Lindley and Smith (1972) showed that $V^{-1} = A_1^{\mathrm{T}} C_1^{-1} A_1 + C_2^{-1}$ and hence from equation (21)

$$p_D = p - \mathrm{tr}(C_2^{-1} V) \tag{22}$$

as an exact version of approximation (16); then $0 \leqslant p_D \leqslant p$, and $p - p_D$ is the measure of the 'shrinkage' of the posterior estimates towards the prior means. If $(C_2^{-1}V)^{-1} = A_1^{\mathrm{T}} C_1^{-1} A_1 C_2 + I_p$ has eigenvalues $\lambda_i + 1, i = 1, \ldots, p$, then

$$p_D = \sum_{i=1}^{p} \frac{\lambda_i}{\lambda_i + 1}, \tag{23}$$

and hence the upper bound for $p_D$ is approached as the eigenvalues of $C_2$ become large, i.e. the prior becomes flat. It can further be shown, in the case $A_1 = I_n$, that $p_D$ is the sum of the squared canonical correlations between data $Y$ and the 'signal' $\theta$.

### 4.2. The 'hat' matrix and leverages

A revealing identity is found by noting that $b = A_1^{\mathrm{T}} C_1^{-1} y$ and the fitted values for the data are given by $\hat{y} = A_1\bar{\theta} = A_1 V b = A_1 V A_1^{\mathrm{T}} C_1^{-1} y$. Thus the hat matrix that projects the data onto the fitted values is $H = A_1 V A_1^{\mathrm{T}} C_1^{-1}$, and

$$p_D = \mathrm{tr}(A_1^{\mathrm{T}} C_1^{-1} A_1 V) = \mathrm{tr}(A_1 V A_1^{\mathrm{T}} C_1^{-1}) = \mathrm{tr}(H). \tag{24}$$

This identity also holds assuming that $\psi$ is unknown with a uniform prior, in which case Lindley and Smith (1972) showed that $V^{-1} = A_1^{\mathrm{T}} C_1^{-1} A_1 + C_2^{-1} - C_2^{-1} A_2 (A_2^{\mathrm{T}} C_2^{-1} A_2)^{-1} A_2^{\mathrm{T}} C_2^{-1}$.

The identification of the effective number of parameters with the trace of the hat matrix is a standard result in linear modelling and has been applied to smoothing (Wahba, 1990) (page 63) and generalized additive models (Hastie and Tibshirani (1990), section 3.5), and is also the conclusion of Hodges and Sargent (2001) in the context of general linear models. The advantage of using the deviance formulation for specifying $p_D$ is that all matrix manipulation and asymptotic approximation is avoided: see Section 4.4 for further discussion. Note that $\mathrm{tr}(H)$ is the sum of terms which in regression diagnostics are identified as the individual *leverages*, the influence of each observation on its fitted value: we shall return to this identity in Section 6.3.

Ye (1998) considered the independent normal model

$$y_i \sim N(\theta_i, \tau^{-1})$$

and suggested that the effective number of parameters should be $\Sigma_i h_i$, where

$$h_i(\theta) = \frac{\partial E_{y|\theta}(\tilde{\theta}_i)}{\partial \theta_i}: \tag{25}$$

the average sensitivity of an unspecified estimate $\tilde{\theta}_i$ to a small change in $y_i$. This is a generalization of the trace of the hat matrix discussed above. In the context of the normal linear models, it is straightforward to show that $E_{Y|\theta}(\bar{\theta}) = H\theta$, and hence $p_D = \mathrm{tr}(H)$ matches Ye's suggestion for model complexity. Further connections with Ye (1998) are described in Section 7.2.

### 4.3. Example: Laird–Ware mixed models

Laird and Ware (1982) specified the mixed normal model as

$$y \sim N(X\alpha + Z\beta, C_1),$$
$$\beta \sim N(0, D),$$

where the covariance matrices $C_1$ and $D$ are currently assumed known. The random effects are $\beta$, and the fixed effects are $\alpha$, and placing a uniform prior on $\alpha$ we can write this model within the general Lindley–Smith formulation (20) by setting $\theta = (\alpha, \beta)$, $A_1 = (X, Z)$, $\psi = 0$ and $C_2$ as a block diagonal matrix with $\infty$ in the top left-hand block, $D$ in the bottom right and 0 elsewhere.

We have already shown that in these circumstances $p_D = \mathrm{tr}\{A_1^{\mathrm{T}} C_1^{-1} A_1 (A_1^{\mathrm{T}} C_1^{-1} A_1 + C_2^{-1})^{-1}\}$, and substituting in the appropriate entries for the Laird–Ware model gives $p_D = \mathrm{tr}(V^* V^{-1})$, where

$$V^* = \begin{pmatrix} X^{\mathrm{T}} C_1^{-1} X & X^{\mathrm{T}} C_1^{-1} Z \\ Z^{\mathrm{T}} C_1^{-1} X & Z^{\mathrm{T}} C_1^{-1} Z \end{pmatrix},$$
$$V = \begin{pmatrix} X^{\mathrm{T}} C_1^{-1} X & X^{\mathrm{T}} C_1^{-1} Z \\ Z^{\mathrm{T}} C_1^{-1} X & Z^{\mathrm{T}} C_1^{-1} Z + D^{-1} \end{pmatrix}$$

which is the precision of the parameter estimates assuming that $D^{-1} = 0$, relative to the precision assuming informative $D$.

### 4.4. Frequentist approaches to model complexity: smoothing and normal non-linear models

A common model in semiparametric regression is

$$y \sim N(X\alpha + \beta, \tau^{-1} C_1),$$
$$\beta \sim N(0, \lambda^{-1} D),$$

where $\beta$ is a vector of length $n$ of function values of the nonparametric part of an interpolation spline (Wahba, 1990; van der Linde, 1995) and $C_1$ and $D$ are assumed known. Motivated by the need to estimate the unknown scale factors $\tau^{-1}$ and $\lambda^{-1}$, for many years the effective number of parameters has been taken to be the trace of the hat matrix (Wahba (1990), page 63) and so, for example, $\hat{\tau}^{-1}$ is the residual sum of squares divided by the 'effective degrees



of freedom' $n - \mathrm{tr}(H)$. In this class of models this measure of complexity coincides with $p_D$. Interest in regression diagnostics (Eubank, 1985; Eubank and Gunst, 1986) and cross-validation to determine the smoothing parameter $\tau/\lambda$ (Wahba (1990), section 4.2) also drew attention to the diagonal entries of the hat matrix as leverage values.

Links to partially Bayesian interpolation models have been provided by Kimeldorf and Wahba (1970) and Wahba (1978, 1983) and further work built on these ideas. For example, another large class of models can be formulated by using the following extension to the Lindley–Smith model:

$$y \sim N\{g(\theta), \tau^{-1} C_1\},$$
$$\theta \sim N(A_2\psi, \lambda^{-1} D)$$

where $g$ is a non-linear expression as found, for example, in pharmacokinetics or neural networks: in many situations $A_2\psi$ will be 0 and $C_1$ and $D$ will be identity matrices. Define

$$q(\theta) = (y - g(\theta))^{\mathrm{T}} C_1^{-1} (y - g(\theta)),$$
$$r(\theta) = (\theta - A_2\psi)^{\mathrm{T}} D^{-1} (\theta - A_2\psi)$$

as the likelihood and prior residual variation. MacKay (1992) suggested estimating $\tau$ and $\lambda$ by maximizing the 'type II' likelihood $p(y|\lambda, \tau)$ derived from integrating out the unknown $\theta$ from the likelihood. Setting derivatives equal to 0 eventually reveals that

$$\hat{\tau}^{-1} = \frac{q(\bar{\theta})}{n - p_D},$$
$$\hat{\lambda}^{-1} = \frac{r(\bar{\theta})}{p_D},$$

which are the fitted likelihood and prior residual variation, divided by the appropriate effective degrees of freedom: $p_D = \mathrm{tr}(H)$ is the key quantity.

These results were derived by MacKay (1992) in the context of 'regularization' in complex interpolation models such as neural networks, in which the parameters $\theta$ are standardized and assumed to have independent normal priors with mean 0 and precision $\lambda$. Then expression (16) may be written

$$p_D \approx p - \lambda\, \mathrm{tr}(V). \tag{26}$$

However, MacKay's use of approximation (26) requires the evaluation of $\mathrm{tr}(V)$, whereas our $p_D$ arises without any additional computation. We would also recommend including $\lambda$ and $\tau$ in the general MCMC estimation procedure, rather than relying on type II maximum likelihood estimates (Ripley (1996), page 167). In this and the smoothing context a fully Bayesian analysis requires prior distributions for $\tau^{-1}$ and $\lambda^{-1}$ to be specified (van der Linde, 2000), and this will both change the complexity of the model and require a choice of estimator of the precisions. We shall now illustrate the form of $p_D$ in the restricted situation of unknown $\tau^{-1}$.

### 4.5. Normal models with unknown sampling precision

Introducing unknown variances as part of the focus confronts us with the need to choose a form for the plug-in posterior estimates. We may illustrate this issue by extending the general hierarchical normal model (20) to the conjugate normal–gamma model with an unknown scale

parameter $\tau$ in both the likelihood and the prior (Bernardo and Smith (1994), section 5.2.1). Suppose that

$$\begin{aligned} y &\sim N(A_1\theta, \tau^{-1}C_1), \\ \theta &\sim N(A_2\psi, \tau^{-1}C_2), \end{aligned} \tag{27}$$

and we focus on $(\theta, \tau)$. The standardized deviance is $D(\theta, \tau) = \tau\, q(\theta) - n\log(\tau)$, where

$$q(\theta) = (y - A_1\theta)^{\mathrm{T}} C_1^{-1}(y - A_1\theta)$$

is the residual variation. Then, for a currently unspecified estimator $\hat{\tau}$,

$$\begin{aligned} p_D &= E_{\theta,\tau|y}(D|\theta,\tau) - D(\bar{\theta},\hat{\tau}) \\ &= E_{\tau|y}[E_{\theta|\tau,y}\{\tau\, q(\theta)\} - n\ \log(\tau)] - \{\hat{\tau}\, q(\bar{\theta}) - n\log(\hat{\tau})\} \\ &= \mathrm{tr}(H) + q(\bar{\theta})(\bar{\tau} - \hat{\tau}) - n\{\overline{\log(\tau)} - \log(\hat{\tau})\} \end{aligned} \tag{28}$$

where $H = A_1^{\mathrm{T}}C_1^{-1}A_1(A_1^{\mathrm{T}}C_1^{-1}A_1 + C_2^{-1})^{-1}$ is the hat matrix which does not depend on $\tau$. Thus the additional uncertain scale parameter adds the second two terms to the complexity of the model.

A conjugate prior $\tau \sim \mathrm{gamma}(a, b)$ leads to a posterior distribution $\tau|y \sim \mathrm{gamma}(a + n/2, b + S/2)$, where

$$S = (y - A_1A_2\psi)^{\mathrm{T}}(C_1 + A_1^{\mathrm{T}}C_2A_1)^{-1}(y - A_1A_2\psi).$$

It remains to choose the estimator $\hat{\tau}$ to place in equation (28), and we shall consider two options.

Suppose that we parameterize in terms of $\tau$ and use

$$\hat{\tau} = \bar{\tau} = \frac{a + n/2}{b + S/2},$$

making the second term in equation (28) 0. Now if $X \sim \mathrm{gamma}(a, b)$, then $E\{\log(X)\} = \psi(a) - \log(b)$ where $\psi$ is the digamma function, and so $\overline{\log(\tau)} = \psi(a + n/2) - \log(b + S/2)$. Hence the term contributing to $p_D$ due to the unknown precision is

$$\begin{aligned} p_D - \mathrm{tr}(H) &= -n\left\{\psi\left(a + \frac{n}{2}\right) - \log\left(a + \frac{n}{2}\right)\right\} \\ &\approx 1 - \frac{2a - \frac{1}{3}}{2a + n} \end{aligned}$$

using the approximation $\psi(x) \approx \log(x) - 1/2x - 1/12x^2$. This term will tend to $1 + 1/3n$ as prior information becomes negligible and hence will be close to the 'correct' value of 1 for moderate sample sizes.

If we were to parameterize in terms of $\log(\tau)$ and to use $\hat{\tau} = \exp\{\overline{\log(\tau)}\}$, the third term in equation (28) is 0 and the second term can be shown to be $1 - O(n^{-1})$. Thus for reasonable sample sizes the choice of parameterization of the unknown precision will make little difference to the measure of complexity. However, in Section 7 we shall argue that the log-scale may be more appropriate owing to the better approximation to likelihood normality.



## 5. Exponential family likelihoods

We assume that we have $p$ groups of observations, where each of the $n_i$ observations in group $i$ has the same distribution. Following McCullagh and Nelder (1989), we define a one-parameter exponential family for the $j$th observation in the $i$th group as

$$\log\{p(y_{ij}|\theta_i, \phi)\} = w_i\{y_{ij}\theta_i - b(\theta_i)\}/\phi + c(y_{ij}, \phi), \tag{29}$$

where

$$\begin{aligned} \mu_i &= E(Y_{ij}|\theta_i, \phi) = b'(\theta_i), \\ V(Y_{ij}|\theta_i, \phi) &= b''(\theta_i)\phi/w_i, \end{aligned}$$

and $w_i$ is a constant. If the canonical parameterization $\Theta$ is the focus of the model, then writing $\bar{b}_i = E_{\theta_i|y}\{b(\theta_i)\}$ we easily obtain that the contribution of the $i$th group to the effective number of parameters is

$$p_{Di}^{\Theta} = 2n_iw_i\{\bar{b}_i - b(\bar{\theta}_i)\}/\phi. \tag{30}$$

These likelihoods highlight the issue of the lack of invariance of $p_D$ to reparameterization, since the mean parameterization $\mu$ will give a different complexity $p_{Di}^{\mu}$. This is first explored within simple binomial and Poisson models with conjugate priors, and then exact and approximate forms of $p_D$ are examined for generalized linear and generalized linear mixed models.

### 5.1. Binomial likelihood with conjugate prior

In the notation of equation (29), $\phi = 1$, $w_i = 1$ and $\theta = \mathrm{logit}(\mu) = \log\{\mu/(1 - \mu)\}$, and the (unstandardized) deviance is

$$D(\mu_i) = -2y_i\log(\mu_i) - 2(n_i - y_i)\log(1 - \mu_i)$$

where $y_i = \Sigma_j y_{ij}$. A conjugate prior $\mu_i = \{1 + \exp(-\theta_i)\}^{-1} \sim \mathrm{beta}(a, b)$ provides a posterior $\mu_i \sim \mathrm{beta}(a + y_i, b + n_i - y_i)$ with mean $(a + y_i)/(a + b + n_i)$. Now, if $X \sim \mathrm{beta}(a, b)$, then $E\{\log(X)\} = \psi(a) - \psi(a + b)$ and $E\{\log(1 - X)\} = \psi(b) - \psi(a + b)$ where $\psi$ is the digamma function, and hence it can be shown that

$$\begin{aligned} \overline{D(\mu_i)} = \overline{D(\theta_i)} &= -2y_i\,\psi(a + y_i) - 2(n_i - y_i)\,\psi(b + n_i - y_i) + 2n_i\,\psi(a + b + n_i) \\ D(\bar{\mu}_i) &= -2y_i\log(a + y_i) - 2(n_i - y_i)\log(b + n_i - y_i) + 2n_i\log(a + b + n_i) \\ D(\bar{\theta}_i) &= -2y_i\,\psi(a + y_i) + 2y_i\,\psi(b + n_i - y_i) \\ &\quad + 2n_i\log[1 + \exp\{\psi(a + y_i) - \psi(b + n_i - y_i)\}], \\ D(\mu_i^{\mathrm{med}}) = D(\theta_i^{\mathrm{med}}) &= -2y_i\log(\mu_i^{\mathrm{med}}) - 2(n_i - y_i)\log(1 - \mu_i^{\mathrm{med}}) \end{aligned}$$

where $\mu_i^{\mathrm{med}}$ denotes the posterior median of $\mu_i$.

Exact $p_{D_i}$s are obtainable by subtraction, and Fig. 1 shows how the value of $p_{D_i}$ depends on the parameterization, the data and the prior. We may also gain further insight into the behaviour of $p_{D_i}$ by considering approximate formulae for the mean and canonical parameterizations by using $\psi(x) \approx \log(x) - 1/2x \approx \log(x - \frac{1}{2})$. This leads to

$$\begin{aligned} p_{D_i}^{\mu} &\approx \frac{y_i}{a + y_i} + \frac{n_i - y_i}{b + n_i - y_i} - \frac{n_i}{a + b + n_i}, \\ p_{D_i}^{\Theta} &\approx \frac{n_i}{a + b + n_i - \frac{1}{2}}. \end{aligned} \tag{31}$$

We make the following observations.

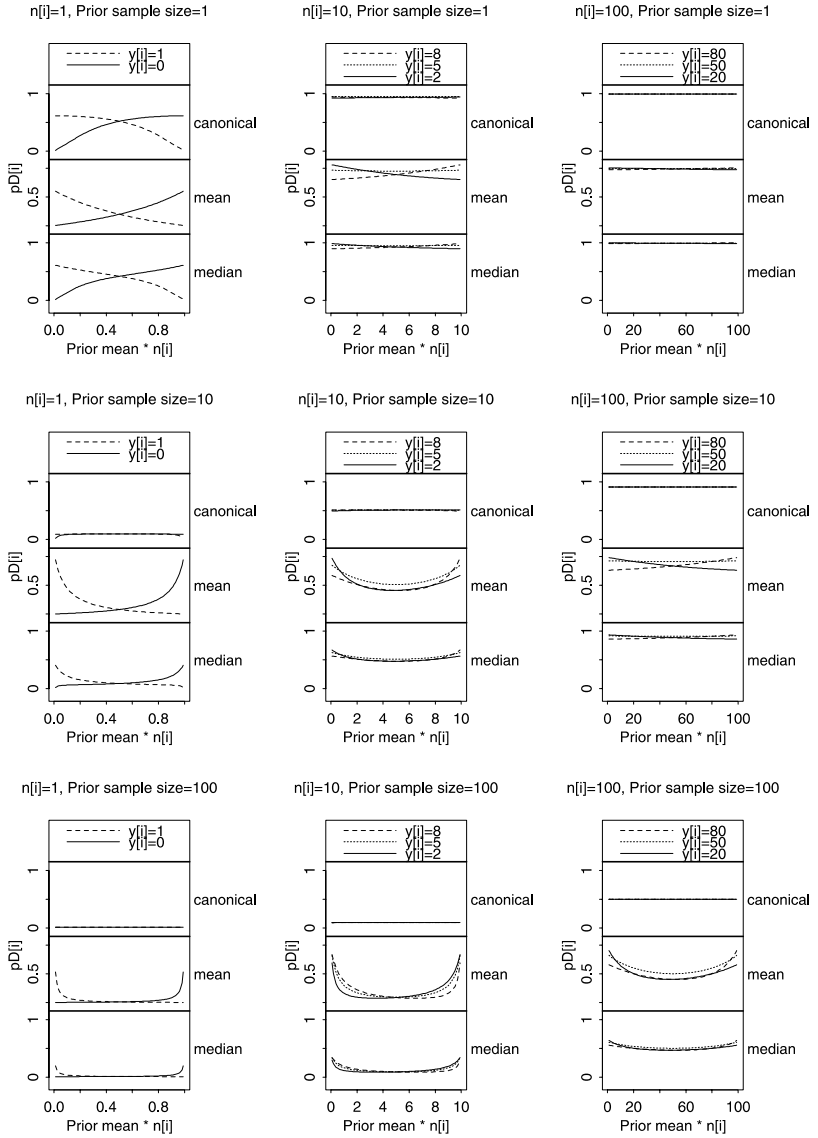


**Fig. 1.** Binomial likelihood—contribution of the $i$th group to the effective number of parameters under various parameterizations (canonical $p_{D_i}^{\Theta}$, mean $p_{D_i}^{\mu}$ and median $p_{D_i}^{\text{med}}$) as a function of the data (sample size $n_i$ and observed proportion $y_i/n_i$) and prior (effective prior sample size $a+b$ and prior mean $a/(a+b)$): we are seeking agreement between alternative parameterizations with little dependence on data



#### 5.1.1. *Behaviour of $p_D$*

For all three parameterizations, as the sample size in each group increases relative to the effective prior sample size, its contribution to $p_{D_i}$ tends towards 1.

#### 5.1.2. *Agreement between parameterizations*

The agreement between parameterizations is generally reasonable except in the situations in which the prior sample size is 10 times that of the data. While the canonical parameterization has $p_{D_i} \approx 1/11$, the mean and median give increased $p_{D_i}$ for extreme prior means.

#### 5.1.3. *Dependence on data*

With the exception of the sparse data and weak prior scenario for which the approximate formulae do not hold, the canonical $p_{D_i}^{\Theta}$ does not depend on the data observed and is approximately the ratio of the sample size to the effective posterior sample size. When the mean and median forms depend on data (say when $n_i = 1$ and $a + b = 10$), $p_{D_i}$ is higher in situations of prior–data conflict.

### 5.2. *Poisson likelihood with conjugate prior*

In the notation of equation (29), $\phi = 1, w_i = 1$ and $\theta = \log(\mu)$, and the (unstandardized) deviance is $D(\mu_i) = -2y_i \log(\mu_i) + 2n_i\mu_i$. A conjugate prior $\mu_i = \exp(\theta_i) \sim \text{gamma}(a, b)$ gives a posterior $\mu_i \sim \text{gamma}(a + y_i, b + n_i)$ with mean $(a + y_i)/(b + n_i)$. If $X \sim \text{gamma}(a, b)$, then $E\{\log(X)\} = \psi(a) - \log(b)$ and hence we can show that

$$\overline{D(\mu_i)} = \overline{D(\theta_i)} = -2y_i\{\psi(a + y_i) - \log(b + n_i)\} + 2n_i\frac{a + y_i}{b + n_i},$$

$$D(\bar{\mu}_i) = -2y_i\{\log(a + y_i) - \log(b + n_i)\} + 2n_i\frac{a + y_i}{b + n_i},$$

$$D(\bar{\theta}_i) = -2y_i\{\psi(a + y_i) - \log(b + n_i)\} + 2n_i\frac{\exp\{\psi(a + y_i)\}}{b + n_i},$$

$$D(\mu_i^{\text{med}}) = D(\theta_i^{\text{med}}) = -2y_i \log(\mu_i^{\text{med}}) + 2n_i\mu_i^{\text{med}}.$$

Exact $p_{D_i}$s are obtainable by subtraction. Fig. 2 shows how the value of $p_{D_i}$ relates to the parameterization, the data and the prior. Using the same approximation as previously, approximate $p_{D_i}$s for the mean and canonical parameterizations are

$$p_{D_i}^{\mu} \approx y_i/(a + y_i),$$
$$p_{D_i}^{\Theta} \approx n_i/(b + n_i).$$

#### 5.2.1. *Behaviour of $p_{D_i}$*

For all three parameterizations, as the sample size in each group increases relative to the effective prior sample size, its contribution to $p_{D_i}$ tends towards 1.

#### 5.2.2. *Agreement between parameterizations*

The agreement between parameterizations is best when there is no conflict between the prior expectation and the data, but it can be substantial when such conflict is extreme. The median

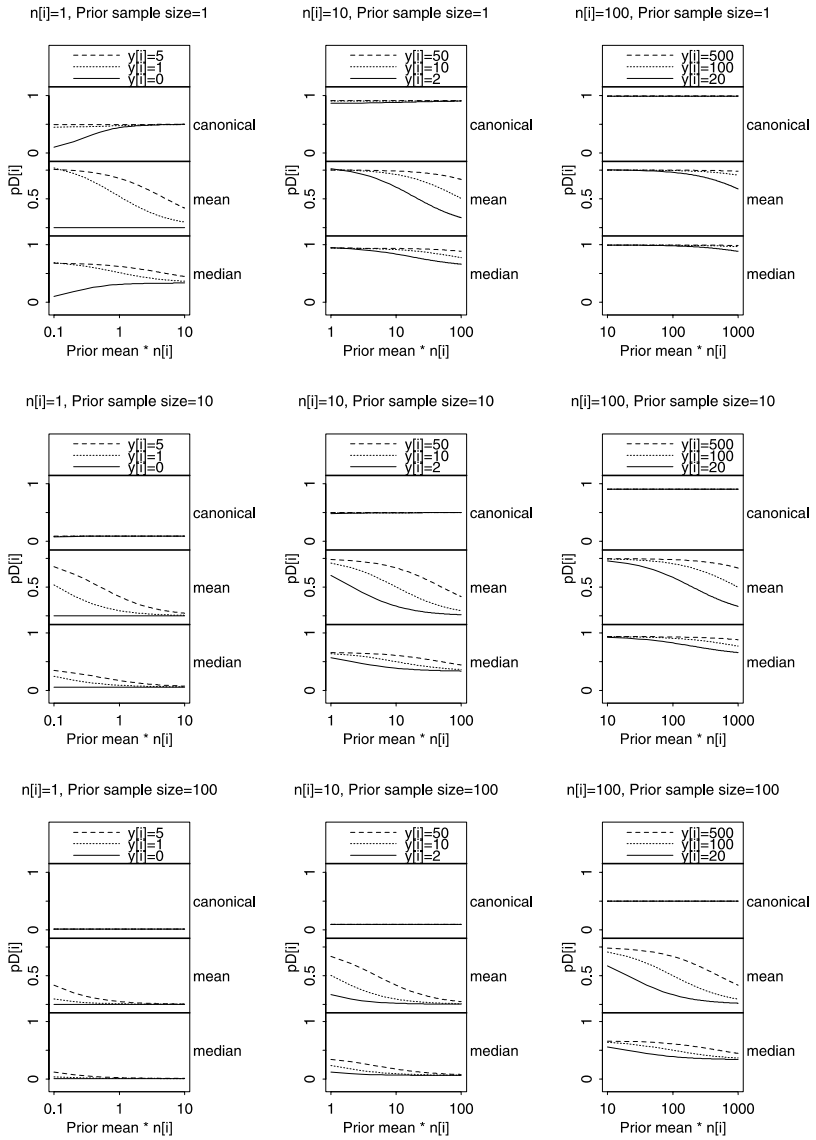


**Fig. 2.** Poisson likelihood—contribution of the $i$th group to the effective number of parameters under various parameterizations (canonical $p_{D_i}^{\Theta}$, mean $p_{D_i}^{\mu}$ and median $p_{D_i}^{\text{med}}$) as a function of the data (sample size $n_i$ and observed total $y_i$) and prior (mean $n_i a/b$ and 'sample size' $b$)



estimator leads to a $p_{D_i}$ that is intermediate between those derived from the canonical and mean parameterizations.

#### 5.2.3. *Dependence on data*

Except in the situation of a single $y_i = 0$ with weak prior information, the approximation for the canonical $p_{D_i}^{\Theta}$ is very accurate and so $p_{D_i}^{\Theta}$ does not depend on the data observed. There can be a substantial dependence for the mean parameterization, with $p_{D_i}^{\mu}$ being higher when the prior mean underestimates the data.

#### 5.2.4. *Conclusion*

In conclusion, for both binomial and Poisson data there is reasonable agreement between the different $p_{D_i}$s provided that the model provides a reasonable fit to the data, i.e. there is not strong conflict between the prior and data. The canonical parameterization appears preferable, both for its lack of dependence on the data and for its generally close approximation to the invariant $p_{D_i}$ based on a median estimator. Thus we would not normally expect the choice of parameterization to have a strong effect, although in Section 8.3 we present an example of a Bernoulli model where this choice does prove to be important.

### 5.3. Generalized linear models with canonical link functions

Here we shall focus on the canonical parameterization in terms of $\theta_i$, both for the reasons outlined above and because its likelihood should better fulfil a normal approximation (Slate, 1994): related identities are available for the mean parameterization in terms of $\mu_i = \mu(\theta_i)$. We emphasize again that the approximate identities that are derived in this and the following section are only for understanding the behaviour of $p_D$ in idealized circumstances (i.e. known precision parameters) and are not required for computation in practical situations.

Following McCullagh and Nelder (1989) we assume that the mean $\mu_i$ of $y_{ij}$ is related to a set of covariates $x_i$ through a link function $g(\mu_i) = x_i^{\mathrm{T}}\alpha$, and that $g$ is the canonical link $\theta(\mu)$. The second-order Taylor series expansion of $D(\theta_i)$ around $D(\bar{\theta}_i)$ yields an approximate normal distribution for working observations and hence derivations of Section 3 apply. We eventually obtain

$$p_D \approx \mathrm{tr}\{X^{\mathrm{T}} W X\, V(\alpha|y)\}$$

where $W$ is diagonal with entries

$$W_i = \frac{w_i}{\phi} n_i\, b''(\bar{\theta}_i),$$

the generalized linear model iterated weights (McCullagh and Nelder (1989), page 40): $\phi$ is assumed known.

Under an $N(\alpha_0, C_2)$ prior on $\alpha$, the prior contribution to the negative Hessian matrix at the mode is just $C_2^{-1}$, so under the canonical link the approximate normal posterior has variance

$$V(\alpha|y) = (C_2^{-1} + X^{\mathrm{T}} W X)^{-1},$$

again producing $p_D$ as a measure of the ratio of the 'working' likelihood to posterior information.

### 5.4. Generalized linear mixed models

We now consider the class of generalized linear mixed models with canonical link, in which $g(\mu_i) = x_i^{\mathrm{T}}\alpha + z_i^{\mathrm{T}}\beta$, where $\beta \sim N(0, D)$ (Breslow and Clayton, 1993) and $D$ is assumed known.

Using the same argument as for generalized linear models (Section 5.3), we find that

$$p_D \approx \mathrm{tr}[(X, Z)^{\mathrm{T}} W(X, Z) V\{(\alpha, \beta)|y\}] \approx \mathrm{tr}(V^* V^{-1}),$$

where

$$V^* = \begin{pmatrix} X^{\mathrm{T}}W^{-1}X & X^{\mathrm{T}}W^{-1}Z \\ Z^{\mathrm{T}}W^{-1}X & Z^{\mathrm{T}}W^{-1}Z \end{pmatrix},$$

$$V = \begin{pmatrix} X^{\mathrm{T}}W^{-1}X & X^{\mathrm{T}}W^{-1}Z \\ Z^{\mathrm{T}}W^{-1}X & Z^{\mathrm{T}}W^{-1}Z + D^{-1} \end{pmatrix}.$$

This matches the proposal of Lee and Nelder (1996) except their $D^{-1}$ is a diagonal matrix of the second derivatives of the prior likelihood for each random effect.

## 6. Diagnostics for fit and influence

### 6.1. Posterior expected deviance as a Bayesian measure of fit or 'adequacy'

The posterior mean of the deviance $E_{\theta|y}\{D(\theta)\} = \overline{D(\theta)}$ has often been used to compare models informally: see, for example, Dempster (1974) (reprinted as Dempster (1997a)), Raghunathan (1988), Zeger and Karim (1991), Gilks *et al.* (1993) and Richardson and Green (1997). These researchers have, however, not been explicit about whether, or how much, such a measure might be traded off against increasing complexity of a model: Dempster (1997b) suggested plotting log-likelihoods from MCMC runs but hesitated to dictate a model choice procedure. We shall discuss this further in Section 7.3. In Section 2.6 we argued that $\overline{D(\theta)}$ already incorporates some penalty for complexity and hence we use the term 'adequacy' and 'Bayesian fit' interchangeably.

### 6.2. Sampling theory diagnostics for lack of Bayesian fit

Suppose that all aspects of the model were assumed true. Then before observing data $Y$ our expectation of the posterior expected deviance is

$$\begin{aligned} E_Y(\bar{D}) &= E_Y[E_{\theta|y}\{D(\theta)\}] \\ &= E_\theta(E_{Y|\theta}[-2\log\{p(Y|\theta)\} + 2\log\{f(Y)\}]) \end{aligned} \tag{32}$$

by reversing the conditioning between $Y$ and $\theta$. If $f(Y) = p\{Y|\hat{\theta}(Y)\}$ where $\hat{\theta}(Y)$ is the standard maximum likelihood estimate, then

$$E_{Y|\theta}\left(-2\log\left[\frac{p(Y|\theta)}{p\{Y|\hat{\theta}(Y)\}}\right]\right)$$

is simply the expected likelihood ratio statistic for the fitted values $\hat{\theta}(Y)$ with respect to the true null model $\theta$ and hence under standard conditions is approximately $E(\chi^2_p) = p$, the dimensionality of $\theta$. From equation (32) we therefore expect, if the model is true, the posterior expected deviance (standardized by the maximized log-likelihood) to be $E_Y(\bar{D}) \approx E_\theta(p) = p$, the number of free parameters in $\theta$. This might be appropriate for checking the overall goodness of fit of the model.

In particular, consider the one-parameter exponential family where $p = n$, the total sample size. The likelihood is maximized by substituting $y_i$ for the mean of $y_i$, and the posterior mean of the standardized deviance has approximate sampling expectation $n$ if the model is true. This will be exact for normal models with known variance, but in general it will only be reliable if each observation provides considerable information about its mean (McCullagh and Nelder (1989),



page 36). Note that comparing $\bar{D}$ with $n$ is precisely the same as comparing the 'classical' fit $D(\bar{\theta})$ with $n - p_D$, the effective degrees of freedom.

It is then natural to consider the contribution $D_i$ of each observation $i$ to the overall mean deviance, so that

$$\bar{D} = \sum_i \bar{D}_i = \sum_i dr_i^2$$

where $dr_i = \pm\sqrt{\bar{D}_i}$ (with the sign given by the sign of $y_i - E(y_i|\bar{\theta})$) termed the Bayesian deviance residual, defined analogously to McCullagh and Nelder (1989), page 39. See Section 8.1 for an application of this procedure.

### 6.3. Leverage diagnostics

In Section 4.1 we noted that in normal linear models the contribution $p_{Di}$ of each observation $i$ to $p_D$ turned out to be its leverage, defined as the relative influence that each observation has on its own fitted value. For $y_i$ conditionally independent given $\theta$, it can be shown that

$$p_{Di} = -2\left(E_{\theta|y}\left[\log\left\{\frac{p(\theta|y_i)}{p(\theta)}\right\}\right] - \log\left\{\frac{p(\bar{\theta}|y_i)}{p(\bar{\theta})}\right\}\right)$$

which reflects its interpretation as the difficulty in estimating $\theta$ with $y_i$.

It may be possible to exploit this interpretation in general model fitting, and as a by-product of MCMC estimation to obtain estimates of leverage for each observation. Such diagnostics are illustrated in Section 8.1.

## 7. A model comparison criterion

### 7.1. Model 'selection'

There has been a long and continuing debate about whether the issue of selecting a model as a basis for inferences is amenable to a strict mathematical analysis using, for example, a decision theoretic paradigm: see, for example, Key *et al.* (1999). Our approach here can be considered to be semiformal. Although we believe that it is useful to have measures of fit and complexity, and to combine them into overall criteria that have some theoretical justification, we also feel that an overformal approach to model 'selection' is inappropriate since so many other features of a model should be taken into account before using it as a basis for reporting inferences, e.g. the robustness of its conclusions and its inherent plausibility. In addition, in many contexts it may not be appropriate to 'choose' a single model. Our development closely follows that of Section 2.

A characteristic that is common to both Bayesian and classical approaches is the concept of an independent replicate data set $Y_{\mathrm{rep}}$, derived from the same data-generating mechanism as gave rise to the observed data. Suppose that the loss in assigning to a set of data $Y$ a probability $p(Y|\tilde{\theta})$ is $\mathcal{L}(Y, \tilde{\theta})$. We assume that we shall favour models $p(Y|\tilde{\theta})$ for which $\mathcal{L}(Y, \tilde{\theta})$ is expected to be small, and thus a criterion can be based on an estimate of $E_{Y_{\mathrm{rep}}|\theta^{\mathrm{t}}}\{\mathcal{L}(Y_{\mathrm{rep}}, \tilde{\theta})\}$.

A natural, but optimistic, estimate of this quantity is the 'apparent' loss $\mathcal{L}\{y, \tilde{\theta}(y)\}$ that is suffered on repredicting the observed $y$ that gave rise to $\tilde{\theta}(y)$. We follow Efron (1986) in defining the 'optimism' that is associated with this estimator as $c_\Theta$, where

$$E_{Y_{\mathrm{rep}}|\theta^{\mathrm{t}}}[\mathcal{L}\{Y_{\mathrm{rep}}, \tilde{\theta}(y)\}] = \mathcal{L}\{y, \tilde{\theta}(y)\} + c_\Theta\{y, \theta^{\mathrm{t}}, \tilde{\theta}(y)\}. \tag{33}$$

Both classical and Bayesian approaches to estimating the optimism $c_\Theta$ will now be examined when assuming a logarithmic loss function $\mathcal{L}(Y, \tilde{\theta}) = -2\log\{p(Y|\tilde{\theta})\}$: as in Section 2, the classical approach attempts to estimate the sampling expectation of $c_\Theta$, whereas the Bayesian approach is based on a direct calculation of the posterior expectation of $c_\Theta$.

### 7.2. Classical criteria for model comparison

From the previous discussion, approximate forms for the expected optimism

$$\pi(\theta^t) = E_{Y|\theta^t}[c_\Theta\{Y, \theta^t, \tilde{\theta}(Y)\}]$$

will, from equation (33), yield criteria for a comparison of models that are based on minimizing

$$\hat{E}_{Y_{\text{rep}}|\theta^t}[\mathcal{L}\{Y_{\text{rep}}, \tilde{\theta}(y)\}] = \mathcal{L}\{y, \tilde{\theta}(y)\} + \hat{\pi}(\theta^t). \tag{34}$$

Efron (1986) derived the expression for $\pi(\theta^t)$ for exponential families and for general loss functions. In particular, for the logarithmic loss function, Efron showed that

$$\pi_E(\theta^t) = 2\sum_i \text{cov}^t(\hat{Y}_i, Y_i), \tag{35}$$

where $\hat{Y}_i$ is the fitted value arising from the estimator $\tilde{\theta}$: if $\tilde{\theta}$ corresponds to maximum likelihood estimation based on a linear predictor with $p$ parameters, then $\pi_E(\theta^t) \approx 2p$. Hence Efron's result can be thought of as generalizing Akaike (1973), who sought to minimize the expected Kullback–Leibler distance between the true and estimated predictive distribution and showed under broad conditions that $\pi(\theta^t) \approx 2p$.

This in turn suggests that $\pi_E/2$, derived from equation (35), may be adopted as a measure of complexity in more complex modelling situations. Ye and Wong (1998) extended the work mentioned in Section 4.2 to show that $\pi_E/2$ for exponential families can be expressed as a sum of the average sensitivity of the fitted values $\hat{y}_i$ to a small change in $y_i$: this quantity is termed by Ye and Wong the 'generalized degrees of freedom' when using a general estimation procedure. In normal models with linear estimators $\hat{y}_i = \tilde{\theta}_i(y) = \Sigma_j h_{ij} y_j$, and so $\pi(\theta^t) = 2\,\text{tr}(H)$. Finally, Ripley (1996) extended the analysis described in Section 2.4 to show that if the model assumed is not true then $\pi(\theta^t) \approx 2p^*$, where $p^*$ is defined in equation (4). See Burnham and Anderson (1998) for a full and detailed review of all aspects of estimation of $\pi(\theta^t)$.

These classical criteria for general model comparison are thus all based on equation (34) and can all be considered as corresponding to a plug-in estimate of fit, plus twice the effective number of parameters in the model. We shall now adapt this structure to a Bayesian context.

### 7.3. Bayesian criteria for model comparison

Gelfand and Ghosh (1998) and Laud and Ibrahim (1995) both attempted strict decision theoretic approaches to model choice based on expected losses on replicate data sets. Our approach is more informal, in aiming to identify models that best explain the observed data, but with the expectation that they are likely to minimize uncertainty about observations generated in the same way. Thus, by analogy with the classical results described above, we propose a *deviance information criterion* DIC, defined as a classical estimate of fit, plus twice the effective number of parameters, to give

$$\text{DIC} = D(\bar{\theta}) + 2p_D \tag{36}$$

$$= \bar{D} + p_D \tag{37}$$



by definition of $p_D$ (10): equation (37) shows that DIC can also be considered as a Bayesian measure of fit or adequacy, penalized by an additional complexity term $p_D$. From the results in Section 3.2, we immediately see that in models with negligible prior information DIC will be approximately equivalent to Akaike's criterion.

An approximate decision theoretic justification for DIC can be obtained by mimicking the development of Ripley (1996) (page 33) and Burnham and Anderson (1998) (chapter 6). Using the logarithmic loss function in equation (33), we obtain

$$c_\Theta\{y, \theta^t, \tilde{\theta}(y)\} = E_{Y_{\text{rep}}|\theta^t}\{D_{\text{rep}}(\tilde{\theta})\} - D(\tilde{\theta})$$

where $-2\log[p\{Y_{\text{rep}}|\tilde{\theta}(y)\}]$ is denoted $D_{\text{rep}}(\tilde{\theta})$ and so on: note in this section that $D$ is an unstandardized deviance ($f(\cdot) = 1$). It is convenient to expand $c_\Theta$ into the three terms

$$c_\Theta = E_{Y_{\text{rep}}|\theta^t}\{D_{\text{rep}}(\tilde{\theta}) - D_{\text{rep}}(\theta^t)\} + E_{Y_{\text{rep}}|\theta^t}\{D_{\text{rep}}(\theta^t) - D(\theta^t)\} + \{D(\theta^t) - D(\tilde{\theta})\}; \tag{38}$$

we shall denote the first two terms by $\mathcal{L}_1$ and $\mathcal{L}_2$ respectively and, since we are taking a Bayesian perspective, replace the true $\theta^t$ by a random quantity $\theta$.

Expanding the first term to second order gives

$$\mathcal{L}_1(\theta, \tilde{\theta}) \approx E_{Y_{\text{rep}}|\theta}\{-2(\tilde{\theta} - \theta)^T L'_{\text{rep},\theta} - (\tilde{\theta} - \theta)^T L''_{\text{rep},\theta}(\tilde{\theta} - \theta)\}$$

where $L_{\text{rep},\theta} = \log\{p(Y_{\text{rep}}|\theta)\}$. Since $E_{Y_{\text{rep}}|\theta}(L'_{\text{rep},\theta}) = 0$ from standard results for score statistics, we obtain after some rearrangement

$$\mathcal{L}_1(\theta, \tilde{\theta}) \approx \text{tr}\{I_\theta(\tilde{\theta} - \theta)(\tilde{\theta} - \theta)^T\}$$

where $I_\theta = E_{Y_{\text{rep}}|\theta}(-L''_{\text{rep},\theta})$ is the assumed Fisher information in $Y_{\text{rep}}$, and hence also in $y$. Making the good model assumption (Section 2.2), this might reasonably be approximated by the observed information at the estimated parameters, so

$$\mathcal{L}_1(\theta, \tilde{\theta}) \approx \text{tr}\{-L''_{\tilde{\theta}}(\tilde{\theta} - \theta)(\tilde{\theta} - \theta)^T\}. \tag{39}$$

Suppose that under a particular model assumption we obtain a posterior distribution $p(\theta|y)$. Then from approximations (38) and (39) our posterior expected optimism when adopting this model and the estimator $\tilde{\theta}$ is

$$E_{\theta|y}(c_\Theta) \approx \text{tr}[-L''_{\tilde{\theta}}\, E_{\theta|y}\{(\theta - \tilde{\theta})(\theta - \tilde{\theta})^T\}] + E_{\theta|y}\{\mathcal{L}_2(y, \theta)\} + E_{\theta|y}\{D(\theta) - D(\tilde{\theta})\}.$$

Using the posterior mean $\bar{\theta}$ as our estimator makes the expected optimism

$$E_{\theta|y}(c_\Theta) \approx \text{tr}(-L''_{\bar{\theta}} V) + E_{\theta|y}\{\mathcal{L}_2(y, \theta)\} + p_D, \tag{40}$$

where $V$ again is defined as the posterior covariance of $\theta$, and $p_D = \bar{D} - D(\bar{\theta})$. Now

$$\mathcal{L}_2(y, \theta) = E_{Y_{\text{rep}}|\theta}[-2\log\{p(Y_{\text{rep}}|\theta)\}] + 2\log\{p(y|\theta)\},$$

and so $E_Y[E_{\theta|Y}\{\mathcal{L}_2(Y, \theta)\}] = E_\theta[E_{Y|\theta}\{\mathcal{L}_2(Y, \theta)\}] = 0$. We have already shown in approximation (15) that $p_D \approx \text{tr}(-L''_{\bar{\theta}} V)$, and hence from expressions (33) and (40) the expected posterior loss when adopting a particular model is

$$D(\bar{\theta}) + E_{\theta|y}(c_\Theta) \approx D(\bar{\theta}) + 2p_D = \text{DIC},$$

neglecting a term $E_{\theta|y}\{\mathcal{L}_2(y, \theta)\}$ which is expected to be 0. This derivation has assumed that

$D$ is an unstandardized deviance: common standardization across models will leave unchanged the property that differences in DIC are estimates of differences in expected loss in prediction.

We make the following observations concerning this admittedly heuristic justification of DIC. First, for the general normal linear model (20), it is straightforward to show that $\mathcal{L}_2(y,\theta) = p-(y-A_1\theta)^{\mathrm{T}}C_1^{-1}(y-A_1\theta)$ where $p$ is the dimensionality of $\theta$, and hence for true $\theta$ has sampling distribution $p-\chi^2_p$ with mean 0 and variance $2p$. This parallels the classical development in which Ripley (1996) (page 34) pointed out that the equivalent term is $O(\sqrt{n})$: we would hope that this factor will tend to cancel when assessing differences in DIC, but this requires further investigation.

Second, this development draws heavily on the approximations in Section 3 and hence encourages parameterizations in which likelihood normality is more plausible.

Third, we are attempting to evaluate the consequences of assuming a particular model, using an analysis that is based on that very assumption. This use of the good model assumption (Section 2.2) argues for the use of DIC in comparing models that have already been shown to be adequate candidates for explaining the observations.

## 8. Examples

$p_D$ and DIC have already been applied by other researchers in a variety of contexts, such as alternative models for diagnostic probabilities in screening studies (Erkanli *et al.*, 1999), longitudinal binary data using Markov regression models (Erkanli *et al.*, 2001), spline models with Bernoulli responses (Biller and Fahrmeir, 2001), multistage models for treatment usage which combine to form a total DIC (Gelfand *et al.*, 2000), complex spatial models for Poisson counts (Green and Richardson, 2000), pharmacokinetic modelling (Rahman *et al.*, 1999) and structures of Bayesian neural networks (Vehtari and Lampinen, 1999). The following examples illustrate the use of $p_D$ and DIC to compare alternative prior and likelihood structures.

### 8.1. The spatial distribution of lip cancer in Scotland

We consider data on the rates of lip cancer in 56 districts in Scotland (Clayton and Kaldor, 1987; Breslow and Clayton, 1993). The data include observed ($y_i$) and expected ($E_i$) numbers of cases for each county $i$ (where the expected counts are based on the age- and sex-standardized national rate applied to the population at risk in each county) plus the 'location' of each county expressed as a list ($\mathcal{A}_i$) of its $n_i$ adjacent counties. We assume that the cancer counts within each county $y_i$ follow a Poisson distribution with mean $\exp(\theta_i)E_i$ where $\exp(\theta_i)$ denotes the underlying true area-specific relative risk of lip cancer. We then consider the following set of candidate models for $\theta_i$, reflecting different assumptions about the between-county variation in (log-) relative risk of lip cancer: model 1,

$$\theta_i = \alpha_0;$$

model 2,

$$\theta_i = \alpha_0 + \gamma_i;$$

model 3,

$$\theta_i = \alpha_0 + \delta_i;$$

model 4,

$$\theta_i = \alpha_0 + \gamma_i + \delta_i;$$

model 5,

$$\theta_i = \alpha_i.$$



An improper uniform prior is placed on $\alpha_0$, independent (proper) normal priors with large variance are specified for each $\alpha_i$ ($i = 1,\ldots,56$), $\gamma_i$ are exchangeable random effects with a normal prior distribution having zero mean and precision $\lambda_\gamma$, and $\delta_i$ are spatial random effects with a conditional autoregressive prior (Besag, 1974) given by

$$\delta_i|\delta_{\setminus i} \sim \text{normal}\left(\frac{1}{n_i}\sum_{j\in\mathcal{A}_i}\delta_j, \frac{1}{n_i\lambda_\delta}\right).$$

A sum-to-zero constraint is imposed on the $\{\delta_i\}$ for identifiability, and weakly informative gamma(0.5,0.0005) priors are assumed for the random effects precision parameters $\lambda_\gamma$ and $\lambda_\delta$. These five models cover the spectrum between the pooled model 1 that makes no allowance for variation between the true risk ratios in each county and the saturated model 5 that assumes independence between the county-specific risk ratios (essentially yielding the maximum likelihood estimates $\hat{\theta}_i = \log(y_i/E_i)$). The random-effects models 2–4 allow the county-specific relative risks to be similar but not identical, with the autoregressive term allowing for the possibility of spatially correlated variation.

We use the saturated deviance (McCullagh and Nelder (1989), page 34)

$$D(\theta) = 2\sum_i [y_i \log\{y_i/\exp(\theta_i)E_i\} - \{y_i - \exp(\theta_i)E_i\}]$$

obtained by taking $-2\log\{f(y)\} = -2\Sigma_i \log\{p(y_i|\hat{\theta}_i)\} = 208.0$ as the standardizing factor (see Section 2.5). This allows calculation of absolute measures of fit (see Section 6.2). For model comparisons, however, it is sufficient to take the standardizing factor as $f(y) = 1$. For each model we ran two independent chains of an MCMC sampler in WinBUGS (Spiegelhalter *et al.*, 2000) for 15000 iterations each, following a burn-in period of 5000 iterations. As suggested by Dempster (1997b), Fig. 3 shows a kernel density smoothed plot of the resulting posterior distributions of the deviance under each competing model. Apart from revealing the obvious unacceptability of model 1, this clearly illustrates the difficulty of formally comparing posterior deviances on the basis of such plots alone.

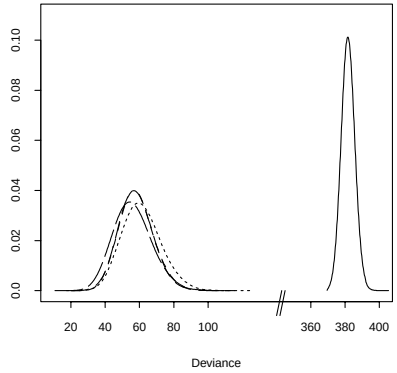


**Fig. 3.** Posterior distributions of the deviance for each model considered in the lip cancer example: ———, model 1; · · · · · · ·, model 2; -------, model 3; – – –, model 4; — —, model 5

**Table 1.** Deviance summaries for the lip cancer data using three alternative parameterizations (mean, canonical and median) for the plug-in deviance†

| *Model* | $\bar{D}$ | $D(\bar{\mu})$ | $p_D^{\mu}$ | $DIC^{\mu}$ | $D(\bar{\theta})$ | $p_D^{\theta}$ | $DIC^{\theta}$ | $D(med)$ | $p_D^{\text{med}}$ | $DIC^{\text{med}}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 1, pooled | 381.7 | 380.7 | 1.0 | 382.7 | 380.7 | 1.0 | 382.7 | 380.7 | 1.0 | 382.7 |
| 2, exchangeable | 61.1 | 18.2 | 42.9 | 104.0 | 17.7 | 43.4 | 104.5 | 17.6 | 43.5 | 104.6 |
| 3, spatial | 58.3 | 26.6 | 31.7 | 89.9 | 27.1 | 31.2 | 89.5 | 27.2 | 31.1 | 89.3 |
| 4, exchangeable + spatial | 57.9 | 26.1 | 31.8 | 89.7 | 26.5 | 31.4 | 89.3 | 26.6 | 31.3 | 89.2 |
| 5, saturated | 55.9 | 0.0 | 55.9 | 111.7 | 3.1 | 52.8 | 108.6 | 1.4 | 54.5 | 110.4 |

†Exchangeable means an exchangeable random effect; spatial is a spatially correlated random effect.

The deviance summaries proposed in this paper are shown for the lip cancer data in Table 1: $\bar{D}$ is simply the mean of the posterior samples of the saturated deviance; $D(\bar{\mu})$ is calculated by plugging the posterior mean of $\mu_i = \exp(\theta_i)E_i$ into the saturated deviance; $D(\bar{\theta})$ is calculated by plugging the posterior means of the relevant parameters ($\alpha_0$, $\alpha_i$, $\gamma_i$ and/or $\delta_i$) into the linear predictor $\theta_i$ and then evaluating the saturated deviance; $D$(med) is calculated by plugging the posterior median of $\theta_i$ (or, equivalently, of $\mu_i$) into the saturated deviance. The results are remarkably similar for the three alternative parameterizations of the plug-in deviance. For fixed effects models we would expect from Section 3.2 that $p_D$ should be approximately the true number of independent parameters. For the pooled model 1, $p_D = 1.0$ as expected, whereas, for the saturated model 5, $p_D$ ranges from 52.8 to 55.9 depending on the parameterization that is used, which is close to the true value of 56 parameters. The models containing spatial random effects (either with or without additional exchangeable effects) both have around 31 effective parameters, whereas the model with only exchangeable random effects has about 12 additional effective parameters. On the basis of the results of Section 5.2 comparing $p_D$ for Poisson likelihoods with different priors, this suggests that the spatial model provides stronger prior information than does the exchangeable model for these data.

Turning to the comparison of DIC for each model, we first note that DIC is subject to Monte Carlo sampling error, since it is a function of stochastic quantities generated under an MCMC sampling scheme. Whereas computing the precise standard errors for our DIC values is a subject of on-going research, the standard errors for the $\bar{D}$-values are readily obtained and provide a good indication of the accuracy of DIC and $p_D$. In any case, in several runs using different initial values and random-number seeds for this example, the DIC and $p_D$-estimates obtained never varied by more than 0.5. As such, we are confident that, even allowing for Monte Carlo error, either of models 3 or 4 is superior (in terms of DIC performance) to models 2 or 5, which are in turn superior to model 1. A comparison of DIC for models 3 and 4 suggests that the two spatial models are virtually indistinguishable in terms of the overall fit: pragmatically, we might prefer reporting model 3 since its DIC is only marginally greater than the more complex model 4.

Considering now the absolute measure of fit suggested in Section 6.2, we compare the values of $\bar{D}$ in Table 1 with the sample size $n = 56$. This suggests that all models except the pooled model 1 provide an adequate overall fit to the data, and that the comparison is essentially based on their complexity alone.

Following the discussion in Section 6, Fig. 4 shows a plot of deviance residuals $\text{dr}_i$ against leverages $p_{D_i}$ for each of the five models considered. The broken curves marked on each plot are of the form $x^2 + y = c$ and points lying along such a parabola will each contribute an amount $\text{DIC}_i = c$ to the overall DIC for that model. For models 2–5, parabolas are marked at values of $c$ = 1, 2, 5, and any data point whose contribution $\text{DIC}_i$ is greater than 2 is labelled by its



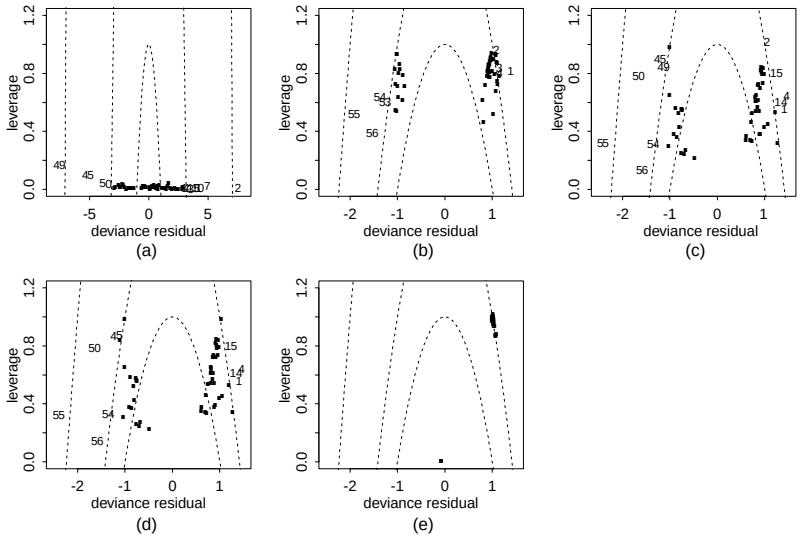


**Fig. 4.** Diagnostics for the lip cancer example—residuals *versus* leverages (the parabolas indicate contributions of 1, 2 or 5 to the total DIC (apart from model 1): (a) model 1; (b) model 2; (c) model 3; (d) model 4; (e) model 5

observation number. For model 1, parabolas are marked at $c$ = 1, 10, 50, since the size of the deviance residuals and individual contributions to DIC are much larger and, for clarity, only points for which $\text{DIC}_i$ is greater than 10 are marked by their observation number. Observations 55 and 56, the only districts with $y_i = 0$, are clearly identified as potential outliers under each of the random-effects models 2–4, as is observation 1 (the district with the highest observed risk ratio $y_i/E_i$). A few other observations (2, 3, 4, 53 and 54) have contributions $\text{DIC}_i$ that are just larger than 2 under model 2: with the exception of the three districts already discussed, these five districts have the most extreme observed risk ratios and so their estimates tend to be shrunk furthest under the exchangeable model. Observations 14, 15, 45 and 50 appear to be outliers in models 3 and 4 which have a spatial effect, but not in the remaining models. A further investigation reveals that the observed risk ratios in these districts are extreme compared with those in each of their neighbouring districts. For example district 50 has only six cases compared with 19.6 expected, whereas each of its three neighbouring districts have high observed counts (17, 16 and 16) relative to those expected (7.8, 10.5 and 14.4). The spatial prior in models 3 and 4 causes the estimated rate in district 50 to be smoothed towards the mean of its neighbours' rates, thus leading to the discrepancy between observed and fitted values, and since the observation still exercises considerable weight on its fitted value the leverage is high as well. However, overall we might not consider that there is sufficient evidence to cast doubt on any particular observations.

### 8.2. *Robust regression using the stack loss data*

Spiegelhalter *et al.* (1996) (pages 27–29) considered a variety of error structures for the oft-analysed stack loss data of Brownlee (1965). Here the response variable $y$, the amount of stack

loss (escaping ammonia in an industrial application), is regresssed on three predictor variables: air flow $x_1$, temperature $x_2$ and acid concentration $x_3$. Assuming the usual linear regression structure

$$\mu_i = \beta_0 + \beta_1 z_{i1} + \beta_2 z_{i2} + \beta_3 z_{i3}$$

where $z_{ij} = (x_{ij} - \bar{x}_{.j})/\mathrm{sd}(x_{.j})$, the standardized covariates, the presence of a few prominent outliers among the $n = 21$ cases motivates a comparison of the following four error distributions: model 1,

$$y_i \sim \text{normal}(\mu_i, \tau^{-1});$$

model 2,

$$y_i \sim \text{DE}(\mu_i, \tau^{-1});$$

model 3,

$$y_i \sim \text{logistic}(\mu_i, \tau^{-1});$$

model 4,

$$y_i \sim t_d(\mu_i, \tau^{-1})$$

(where DE denotes the double-exponential (Laplace) distribution and $t_d$ denotes Student's $t$-distribution with $d$ degrees of freedom).

A well-known alternative to the direct fitting of many symmetric but non-normal error distributions is through scale mixtures of normals (Andrews and Mallows, 1974). From page 210 of Carlin and Louis (2000), we have the alternate $t_d$-formulation model 5,

$$y_i \sim \text{normal}\left(\mu_i, \frac{1}{w_i \tau}\right),$$
$$w_i \sim \frac{1}{d}\chi^2_d = \text{gamma}\left(\frac{d}{2}, \frac{d}{2}\right).$$

Unlike our other examples the form of the likelihood changes with each model, so we must use the full normalizing constants when computing $-2\log\{p(y|\mu, \tau)\}$.

Following Spiegelhalter *et al.* (1996) we set $d = 4$, and for each model we placed essentially flat priors on the $\beta_j$ (actually normal with mean 0 and precision 0.00001) and $\log(\tau)$ (actually gamma(0.001,0.001) on $\tau$) and ran the Gibbs sampler in BUGS for 5000 iterations following a burn-in period of 1000 iterations.

Replacing $\tau$ and $w_i$ by their posterior means where necessary for the $D(\bar{\theta})$-calculation, the resulting deviance summaries are shown in Table 2 (note that the mean parameterization and the canonical parameterization are equivalent here, since the mean $\mu_i$ is a linear function of the canonical $\beta$-parameters). Beginning with a comparison of the first four models, the estimates of $p_D$ are all just over 5, the correct number of parameters for this example. The DIC-values imply that model 2 (double exponential) is best, followed by the $t_4$-, the logistic and finally the normal models. Clearly this order is consistent with the models' respective abilities to accommodate outliers.

Turning to the normal scale mixture representation for the $t_4$-likelihood (model 5), the $p_D$-value is 7.6, suggesting that the $w_i$ random effects contribute only an extra 2–2.5 parameters. However, the model's smaller DIC-value implies that the extra mixing parameters are



**Table 2.** Deviance results for the stack loss data

| *Model* | $\bar{D}$ | $D(\bar{\theta})$ | $p_D$ | *DIC* |
|---|---|---|---|---|
| 1, normal | 110.1 | 105.0 | 5.1 | 115.2 |
| 2, double exponential | 107.9 | 102.3 | 5.6 | 113.5 |
| 3, logistic | 109.5 | 104.2 | 5.3 | 114.8 |
| 4, $t_4$ | 108.7 | 103.2 | 5.5 | 114.2 |
| 5, $t_4$ as scale mixture | 102.1 | 94.5 | 7.6 | 109.7 |

worthwhile in an overall quality-of-fit sense. We emphasize that the results from models 4 and 5 need not be equal since, although they lead to the same marginal likelihood for the $y_i$, they correspond to different prediction problems.

Finally, plots of deviance residuals *versus* leverages (which are not shown) clearly identify the observations determined to be 'outlying' by several previous researchers who analysed this data set.

### 8.3. Longitudinal binary observations: the six-cities study

To illustrate how the mean and canonical parameterizations (introduced in Section 5 and further discussed in Section 9) can sometimes lead to different conclusions, our next example considers a subset of data from the six-cities study, a longitudinal study of the health effects of air pollution: see Fitzmaurice and Laird (1993) for the data and a likelihood-based analysis. The data consist of repeated binary measurements $y_{ij}$ of the wheezing status (1, yes; 0, no) of child $i$ at time $j$, $i = 1, \ldots, I$, $j = 1, \ldots, J$, for each of $I = 537$ children living in Stuebenville, Ohio, at $J = 4$ time points. We are given two predictor variables: $a_{ij}$, the age of child $i$ in years at measurement point $j$ (7, 8, 9 or 10 years), and $s_i$, the smoking status of child $i$'s mother (1, yes; 0, no). Following the Bayesian analysis of Chib and Greenberg (1998), we adopt the conditional response model

$$Y_{ij} \sim \text{Bernoulli}(p_{ij}),$$
$$p_{ij} \equiv \Pr(Y_{ij} = 1) = g^{-1}(\mu_{ij}),$$
$$\mu_{ij} = \beta_0 + \beta_1 z_{ij1} + \beta_2 z_{ij2} + \beta_3 z_{ij3} + b_i,$$

where $z_{ijk} = x_{ijk} - \bar{x}_{..k}$, $k = 1, 2, 3$, and $x_{ij1} = a_{ij}$, $x_{ij2} = s_i$ and $x_{ij3} = a_{ij}s_i$, a smoking–age interaction term. The $b_i$ are individual-specific random effects, initially given an exchangeable $N(0, \lambda^{-1})$ specification, which allow for dependence between the longitudinal responses for child $i$. The model choice issue here is to determine the most appropriate link function $g(\cdot)$ among three candidates, namely the logit, the probit and the complementary log–log-links. More formally, our three models are model 1,

$$g(p_{ij}) = \text{logit}(p_{ij}) = \log\{p_{ij}/(1 - p_{ij})\},$$

model 2,

$$g(p_{ij}) = \text{probit}(p_{ij}) = \Phi^{-1}(p_{ij}),$$

and model 3,

$$g(p_{ij}) = \text{cloglog}(p_{ij}) = \log\{-\log(1 - p_{ij})\}.$$

**Table 3.** Results for both parameterizations of the Bernoulli panel data

| *Model* | $\bar{D}$ | *Results for the canonical parameterization* | | | *Results for the mean parameterization* | | |
|---|---|---|---|---|---|---|---|
| | | $D(\bar{\theta})$ | $p_D$ | *DIC* | $D(\bar{\theta})$ | $p_D$ | *DIC* |
| 1, logit | 1166.4 | 917.7 | 248.7 | 1415.1 | 997.5 | 168.9 | 1335.3 |
| 2, probit | 1148.6 | 885.9 | 262.7 | 1411.3 | 989.9 | 158.7 | 1307.3 |
| 3, complementary log–log | 1180.9 | 956.5 | 224.4 | 1405.3 | 1013.7 | 167.2 | 1348.1 |

Since the Bernoulli likelihood is unaffected by this choice, in all cases the deviance takes the simple form

$$D = -2\sum_{i,j}\{y_{ij}\log(p_{ij}) + (1 - y_{ij})\log(1 - p_{ij})\}.$$

Placing flat priors on the $\beta_k$ and a gamma(0.001,0.001) prior on $\lambda$, and running the Gibbs sampler for 5000 iterations following a burn-in period of 1000 iterations produces the deviance summaries in Table 3 for the canonical and mean parameterizations: the canonical parameterization constructs $\bar{\theta}$ as the mean of the linear predictors $\beta$ and $b_i$, and then uses the appropriate linking transformation (logit, probit or complementary log–log) to obtain the imputed means for the $p_{ij}$. The mean parameterization simply uses the means of the $p_{ij}$ themselves when computing $D(\bar{\theta})$. Natarajan and Kass (2000) have pointed out potential problems with the gamma(0.001,0.001) prior on $\lambda$, but in this context the 537 random effects ensure that these findings are robust to the choice of prior for $\lambda$.

The posterior standard deviation $\sqrt{\lambda^{-1}}$ of the random effects is estimated to be 2.2 (standard deviation 0.2), which indicates extremely high unexplained overdispersion and hence considerable prior–data conflict: this should warn us of a potential lack of robustness in our procedure. We have a sample size of $n_i = 4$ for each of $I = 537$ individuals, and an average $p_{D_i}$ for the canonical parameterization of around 0.4–0.5. From approximation (31), this indicates a prior sample size $a + b$ of around 4–6. Referring to the evidence in Fig. 1 concerning low prior and observation sample sizes ($n_i = 1$; $a + b = 1$), we might expect the mean parameterization to display decreased complexity compared with the canonical, and this is borne out in the results. DIC prefers the complementary log–log-link under the canonical parameterization, but the probit link under the mean parameterization. We repeat that we prefer the canonical results because of the improved normality of the likelihoods and their lack of dependence on observed data: however, none of the models explain the data very well, and the lack of consensus suggests caution in using any of the models.

## 9. Discussion

Here we briefly discuss relationships to other suggestions and give some guidance on the practical use of the techniques described in this paper.

### 9.1. Relationship of $p_D$ and DIC to other suggestions

#### 9.1.1. Cross-validation

Stone (1977) showed the asymptotic equivalence of model comparison based on cross-validation and AIC, whereas Wahba (1990) (page 52) showed how a generalized cross-validation criterion leads to the use of $n - \mathrm{tr}(H)$ as a denominator in the estimation of residual mean-squared error. We would expect our measure of model complexity $p_D$ to be strongly related to cross-validatory assessment, but this requires further investigation.



#### 9.1.2. Other predictive loss functions

Kass and Raftery (1995) criticized Akaike (1973) for using a plug-in predictive distribution as we have done in Section 7.3, rather than the full predictive distribution obtained by integrating out the unknown parameters. A criterion based on this predictive distribution is also invariant to reparameterizations. Laud and Ibrahim (1995) and Gelfand and Ghosh (1998) suggested minimizing a predictive 'discrepancy measure' $E\{d(Y_{\mathrm{new}}, y)|y\}$, where $Y_{\mathrm{new}}$ is a draw from the posterior predictive distribution $p(Y_{\mathrm{new}}|y)$, and we might for instance take $d(Y_{\mathrm{new}}, y) = (Y_{\mathrm{new}} - y)^{\mathrm{T}}(Y_{\mathrm{new}} - y)$. They showed that their measures also have attractive interpretations as weighted sums of 'goodness of fit' and 'predictive variability penalty' terms. However, a proper choice of the criterion requires fairly involved analytic work, as well as several subjective choices about the utility function that is appropriate for the problem at hand. Furthermore, the one-way ANOVA model in Section 2.5 gives rise to a fit term equivalent to $D(\bar{\theta})$, and a predictive variability term equal to $p_D + p$. Thus their suggestion is equivalent in this context to the comparison by our Bayesian measure of fit $\bar{D}$ which, although invariant to parameterization, does not seem to penalize complexity sufficiently.

In general the use of a plug-in estimate appears to 'cost' an extra penalty of $p_D$.

#### 9.1.3. Bayes factors

Bayes factors are criteria based on a comparison of the marginal likelihoods (1) (Kass and Raftery, 1995), and a common approximation is the Bayesian (or Schwarz) information criterion (Schwarz, 1978), which for a model with $p$ parameters and $n$ observations is given by

$$\mathrm{BIC} = -2\log\{p(y|\hat{\theta})\} + p\log(n).$$

Bernardo and Smith (1994) (chapter 6) argued that this formulation may only be appropriate in circumstances where it was really believed that one and only one of the competing models was in fact true, and the crucial issue was to choose this correct model, and that in other circumstances criteria based on short-term prediction, such as cross-validation, may be more appropriate. We support this view and refer to Han and Carlin (2001) for a review of some of the computational and conceptual difficulties in using Bayes factors to compare complex hierarchical models. Whether DIC can be justified as a basis for model averaging remains open for investigation.

### 9.2. Practical issues in using DIC

#### 9.2.1. Invariance

$p_D$ may be only approximately invariant to the chosen parameterization, since different fitted deviances $D(\bar{\theta})$ may arise from substituting posterior means of alternative choices of $\theta$. The example in Section 8.3 shows that this choice could be important with Bernoulli data.

In Section 5 we explored the use of the posterior median as an estimator leading to an invariant $p_D$. This has two possible disadvantages: we do not have a proof that $p_D$ will be positive and some additional computational difficulty in that the full sample needs to be retained. In addition the approximate properties based on Taylor series expansions in Section 3 may not hold, although

this may be only of theoretical interest. Currently we recommend calculation of DIC on the basis of several different estimators, with a preference for posterior means based on parameterizations obeying approximate likelihood normality.

#### 9.2.2. *Focus of analysis*

As we saw in the stack loss example of Section 8.2, there may be sensitivity to apparently innocuous restructuring of the model: this is to be expected since by making such changes we are altering the definition of a replicate data set, and hence one would expect DIC to change. For example, consider a model comprising a mixture of normal distributions. If this assumption was solely to obtain a flexible functional form, then the appropriate likelihood would comprise the mixture. If, however, we were interested in the membership of individual observations, then the likelihoods would be normal and the membership variables would contribute to the complexity of the model. Thus the parameters in the focus of a model should ideally depend on the purpose of the investigation, although in practice it is likely that the focus may be chosen on computational grounds as providing likelihoods that are available in closed form.

#### 9.2.3. *Nuisance parameters*

Strictly speaking, nuisance parameters should first be integrated out to leave a likelihood depending solely on parameters in focus. In practice, however, parameters such as variances are likely to be included in the focus and add to the estimated complexity: we would recommend posterior means of log-variances as estimators.

#### 9.2.4. *What is an important difference in DIC?*

Burnham and Anderson (1998) suggested models receiving AIC within 1–2 of the 'best' deserve consideration, and 3–7 have considerably less support: these rules of thumb appear to work reasonably well for DIC. Certainly we would like to ensure that differences are not due to Monte Carlo error: although this is straightforward for $\bar{D}$, Zhu and Carlin (2000) have explored the difficulty of assessing the Monte Carlo error on DIC.

#### 9.2.5. *Asymptotic consistency*

As with AIC, DIC will not consistently select the true model from a fixed set with increasing sample sizes. We are not greatly concerned about this: we neither believe in a true model nor would expect the list of models being considered to remain static as the sample size increased.

### 9.3. Conclusion

In conclusion, our suggestions have a similar 'information theoretic' background to frequentist measures of model complexity and criteria for model comparison but are based on expectations with respect to parameters in place of sampling expectations. DIC can thus be viewed as a Bayesian analogue of AIC, with a similar justification but wider applicability. It is also applicable to any class of model, involves negligible additional analytic work or Monte Carlo sampling and appears to perform reasonably across a range of examples. We feel that $p_D$ and DIC deserve further investigation as tools for model assessment and comparison.

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## Discussion on the paper by Spiegelhalter, Best, Carlin and van der Linde

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This is a wonderful paper containing a wide array of interesting ideas. It seems to me very much like a first step (and in the right direction) and I am sure that it will be seen as both a focus and a source of inspiration for future developments in this area.

As the authors point out, their $p_D$ and the deviance information criterion (DIC) statistics have already been widely used within the Bayesian literature. Given this history and in the previous absence of a published source for these ideas, it is easy to misunderstand what $p_D$ actually does. Certainly, before reading this paper, but having read several others which use the DIC, I thought that the $p_D$-statistic was a clever way of avoiding the problem that Bayesians have when it comes to calculating the number of parameters in any hierarchical model. Essentially the problem is one of deciding which variables in the posterior are model parameters and which are hyperparameters arising from the prior. However, $p_D$ does not help us here and that is why we have Section 2.1 explaining that this choice is up to the reader. The authors refer to this as choosing the 'focus' for the analysis. Sadly, in many cases the calculation of $p_D$ will be impossible for the focus of primary interest since the deviance will not be available in closed from (this includes random effects and state space models, for example), so this remains an open problem.

What $p_D$ *does* do is to tell you, once you have chosen your focus, how many parameters you lose (or even gain?) by being Bayesian. The number of degrees of freedom (or parameters) in a model is clear from the (focused) likelihood. However, by combining the likelihood with the prior we almost always impose additional restrictions on the parameter space, effectively reducing the degrees of freedom of our model. Take the authors' saturated model of Section 8.1, in which parameters $\alpha_1, \ldots, \alpha_{56}$ are given a prior with some unknown mean $\mu$ and fixed variance $\sigma^2$. Clearly, in the limit as $\sigma^2$ goes to 0, we essentially remove the 56 individual parameters $\alpha_i$ and effectively replace them with a single parameter $\mu$. I guess that this is fairly obvious with hindsight as is the case with many great ideas. None-the-less it is a credit to the authors firstly for seeing it and, more importantly, for actually deriving a procedure for dealing with it.

This prior-induced parameter reduction can be clearly observed in Fig. 5 in which we plot the value of $p_D^\theta$ against $\log(\sigma^2)$ both for a hyperprior $\mu \sim N(0, 1000)$ and for $\mu = 0$ (the authors are unclear about which, if either, they actually use in Section 8.1). We can see that, as $\sigma^2$ decreases, the effective number of parameters decreases to either 1 or 0 depending on whether or not $\mu$ itself is a parameter, i.e. which prior is chosen. It is interesting to note the rapid decline in $p_D$ for variances between 1 and 0.01, but what is particularly interesting about this plot is that, as $\sigma^2$ increases, $p_D$ converges to a fixed maximum well below 56, the number of parameters in the likelihood. As an experiment, if we take $\sigma^2 = 10^{30}$ or even the Jeffreys prior for the $\mu_i$, a value for $p_D$ exceeding 53.1 is never obtained (modulo Monte Carlo error). This suggests that we automatically lose three parameters just by being Bayesian, even if we are as vague as we could possibly be with our prior. Quoting Bernardo and Smith (1994), page 298, 'every prior specification has *some* informative posterior or predictive implications .... There is no "objective" prior that represents ignorance.' Of course, the authors' Table 1 suggests that if we took the median as the basis for the calculation of $p_D$ then we might obtain different results; indeed we seem to regain several parameters this way! Unfortunately, analytic investigation of the $p_D$-statistic is essentially limited to the case where we take $\tilde{\theta}(y)$ to be the posterior mean, so we have little idea of the extent and nature of the variability across parameterizations. This choice is likely to have a significant effect on any inference based on the corresponding $p_D$-statistic and further (no doubt simulation-based) investigation along these lines would certainly be very helpful.

As well as the construction of the $p_D$-statistic, the paper also derives a new criterion for model comparison labelled the DIC. The authors provide a heuristic justification for the DIC, but there are clearly several alternatives. One obvious extension of the usual Akaike information criterion (AIC) statistic to

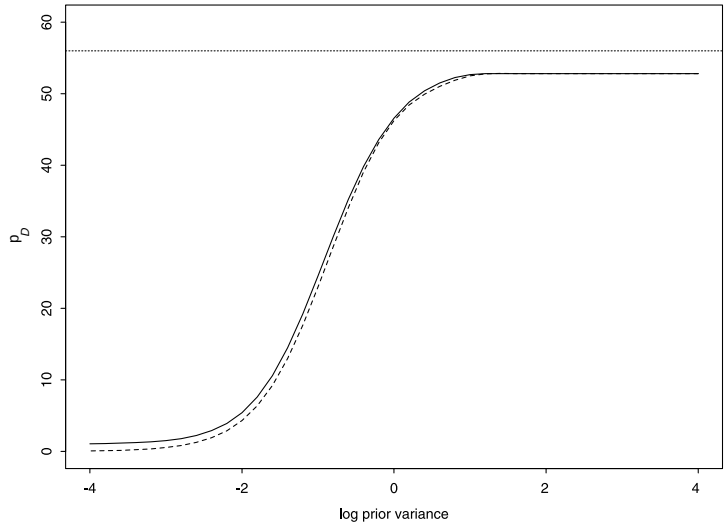


**Fig. 5.** Plot of $p_D^\theta$ for the saturated model of Section 8.1 demonstrating its dependence on the prior variance for the random effects: ———, $p_D$-statistic with an $N(0, 1000)$ hyperprior for $\mu$: - - - - -, corresponding value when we fix $\mu = 0$; · · · · · · · , number of parameters in the likelihood

the Bayesian context is to calculate its posterior expectation, $\text{EAIC} = \overline{D(\theta)} + 2p$ (rather than evaluating it at the posterior mode under a flat prior), or to take the deviance calculated at the posterior mean, i.e. taking $D(\bar{\theta}) + 2p$. Of course, as with the DIC, posterior medians, modes etc. could also be taken and similar extensions could be applied to the corrected AIC statistic and the Bayesian information criterion for example. Further, the number of parameters in each of these expressions might be replaced by $p_D$ to gain even more potential criteria. Table 4 gives the posterior model probabilities and posterior-averaged information criteria (based on $p$, rather than $p_D$), including DIC, for autoregressive models of various orders fitted to the well-known lynx data (Priestley (1981), section 5.5). We note the broad agreement between the DIC, EAIC and $\text{EAIC}_\text{c}$ (as is common in my own experience and, I think, expected by the authors), but that EBIC locates an entirely different model. We note also that the posterior model probabilities correctly identify the fact that two models appear to describe the data well and it is the only criterion to identify correctly the existence of two distinct modes in the posterior.

Given the number of approximations and assumptions that are required to obtain the DIC it can only really be used as a broad brush technique for discriminating between obviously disparate models, in much the same way as any of the alternative information criteria suggested above might be used. However, in many realistic applications there may be two or more models with sufficiently similar DIC that it is impossible to choose between the two. The only sensible choice in this circumstance is to model-average (see Section 9.1.3). Burnham and Anderson (1998), section 4.2, suggested the use of AIC weights and these are also given in Table 4 together with the corresponding weights for the other criteria. Essentially, these are obtained by subtracting from each AIC the value associated with the 'best' model and then setting

$$w_k \propto \exp\{-\Delta\text{AIC}(k)/2\}$$

where $\Delta\text{AIC}(k)$ denotes the transformed AIC-value for model $k$. These weights are then normalized to sum to 1 over the models under consideration.

Note the distinct differences between the weights and the posterior model probabilities given in Table 4, suggesting that only one or the other can really make any sense. We note here that similar comparisons have been made in the context of other examples. In the context of a log-linear contingency



**Table 4.** Effective number of parameters, values of DIC and the posterior expectation of various information criteria for fitting an autoregressive model of order $k$ (with $k + 1$ parameters including the error variance) to the lynx data†

| $k$ | $p_D$ | $DIC$ | $EAIC$ | $EBIC$ | $EAIC_\text{c}$ | $\pi(K = k)$ | $w_k^{\text{DIC}}$ | $w_k^{\text{EAIC}}$ | $w_k^{\text{EBIC}}$ | $w^{\text{EAIC}_\text{c}}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1.88 | 206.66 | 206.78 | 209.51 | 206.81 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| 2 | 2.85 | 126.58 | 127.72 | **133.19** | 127.83 | **0.243** | 0.000 | 0.003 | **0.858** | 0.011 |
| 3 | 3.78 | 127.06 | 129.27 | *137.48* | 129.50 | 0.016 | 0.000 | 0.001 | **0.101** | 0.005 |
| 4 | 4.76 | 125.52 | 128.75 | 139.70 | 129.12 | 0.007 | 0.000 | 0.002 | 0.033 | 0.006 |
| 5 | 5.70 | 125.23 | 129.52 | 143.20 | 130.08 | 0.002 | 0.000 | 0.001 | 0.006 | 0.004 |
| 6 | 6.62 | 126.30 | 131.68 | 148.09 | 132.46 | 0.001 | 0.000 | 0.004 | 0.000 | 0.001 |
| 7 | 7.60 | 122.34 | 128.72 | 147.88 | 129.78 | 0.002 | 0.000 | 0.002 | 0.001 | 0.004 |
| 8 | 8.61 | 121.81 | 129.19 | 151.08 | 130.56 | 0.002 | 0.000 | 0.001 | 0.000 | 0.003 |
| 9 | 9.58 | 122.75 | 131.16 | 155.79 | 132.89 | 0.001 | 0.000 | 0.001 | 0.000 | 0.001 |
| 10 | 10.54 | 118.94 | 128.40 | 155.76 | 130.53 | 0.002 | 0.001 | 0.002 | 0.000 | 0.003 |
| 11 | 11.33 | **106.51** | **117.16** | 147.26 | **119.75** | 0.154 | **0.431** | **0.566** | 0.001 | **0.624** |
| 12 | 12.61 | *106.89* | *118.27* | 151.10 | *121.36* | **0.268** | **0.356** | **0.325** | 0.000 | **0.280** |
| 13 | 13.56 | *108.74* | *121.17* | 156.74 | *124.81* | 0.135 | 0.142 | 0.076 | 0.000 | 0.050 |
| 14 | 14.46 | 110.77 | 124.30 | 162.61 | 128.54 | 0.067 | 0.051 | 0.016 | 0.000 | 0.008 |
| 15 | 15.37 | 112.896 | 127.42 | 168.47 | 132.32 | 0.000 | 0.019 | 0.003 | 0.000 | 0.001 |

†Criterion entries in bold indicate the model minimizing the relevant criterion, whereas those in italics denote alternative plausible models under the rules of thumb discussed in Section 9.2.4. Probabilities $\pi$ or weights $w$ in bold denote the top two models in each case. Here, $\text{EAIC}_\text{c}$ denotes the posterior mean of the corrected EAIC (Burnham and Anderson, 1998), $\pi(K = k)$ the corresponding posterior model probability under a flat prior across models and the $w_k^X$ the corresponding Akaike weights (or equivalent). The posterior model probabilities were kindly provided by Ricardo Ehlers.

table analysis, King (2001), Table 2.5, found that two models have posterior probability 0.557 and 0.057 but corresponding DIC weights of 0.062 and 0.682 respectively. Similar examples in which the DIC and posterior model probabilities give wildly different results are provided by King and Brooks (2001). Do the authors have any feel for why these two approaches might give such different results? Which would they recommend be used and do they have any suggestions for alternative DIC-based weights for model averaging which might lead to more sensible results? Surely, the only sensible approach is to calculate posterior model probabilities via transdimensional Markov chain Monte Carlo methods. When, then, do the authors suggest that the DIC might be used? What, in practical terms is the question that the DIC is answering as opposed to the posterior model probabilities?

The incorporation of the DIC-statistic into WinBUGS 1.4 ensures its ultimate success, but I have grave misgivings concerning the blind application of a 'default' DIC-statistic for model determination problems particularly given its heuristic derivation and the series of essentially arbitrary assumptions and approximations on which it is based. The authors 'recommend calculation of DIC on the basis of several different estimators'. The option to choose different parameterizations is not available in the beta version of WinBUGS 1.4; will it be added to later versions? What about options for the all-important choice of focus? What do the authors suggest we do when the same parameterization is not calculable for all models being compared? Could not the choice of parameterization for each model adversely influence the results, particularly for models with large numbers of parameters (where a small percentage change in $p_D$ might mean a large absolute change in the corresponding DIC)?

The paper, like any good discussion paper, leaves various other open questions. For example: why take $\mathbb{E}_{\theta|y}[d_\Theta]$ in equation (9) and not the mode or median; how should we decide when to take $\hat{\theta}$ to be the mean, median, mode etc. as this will surely lead to different comparative results for the DIC; when is $p_D$ negative and why; in an entirely practical sense, how does model comparison with the DIC compare with that via posterior model probabilities and why do they differ—can both be 'correct' in any meaningful way? On page 613, the authors write '$p_D$ and DIC deserve *further investigation* as tools for model assessment and comparison' and I would certainly agree that they do. I have very much enjoyed thinking about some of these ideas over the past few weeks and I am very grateful to the authors for the opportunity and motivation to do so. It therefore gives me great pleasure to propose the vote of thanks.

**Jim Smith** (*University of Warwick, Coventry*)

I shall not address technical inaccuracies but just present four foundational problems that I have with the model selection in this paper.

(a) Bayesian models are designed to make plausible predictive statements about future observables. The predictive implications of all the prior settings on variances in the worked examples in Section 8 are unbelievable. They do not represent carefully elicited expert judgments but the views of a vacuous software user. Early in Section 1 the authors state that they want to identify succinct models 'which appear to describe the information [about wrong "true" parameter values (see Section 2.2)?] in the *data* accurately'. But in a Bayesian analysis a separation between information in the data and in the prior is artificial and inappropriate. For example where do I input extraneous data used as the basis of my prior? When do I stop calling this data (and so include it in $D(\cdot)$) and instead call it prior information? This forces the authors to use default priors.

A Bayesian analysis on behalf of a remote auditing expert (Smith, 1996) might require the selection of a prior that is robust within a *class* of belief of different experts (e.g. Pericchi and Walley (1991)). Default priors can sometimes be justified for simple models. Even then, models within a selection class need to have compatible parameterizations: see Moreno *et al.* (1998). However, in examples where 'the number of parameters outnumbers observations'—they claim their approach addresses—default priors are unlikely to exhibit any robustness. In particular, outside the domain of vague location estimation or separating variance estimation (discussed in Section 4), apparently default priors can have strong influence on model implications and hence selection.

(b) Suppose that we need to select models whose predictive implications we do not believe. Surely we should try to ensure that prior information in each model corresponds to predictive statements that are comparable. Such issues, not addressed here, are considered by Madigan and Raftery (1991) for simple discrete Bayesian models. But outside linear models with known variances this is a difficult problem. Furthermore it is well known that calibration is a fast function (Cooke, 1991). In particular apparently inconsequential deviations from the features of a model 'not in focus' tend to dominate $D(\theta)$ and $\overline{D(\theta)}$. A trivial example of this occurs when we plan to forecast $X_2$ having observed an independent identically distributed $X_1 = 0.01$ which under models M1 and M2 have respective Gaussian distributions $N(100, 10000)$ and $N(0, 0.001)$. Then, for most priors, model M1 is strongly preferred although its predictions about $X_2$ are less 'useful' (Section 2.2). The authors' premise that all the models they entertain are 'wrong' allows these calibration issues to bite theoretically even in the limit, unlike their asymptotically consistent rivals. The authors, however, do no more than to acknowledge the existence of this core difficulty after the example in Section 8.3.

(c) Suppose that problems (a) and (b) do not bite. Then the 'vector of parameters of focus' (POF) will have a critical influence on any ensuing inference. How in practice do we specify this? The authors state without elaboration that this 'should depend on the purpose of the investigation' (Section 9.2.2). But it appears that in practice the POF is calculated on 'computational grounds', their software capability driving their inference.

The high influence of the choice of the POF is illustrated in the example in Section 8.2. Here models 4 and 5 are predictively identical but model 5 has a significantly smaller deviance information criterion DIC than model 4. The authors conclude that 'the extra mixing parameters are worthwhile': why? In what practical sense is this helpful? This example illustrates that the unguided choice of the POF will often be inferentially critical. Incidentally in this example the order of DIC is not (as stated) consistent with the thickness of tails of the sample distribution, the thickest-tailed distribution being model 4.

(d) But ignoring all these difficulties there still remains the acknowledged choice of (re)parameterization governing the choice of $\bar{\theta}$ which initially we shall assume to be the mean. Consider the case when the POF $\theta$ is one dimensional with strictly increasing posterior distribution function $F(\theta|y)$, and $G_\mu$ is a distribution function of a random variable with mean $\mu$. Then the reparameterization of $\theta$ to $\phi_\mu = G_\mu^{-1}\{F(\theta|y)\}$ has $E(\phi_\mu) = \mu$. Thus $D(\bar{\theta})$ (or $D(\bar{\phi})$) is arbitrary within the range of $D(\cdot)$. Thus, contrary to Section (5.1.4), the choice of parameterization of $\theta$ with non-degenerate posterior will always be critical. But no *general* selection guidance is given here. In observation (c) of Section 2.6 the authors suggest the use of the posterior median instead of the mean if this can be calculated easily from their output: not a solution when the POF is more than one dimensional. Even familiar transforms of marginal medians to contrasts and means or means and variances to means and coefficients of variation will not exhibit the required sorts of invariance.



There may be theoretical reasons to use DIC but I do not believe that this paper gives them. So my suggestion to a practitioner would be: if you must use a formal selection criterion do not use DIC. I second the vote of thanks.

The vote of thanks was passed by acclamation.

**Aki Vehtari** (*Helsinki University of Technology*)

The authors mention that the deviance information criterion DIC estimates the expected loss, with deviance as the loss function. This connection should be emphasized more. It should be remembered that the estimation of the expected deviance was Akaike's motivation for deriving the very first information criterion AIC (Akaike, 1973). In prediction and decision problems, it is natural to assess the predictive ability of the model by estimating the expected utilities, as the principle of rational decisions is based on maximizing the expected utility (Good, 1952) and the maximization of expected likelihood maximizes the information gained (Bernardo, 1979). It is often useful to use other than likelihood-based utilities. For example, in classification problems it is much more meaningful for the application expert to know the expected classification accuracy than just the expected deviance value (Vehtari, 2001). Given an arbitrary utility function $u$, it is possible to use Monte Carlo samples to estimate $E_\theta[\bar{u}(\theta)]$ and $\bar{u}(E_\theta[\theta])$, and then to compute an expected utility estimate as

$$\bar{u}_{\mathrm{DIC}} = \bar{u}(E_\theta[\theta]) + 2\{E_\theta[\bar{u}(\theta)] - \bar{u}(E_\theta[\theta])\},$$

which is a generalization of DIC (Vehtari, 2001).

The authors also mention the known asymptotic relationship of AIC to cross-validation (CV). Equally important is to note that the same asymptotic relationship holds also for NIC (Stone (1977), equation (4.5)). The asymptotic relationship is not surprising, as it is known that CV can also be used to estimate expected utilities with Bayesian justification (Bernardo and Smith (1994), chapter 6, Vehtari (2001) and Vehtari and Lampinen (2002a)). Below some main differences between CV and DIC are listed. See Vehtari (2001) and Vehtari and Lampinen (2002b) for full discussion and empirical comparisons. CV can use full predictive distributions. In the CV approach, there are no parameterization problems, as it deals directly with predictive distributions. CV estimates the expected utility directly, but it can also be used to estimate the effective number of parameters if desired. In the CV approach, it is easy to estimate the distributions of the expected utility estimates, which can for example be used to determine automatically whether the difference between two models is 'important'. Importance sampling leave-one-out CV (Gelfand *et al.*, 1992; Gelfand, 1996) is computationally as light as DIC, but it seems to be numerically more unstable. $k$-fold CV is very stable and reliable, but it requires $k$ times more computation time to use. $k$-fold CV can also handle finite range dependences in the data. For example, in the six-cities study, the wheezing statuses of a single child at different ages are not independent. DIC, which assumes independence, underestimates the expected deviance. In $k$-fold CV it is possible to group the dependent data and to handle independent groups and thus to obtain better estimates (Vehtari, 2001; Vehtari and Lampinen, 2002b).

**Martyn Plummer** (*International Agency for Research on Cancer, Lyon*)

I congratulate the authors on their thought-provoking paper. I would like to offer one constructive suggestion and one criticism.

Firstly, I have a proposal for a modified definition of the effective number of parameters $p_D$. Starting from the Kullback–Leibler information divergence between the predictive distributions at two different values of $\theta$

$$I(\theta^0, \theta^1) = E_{Y_{\mathrm{rep}}|\theta^0}\left[\log\left\{\frac{p(Y_{\mathrm{rep}}|\theta^0)}{p(Y_{\mathrm{rep}}|\theta^1)}\right\}\right],$$

I suggest that $p_D$ be defined as the expected value of $I(\theta^0, \theta^1)$ when $\theta^0$ and $\theta^1$ are independent samples from the posterior distribution of $\theta$. This modified definition yields exactly the same expression for $p_D$ in the normal linear model with known variance. In general, it should give a similar estimate of $p_D$ when $\theta$ has an asymptotic normal distribution. This version of $p_D$ can also be decomposed into influence diagnostics when the likelihood factorizes as in Section 6.3. It has the theoretical advantages of being non-negative and co-ordinate free. A practical advantage is that $p_D$ can be estimated via Markov chain Monte Carlo sampling using two parallel chains by taking the sample average of

$$\log\left\{\frac{p(Y^0_{\mathrm{rep}}|\theta^0)}{p(Y^0_{\mathrm{rep}}|\theta^1)}\right\}$$

where the superscript denotes the chain to which each quantity belongs. The Monte Carlo error of this estimate is easily calculated and the difficulties discussed by Zhu and Carlin (2000) can thus be avoided.

For exponential family models, $I(\theta^0, \theta^1)$ can be expressed in closed form and there is no need to simulate replicate observations $Y_{\text{rep}}$. When the scale parameter $\phi$ is known, the expression for $p_{D_i}$ simplifies to

$$p_{D_i} = n_i w_i \operatorname{cov}\{\theta_i, \mu(\theta_i)|Y\} / \phi.$$

This gives a surprising resolution to the problem of whether to use the canonical or mean parameterization to estimate $p_D$.

On a more negative note, I am not convinced by the heuristic derivation of the deviance information criterion DIC in Section 7.3. I followed this derivation for the linear model of Section 4.1, for which it is not necessary to make any approximations. The term with expectation 0, neglected in the final expression, is $p - p_D - D(\tilde{\theta})$. Adding this to DIC gives an expected loss of $p + p_D$ which is not useful as a model choice criterion. I am not suggesting that the use of DIC is wrong, but a formal derivation is lacking.

**Mervyn Stone** (*University College London*)

The paper is rather economical with the 'truth'. The *truth* of $p^{\text{t}}(Y)$ corresponds fixedly to the *conditions* of the experimental or observational set-up that ensures independent future replication $Y_{\text{rep}}$ or internal independence of $y = \mathbf{y} = (y_1, \ldots, y_n)$ (not excluding an implicit concomitant $x$). For $p^{\text{t}}(Y) \approx p(Y|\theta^{\text{t}})$, $\theta$ must parameterize a scientifically plausible family of alternative distributions of $Y$ under those conditions and is therefore a *necessary* 'focus' if the 'good [true] model' idea is to be invoked: think of tossing a bent coin. Changing focus is not an option.

Any connection of $p_D$ with cross-validatory assessment would need truth as $p^{\text{t}}(\mathbf{y}) = p^{\text{t}}(y_1) \ldots p^{\text{t}}(y_n)$. If $l = \log(p)$ is an acceptable measure of predictive success, $A = \Sigma_i l(y_i|\tilde{\theta}_{-i})$ is a one-out estimate of $E_{p^{\text{t}}(\mathbf{y})}[\Sigma_i l\{Y_i|\hat{\theta}(\mathbf{y})\}]$. Multiplied by $-2$, this connects with equation (33) only when the $\theta$-model is true with $Y_1, \ldots, Y_n$ independent.

Extending Stone (1977) to the posterior mode for prior $p(\theta)$, with $n$ large, $A \approx L_{\tilde{\theta}}(\mathbf{y}) - \Pi(\mathbf{y})$ where

$$\Pi(\mathbf{y}) = -\operatorname{tr}\{L''_{\tilde{\theta}} + l''(\tilde{\theta})\}^{-1} \sum_i l'_{\tilde{\theta}}(y_i) l'_{\tilde{\theta}}(y_i)^{\mathrm{T}}$$

and $l(\theta) = \log\{p(\theta)\}$. If $l''(\tilde{\theta})$ is negative definite, the typically non-negative penalty $\Pi(\mathbf{y})$ is smaller for the posterior mode than for the maximum likelihood estimate. For the maximum likelihood estimate, $l''(\tilde{\theta}) = \mathbf{O}$ gives $\Pi(\mathbf{y})$ estimating $p^*$, but the general form probably gives Ripley's $p^*$.

If Section 7.3 could be rigorously developed (the use of $E_{\mathbf{Y}}$ does look suspicious!), another connection (via equation (33)) might be that DIC $\approx -2A$. But, since Section 7.3 invokes the 'good model' assumption and small $|\tilde{\theta} - \theta|$ for the Taylor series expansion (i.e. large $n$), such a connection would be as contrived as that of $A$ with the Akaike information criterion: why not stick with the pristine (nowadays calculable) form of $A$—which does not need large $n$ or truth, and which accommodates estimation of $\theta$ at the independence level of a hierarchical Bayesian model? If sensitivity of the logarithm to negligible probabilities is objectionable, Bayesians should be happy to substitute a subjectively preferable measure of predictive success.

**Christian P. Robert** (*Université Paris Dauphine*) **and D. M. Titterington** (*University of Glasgow*)

A question that arises regarding this thought challenging paper was actually raised in the discussion of Aitkin (1991), namely that the data seem to be used *twice* in the construction of $p_D$. Indeed, $y$ is used the first time to produce the posterior distribution $\pi(\theta|y)$ and the associated estimate $\tilde{\theta}(y)$. The (Bayesian) deviance criterion then computes the posterior expectation of the *observed* likelihood $p(y|\theta)$,

$$\int \log\{p(y|\theta)\}\, \pi(\mathrm{d}\theta|y) \propto \int \log\{p(y|\theta)\}\, p(y|\theta)\, \pi(\mathrm{d}\theta),$$

and thus uses $y$ again, similarly to Aitkin's posterior Bayes factor

$$\int p(y|\theta)\, \pi(\mathrm{d}\theta|y).$$

This repeated use of $y$ would appear to be a potential factor for overfitting.

It thus seems more pertinent (within the Bayesian paradigm) to follow an integrated approach along the lines of the posterior *expected* deviance of Section 6.2,



$$\int E_{Y|\theta}[-2\log\{p(Y|\theta)\} + 2\log\{f(Y)\}]\pi(\mathrm{d}\theta|y)$$

because this quantity would be strongly related to the posterior *expected* loss defined by the logarithmic deviance,

$$d(\theta, \tilde{\theta}) = E_{Y|\theta}[\log\{p(Y|\theta)\} - \log\{p(Y|\tilde{\theta})\}],$$

advocated in Robert (1996) and Dupuis and Robert (2002) as an intrinsic loss adequate for model fitting. In fact, the connection between $p_D$, the deviance information criterion and the logarithmic deviance would suggest the use of this loss $d(\theta, \tilde{\theta})$ to compute the estimate plugged in $p_D$ as the intrinsic Bayes estimator

$$\begin{aligned}\theta^{\pi}(y) &= \arg\min_{\tilde{\theta}}\{E_{\theta|y}(E_{Y|\theta}[\log\{p(Y|\theta)\} - \log\{p(Y|\tilde{\theta})\}])\} \\ &= \arg\max[E_{Y|y}\{p(Y|\tilde{\theta})\}]\end{aligned}$$

where the last expectation is computed under the predictive distribution. Not only does this make sense because of the aforementioned connection, but it also provides an estimator that is completely invariant to reparameterization and thus avoids the possibly difficult choice of the parameterization of the problem. (See Celeux *et al.* (2000) for an illustration in the set-up of mixtures.)

**J. A. Nelder** (*Imperial College of Science, Technology and Medicine, London*)

My colleague Professor Lee has made some general points connecting the subject of this paper to our work on likelihood-based hierarchical generalized linear models. I want to make one specific point and two general ones.

(a) Professor Dodge has shown that, of the 21 observations in the stack loss data set, only five have not been declared to be outliers by someone! Yet there is a simple model in which no observation appears as an outlier. It is a generalized linear model with gamma distribution, log-link and linear predictor $x_2 + \log(x_1) * \log(x_3)$. This gives the following entries for Table 2 in the paper

98.3 92.1 6.2 104.5

(I am indebted to Dr Best for calculating these). It is clearly better than the existing models used in Table 2.

(b) This example illustrates my first general point. I believe that the time has passed when it was enough to assume an identity link for models while allowing the distribution only to change. We should take as our base-line set of models at least the generalized linear model class defined by distribution, link and linear predictor, with choice of scales for the covariates in the last named.

(c) My second general point is that there is, for me, not nearly enough model checking in the paper (I am assuming that the use of such techniques is not against the Bayesian rules). For example, if a set of random effects is sufficiently large in number and the model postulates that they are normally distributed, their estimates should be graphed to see whether they look like a sample from such a distribution. If they look, for example, strongly bimodal, then the model must be revised.

**Anthony Atkinson** (*London School of Economics and Political Science*)

This is an interesting paper which tackles important problems. In my comments I concentrate on regression models: the points extend to the more complicated models at the centre of the authors' presentation.

It is stressed in Section 7.1 that information criteria assume a replication of the observations; in regression this would be with the same $X$-matrix. But, the simulations of Atkinson (1980) showed that, to predict over a different region, higher values of the penalty coefficient than two in equation (36) are needed. Do the authors know of any analytical results in this area?

Information criteria for model selection are based on aggregate statistics. Fig. 4 shows an alternative and more informative breakdown of one criterion into the contributions of individual observations than that given by Weisberg (1981). However, it does not show the effect of the deletion of observations on model choice. Atkinson and Riani (2000) used the forward search to analyse the stack loss data, for which symmetrical error distributions were considered in Section 8.2. Their Fig. 4.28 shows that the square-root transformation is the only one supported by all the data. The forward plot of residuals, Fig. 3.27, is stable, with observations 4 and 21 outlying. This diagnostic technique complements the choice of a model using information criteria calculated over a set of models that is too narrow.

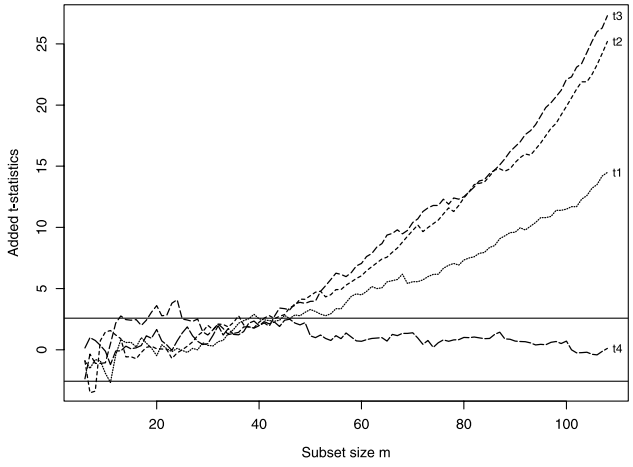


**Fig. 6.** Transformed surgical unit data: forward plot of the four added variable $t$-statistics: three variables are needed in the model—$x_4$ is not significant

An example of model choice potentially confounded by the presence of several outliers is provided by 108 observations on the survival of patients following liver surgery from Neter *et al.* (1996), pages 334 and 438. There are four explanatory variables. Fig. 6 shows the evolution of the added variable $t$-tests for the variables during the forward search with log(survival time) as the response: the evidence for the importance of all variables except $x_4$ increases steadily during the search. Atkinson and Riani (2002) modify the data to produce two different effects. The forward plots of the $t$-tests in Fig. 7(a) show that now $x_1$

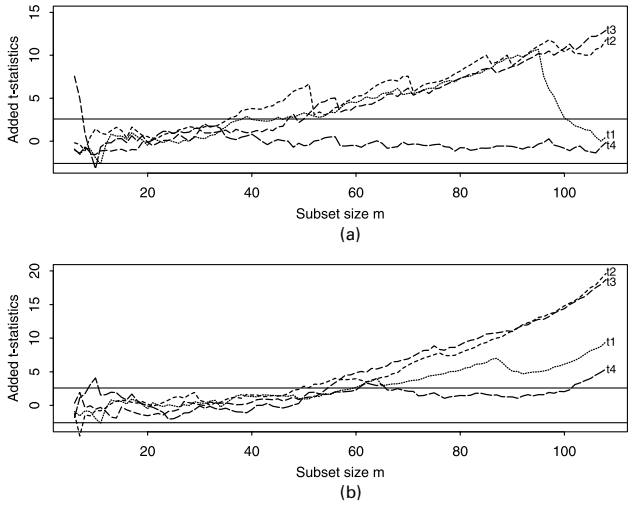


**Fig. 7.** Modified transformed surgical unit data: (a) outliers render $x_1$ non-significant; (b) now the outliers make $x_4$ significant (both (a) and (b) show forward plots of added variable $t$-statistics)



is non-significant at the end of the search. The plot identifies the group of modified observations which have this effect on the $t$-test for $x_1$. Fig. 7(b) shows the effect of a different contamination, which makes $x_4$ significant at the end of the search.

The use of information criteria in the selection of models is a first step, which needs to be complemented by diagnostic tests and plots. These examples show that the forward search is an extremely powerful tool for this purpose. It also requires many fits of the model to subsets of the data. Can it be combined with the appreciable computations of the authors' Markov chain Monte Carlo methods?

**A. P. Dawid** (*University College London*)

This paper should have been titled 'Measures of Bayesian model complexity and fit', for it is the models, not the measures, that are Bayesian. Once the ingredients of a problem have been specified, any relevant question has a unique Bayesian answer. Bayesian methodology should focus on specification issues or on ways of calculating or approximating the answer. Nothing else is required.

Classical criteria overfit complex models, necessitating some form of penalization, and this paper lies firmly in that tradition. But with Bayesian techniques (Kass and Raftery, 1995) overfitting is not a problem: the marginal likelihood automatically penalizes model complexity without any need for further adjustment. In particular, Bayesian model choice is consistent in the 'good model' case (Dawid, 1992a). In Section 9.2.5 the authors brush aside the failure of their deviance information criterion procedure to share this consistency property; but should we not seek reassurance that a procedure performs well in those simple cases for which its performance can be readily assessed, before trusting it on more complex problems?

I contest the view (Section 9.1.3) that likelihood is relevant only under the good model assumption: from a decision theoretic perspective, we can always regard the 'log-loss' scoring rule $S(p, y) := -\log\{p(y)\}$ as a measure of the inadequacy of an assessed density $p(\cdot)$ in the light of empirical data $y$ (Dawid, 1986). Moreover, when $y$ is a sequence $y^n = (y_1, \ldots, y_n)$ of not necessarily independent or identically distributed variables, we have

$$-\log\{p(y^n)\} = \sum_{i=1}^{n} -\log\{p(y_i|y^{i-1})\}, \tag{41}$$

the $i$th term measuring the performance of the Bayesian probability forecast for $y_i$ on the basis of analysis of earlier data only (Cowell *et al.* (1999), chapters 10 and 11). This representation clearly demonstrates why unadjusted marginal likelihood offers a valid measure of model fit: each 'test' observation $y_i$ is always entirely disjoint from the associated 'training' data $y^{i-1}$. If desired, we can generalize this prequential formulation of marginal likelihood by inserting other loss functions (Dawid, 1992b) or using other model fitting methods (Skouras and Dawid, 1999). Such procedures exhibit a natural consistency property even under model misspecification (Dawid, 1991; Skouras and Dawid, 2000).

One place where a Bayesian might want a measure of model complexity is as a substitute for $p$ in the Bayes information criterion approximation to marginal likelihood, e.g. for hierarchical models. But in such cases the definition of the sample size $n$ can be just as problematic as that of the model dimension $p$. What we need is a better substitute for the whole term $p \log(n)$.

**Andrew Lawson and Allan Clark** (*University of Aberdeen*)

We would like to make several comments on this excellent paper.

Our prime concern here is the fact that the deviance information criterion DIC is not designed to provide a sensible measure of model complexity when the parameters in the model take the form of locations in some $\mathcal{R}$-dimensional space. In the spatial context, this could mean the locations of cluster centres or, more generally, the components of a mixture. Clearly the averaging of parameters in these contexts is nonsensical but is a fundamental ingredient of DIC's penalty term $D(\bar{\theta})$. Even if an alternative measure of central tendency is used it remains inappropriate to average over configurations where locations in the chosen space are parameters (e.g. cluster detection modelling in spatial epidemiology (McKeague and Loiseaux, 2002; Gangnon and Clayton, 2002). In the case of the Bayes information criterion, however, it might be possible to replace the penalty $p \ln(n)$ by an average number of parameters (in a reversible jump context) such as $\bar{p} \ln(n)$, where $p$ is the number of parameters and $n$ the sample size. This would at least approximately accommodate the varying dimension but would not require the averaging of parameters (as compared with DIC). This was suggested in Lawson (2000).

The second point of concern is the relationship of the goodness of fit to convergence of the Markov chain Monte Carlo samplers for which DIC is designed. If posterior marginal distributions are multimodal then

the conventional convergence diagnostic will fail (as they will usually find too much variability in individual chains), and also DIC will average over the modes.

We are also somewhat concerned and puzzled by the results for the Scottish lip cancer data set. In Table 1, excepting the saturated model, the largest penalty terms are for the exchangeable model and not those with either spatial or spatial and exchangeable components. We also note that it is not strictly appropriate to fit a spatial-only model without the exchangeable component.

Finally we note that alternative approaches have recently been proposed (Plummer, 2002).

**José M. Bernardo** (*Universitat de València*)

This interesting paper discusses rather polemic issues and offers some reasonable suggestions. I shall limit my comments to some points which could benefit from further analysis.

(a) The authors point out that their proposal is not invariant under reparameterization and show that differences may be large. The use of the median would make the result invariant in one dimension, but it is not trivial to extend this to many dimensions. An attractive, general invariant estimator is the *intrinsic* estimator obtained by minimizing the *reference* posterior expectation of the intrinsic loss $\delta(\hat{\theta}, \theta)$ (Bernardo and Suarez, 2002) defined as the *minimum* logarithmic divergence between $p(x|\hat{\theta})$ and $p(x|\theta)$. Under regularity conditions and moderate or large samples, this is well approximated by $(E[\theta|\mathbf{x}] + M[\theta|\mathbf{x}])/2$, the average between the reference posterior mean and mode. Other invariant estimators may be obtained by minimizing the posterior expectation of $\delta(\hat{\theta}, \theta)$ obtained from either a proper subjective prior or an improper prior which, as the reference prior, is obtained from an algorithm which is invariant under reparameterization.

(b) The authors use 'essentially flat' or 'weakly informative' priors, i.e. conjugate-like priors with very small parameter values. This is dangerous and is *not* recommended. There is no reason to believe that those priors are weakly informative on the parameters of interest. Indeed, these limiting proper priors can have hidden undesirable features such as strong biases (cf. the Stein paradox). Moreover, they may approximate a prior function which would result in an improper posterior and using a 'vague' proper prior in that case does not solve the problem; the answer will then typically be extremely sensitive to the hyperparameters chosen for the vague proper prior and, since the Markov chain Monte Carlo algorithm will converge because the posteriors are guaranteed to be proper, one might not notice anything wrong. If full, credible, subjective elicitation is not possible then one should use formal methods to derive an appropriate reference prior.

(c) The authors' brief comment (in Section 9.2.4) on the calibration of the deviance information criterion DIC is too short to offer guidance. With Bayes factors, we have a direct interpretation of the numbers obtained. The Bayesian reference criterion (Bernardo, 1999) is defined in terms of natural information units (and may also be described in terms of log-odds). Is there a natural interpretation for DIC?

(d) The important particular case of nested models is not discussed in the paper. Would the authors comment on the behaviour on DIC in that case (and hence on their implication on precise hypothesis testing)? For instance, what is DIC's recommendation for the simple canonical problem of testing a value for a normal mean? It seems to me that, like Akaike's information criterion or the Bayesian reference criterion (but not the Bayes information criterion or Bayes factors), DIC would avoid Lindley's paradox. Is this so?

**Sujit K. Sahu** (*University of Southampton*)

This impressive paper shows how the very complicated business of model complexity can be assessed easily by using Markov chain Monte Carlo methods. My comments mostly concern the foundational aspects of the methods proposed and the interrelationship of the deviance information criterion DIC and other Bayesian model selection criteria.

The paper provides a long list of models and the associated $p_D$, the effective number of parameters. In each of these cases $p_D$ is interpreted nicely in terms of model quantities. However, there is an unappealing feature of $p_D$ that I would like to point out in the discussion below.

Consider the set-up leading to equation (23). Assume further that $A_1 = \mathbf{1}$, $C_1 = 1$ and $C_2 = \tau^2$. Thus the likelihood is $N(\theta, 1)$ and the prior is $N(0, \tau^2)$. Then equation (23) yields that

$$p_D = \frac{1}{1 + 1/n\tau^2}.$$

Assuming $\tau^2$ to be finite it is seen that $p_D$ increases to 1 as $n \to \infty$. The unappealing point is that the



effective number of parameters is larger for larger sample sizes; conventional intuition suggests otherwise. The number of unknowns (i.e. the effective number of parameters) should decrease as more data are obtained under this very simple static model. In spite of the authors' views on asymptotics or consistency, this point deserves further explanation as it is valid even when small sample sizes are considered.

In Section 9.1 the relationship between DIC and other well-known Bayesian model selection criteria including the Bayes factor is discussed. Although DIC is not to be viewed as a formal model choice criterion (according to the authors), it is often (and it will be) used to perform model selection; see for example the references cited by the authors. In this regard a more precise statement about the relationship between the Bayes factor and DIC can be made. I illustrate this with the above simple example taken from the paper.

Assume that the observation model is $N(\theta, 1)$ and the prior for $\theta$ is $N(0, \tau^2)$. Suppose that model 0 specifies that $H_0 : \theta = 0$ and model 1 says that $H_1 : \theta \neq 0$. I assume that both $n$ and $\tau^2$ are finite and thus avoid the problems with interpretation of the Bayes factor and Lindley's paradox. Using the Bayes factor, model 0 will be selected if

$$n\bar{y}^2 < (1 + n\tau^2)\frac{\log(1 + n\tau^2)}{n\tau^2}.$$

In contrast, DIC selects model 0 if

$$n\bar{y}^2 < (1 + n\tau^2)\frac{2}{2 + n\tau^2}.$$

Clearly, if DIC selects model 0 then the Bayes factor will also select model 0. It is also observed that the Bayes factor allows for higher $|\bar{y}|$-values without rejecting the simpler model. In effect DIC is seen to have the much discussed poor behaviour of a conventional significance test which criticizes the simpler null hypothesis too much and often rejects it when it should not.

**Sylvia Richardson** (*Imperial College School of Medicine, London*)

I restrict my comments on this far-reaching paper to the use of the deviance information criterion DIC for choosing within a family of models and the behaviour of $p_D$ as a penalization.

My first remark concerns the spatial example of Section 8. The DIC-values for the 'spatial' and the 'spatial plus exchangeable' models are nearly identical. Thus, the authors resort to external pragmatic considerations for preferring the simpler model, while the more complex one is not penalized.

**Table 5.** Performance of DIC for mixture models with different numbers of components

| | *Results for the following values of k:* | | | | |
|---|---|---|---|---|---|
| | *k = 2* | *k = 3* | *k = 4* | *k = 5* | *k = 6* |
| *Bimod (n = 200)* | | | | | |
| DIC($k$) | 566.7 | 567.7 | 568.5 | 569.2 | 570.0 |
| $E(D\|y, k)$ | 563.4 | 563.7 | 564.1 | 564.5 | 565.0 |
| $p_D$ | 3.3 | 4 | 4.4 | 4.7 | 5 |
| *Skew (n = 200)* | | | | | |
| DIC($k$) | 545.5 | 535.9 | 535.5 | 535.7 | 535.8 |
| $E(D\|y, k)$ | 540.3 | 530.1 | 530.0 | 530.2 | 530.4 |
| $p_D$ | 5.2 | 5.8 | 5.5 | 5.5 | 5.4 |
| *North–south (n = 94)* | | | | | |
| DIC($k$) | 110.5 | 110.9 | 110.9 | 110.5 | 110.8 |
| $E(D\|y, k)$ | 94.2 | 91.9 | 89.6 | 87.7 | 86.2 |
| $p_D$ | 16.3 | 19.0 | 21.3 | 22.8 | 24.6 |

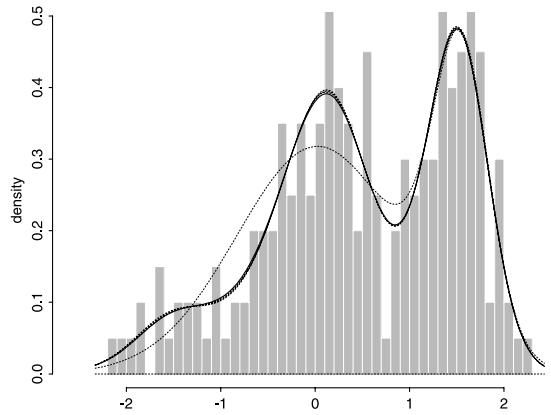


**Fig. 8.** Predictive densities for the skew data set: ·····, $k = 2$; ———, unconditional (results for $k = 3, 4, 5$ are superimposed)

Turning to mixture models and the comparison between models with different numbers of components, I discuss two situations. The first concerns simple Gaussian mixtures with an unknown number of components; $y_i \sim \Sigma_{j=1}^{k} w_j f(\cdot|\theta_j)$, $i = 1, \ldots, n$, where $f(\cdot|\theta_j)$ is Gaussian. To calculate DIC in this setting, let us focus on mixtures as flexible distributions and use the conditional density for a new observation $y^* : g(y^*) = p(y^*|y, w, \theta, k)$ to calculate the deviance $D(g) = -2\,\Sigma_{i=1}^{n} \log\{g(y_i)\}$ and take its expectation over the Markov chain Monte Carlo run, conditional on $k$. We have $p_D(k) = E\{D(g)\} - D(\hat{g}_k)$, where $\hat{g}_k = p(y^*|y, k)$.

Two cases of Gaussian mixtures were simulated (one replication): a well-separated bimodal mixture (bimod), 0.5 $N(-1.5, 0.5) + 0.5$ $N(1.5, 0.5)$, and an overlapping skewed bimodal mixture (skew): 0.75 $N(0, 1) + 0.25$ $N(1.5, 0.33)$, each with 200 data points.

In the clear-cut bimod case, DIC($k$) is lower for $k = 2$, with a small incremental increase in both $E(D|y, k)$ and $p_D$ as extra components are being fitted (Table 5). In the more challenging skew case, the pattern of DIC-values shows that this data set requires more than two components to be adequately fitted, but the values of DIC and $p_D$ stay surprisingly flat between three and six components. Note that the predictive density plots conditional on $k = 3, 4, 5$ are completely superimposed (Fig. 8), indicating that more than three components can be considered as overfitting the data, in the sense that they give alternative explanations that are no better but involve increasing numbers of parameters.

The second situation is that of spatial mixture models proposed in Green and Richardson (2002) in the context of disease mapping. DIC was calculated by focusing on area-specific risk. Referring, for example, to the simple north–south (two-component) contrast defined in that paper, we find that DIC stays stable as $k$ increases, decreasing $E(D|y, k)$ values being compensated by increasing $p_D$. On the basis of a mean-square error criterion between the estimated and the underlying risk surface, a deterioration of the fit would be seen with values of 0.14, 0.15 and 0.16 for $k = 2, 3, 4$ respectively.

Thus $p_D$ acts as a sufficient penalization only in the simplest case. In other cases, DIC does not distinguish between alternative fits with increasing number of parameters.

**Peter Green** (*University of Bristol*)

I have two rather simple comments on this interesting, important and long-awaited paper.

The first concerns using basic distribution theory to give a surprising new perspective on $p_D$ in the normal case, perhaps identifying a missed opportunity in exposition.

Consider first a decomposition of data as focus plus noise:

$$Y = X + Z$$

where $X$ and $Z$ are independent $n$-vectors, normally distributed with fixed means and variances, and var($Z$)



is non-singular. The deviance is

$$D(X) = (Y - X)^{\mathrm{T}} \operatorname{var}(Z)^{-1}(Y - X)$$

and so

$$p_D = E[D(X)|Y] - D(E[X|Y]) = \operatorname{tr}\{\operatorname{var}(Z)^{-1}\operatorname{var}(Z|Y)\}, \tag{42}$$

using the standard expression for the expectation of a quadratic form. Several results in the paper have this form, possibly in disguise. However,

$$\begin{aligned}\operatorname{var}(Z|Y) &= \operatorname{var}(Z) - \operatorname{cov}(Z, Y)\operatorname{var}(Y)^{-1}\operatorname{cov}(Y, Z)\\ &= \operatorname{var}(Z) - \operatorname{var}(Z)\operatorname{var}(Y)^{-1}\operatorname{var}(Z)\\ &= \operatorname{var}(Z)\operatorname{var}(Y)^{-1}\{\operatorname{var}(Y) - \operatorname{var}(Z)\},\end{aligned}$$

yielding the much more easily interpretable

$$p_D = \operatorname{tr}\{\operatorname{var}(Y)^{-1}\operatorname{var}(X)\}. \tag{43}$$

This allows a very clean derivation of examples in Sections 2.5 and 4.1–4.3. For example, in the Lindley and Smith model we have $\operatorname{var}(Z) = C_1$ and $\operatorname{var}(X) = A_1 C_2 A_1^{\mathrm{T}}$, and so

$$p_D = \operatorname{tr}\{(A_1 C_2 A_1^{\mathrm{T}} + C_1)^{-1} A_1 C_2 A_1^{\mathrm{T}}\} = \operatorname{tr}\{A_1^{\mathrm{T}} C_1^{-1} A_1 (A_1^{\mathrm{T}} C_1^{-1} A_1 + C_2^{-1})^{-1}\},$$

as in equation (21) of the paper.

Turning now to hierarchical models, consider a decomposition into $k$ independent terms

$$Y = Z_1 + Z_2 + \ldots + Z_k,$$

where all $Z_i$ are normal, and var($Z_k$) is non-singular. These represent all the various terms of the model: fixed effects with priors, random effects with different structures, errors at various levels; again all means and variances are fixed. Then for any level $l = 1, 2, \ldots, k - 1$ we may take the sum of the first $l$ terms as the focus and the rest as noise.

Version (42) of $p_D$ above is then not very promising:

$$p_D(l) = \operatorname{tr}\left\{ \operatorname{var}\left( \sum_{i=l+1}^{k} Z_i \right)^{-1} \operatorname{var}\left( \sum_{i=l+1}^{k} Z_i \middle| Y \right) \right\},$$

but expression (43) gives the more compelling

$$p_D(l) = \operatorname{tr}\left\{ \operatorname{var}(Y)^{-1} \operatorname{var}\left( \sum_{i=1}^{l} Z_i \right) \right\}. \tag{44}$$

Thus $p_D$ has generated a decomposition of the overall degrees of freedom $n = \Sigma_l \operatorname{tr}\{\operatorname{var}(Y)^{-1}\operatorname{var}(Z_l)\}$ into non-negative terms attributable to the levels $l = 1, 2, \ldots, k$, just as in frequentist nested model analysis of variance. (We must take care with improper priors in using expression (44), and terms should be treated as limits as precisions go to 0.) Of course, expressions (43) and (44) fail to hold with unknown variances or with non-normal models, but the observations above do provide further motivation for accepting $p_D$ as a measure of complexity, and suggest exploring more thoroughly its role in hierarchical models.

My second point notes that the paper has no examples with discrete 'parameters'. Conditional distributions in hierarchical models with purely categorical variables can be computed by using probability propagation methods (Lauritzen and Spiegelhalter, 1988), avoiding Markov chain Monte Carlo methods, so that $p_D$ is again a cheap local computation. Presumably marginal posterior modes would be used for $\tilde{\theta}$. Certainly this is a context where $p_D$ can be negative. Can connections be drawn with existing model criticism criteria in probabilistic expert systems?

The following contributions were received in writing after the meeting.

**Kenneth P. Burnham** (*US Geological Survey and Colorado State University, Fort Collins*)

This paper is an impressive contribution to the literature and I congratulate the authors on their achievements therein. My comments focus on the model selection aspect of the deviance information criterion DIC. My perspectives on model selection are given in Burnham and Anderson (2002), which has a focus on the Akaike information criterion AIC as derived from Kullback–Leibler information theory. A lesson that we learned was that, if the sample size $n$ is small or the number of estimated parameters $p$ is large relative to $n$, a modified AIC should be used, such as $\mathrm{AIC}_c = \mathrm{AIC} + 2p(p+1)/(n-p-1)$. I wonder whether DIC needs such a modification or if it really automatically adjusts for a small sample size or large $p$, relative to $n$. This would be a useful issue for the authors to explore in detail.

At a deeper level I maintain that model selection should be multimodel inference rather than just inference based on a single best model. Thus, model selection to me has become the computation of a set of model weights (probabilities in a Bayesian approach), based on the data and the set of models, that sum to 1. Given these weights and the fitted models (or posterior distributions), model selection uncertainty can be assessed and model-averaged inferences made. The authors clearly have this issue in mind as demonstrated by the last sentence of Section 9.1.3. I urge them to pursue this much more general implementation of model selection and to seek a theoretical or empirical basis for it with DIC.

There is a matter that I am confused about. The authors say '... we essentially reduce all models to non-hierarchical structures' (third page), and 'Strictly speaking, nuisance parameters should first be integrated out ...' (Section 9.2.3). Does this mean that we cannot make full inferences about models with random effects? Can DIC be applied to random-effects models? It seems so on the basis of their lip cancer example (Section 8.1). Can I have a model with fixed effects $\boldsymbol{\tau}$, random effects $\phi_1, \ldots, \phi_k$, with postulated distribution $g(\phi|\boldsymbol{\theta})$, $\boldsymbol{\theta}$ as fixed effects (plus priors on all fixed effects) and have my focus be all of $\boldsymbol{\tau}$, $\boldsymbol{\phi}$ and $\boldsymbol{\theta}$? Thus, I obtain shrinkage-type inferences about the $\phi_i$; I do not integrate out the $\phi$ (AIC has been adapted to this usage).

The authors make a point (page 612) that I wish to make more strongly. It will usually not be appropriate to 'choose' a single model. Unfortunately, standard statistical model selection has been to select a single model and to ignore any selection uncertainty in the subsequent inferences.

**Maria DeIorio** (*University of Oxford*) **and Christian P. Robert** (*Université Paris Dauphine*)

Amidst the wide scope of possible extensions of their paper, the authors mention the case of mixtures

$$\sum_{j=1}^{k} p_j \, f(x|\theta_j),$$

which is quite interesting, as it illustrates the versatility of the deviance information criterion DIC under different representations of the same model.

In this set-up, if the $p_j$s are known, the associated *completed* likelihood is

$$L\{\boldsymbol{\theta}|(x_1, z_1), \ldots, (x_n, z_n)\} \propto \prod_{i=1}^{n} f(x_i|\theta_{z_i}) = \prod_{j=1}^{k} \prod_{i:z_i=j} f(x_i|\theta_j). \tag{45}$$

Therefore, conditional on the latent variables $\mathbf{z} = (z_1, \ldots, z_n)$, and setting the saturated deviance $f(x)$ to 1, define

$$[\mathrm{DIC}|\mathbf{z}] = \sum_{j=1}^{k} \sum_{i:z_i=j} (-4E[\log\{f(x_i|\theta_j)\}|\mathbf{x}, \mathbf{z}\} + 2 \log\{f(x_i|\hat{\theta}_j)\}])$$

where $\hat{\theta}_j = E(\theta_j|\mathbf{x}, \mathbf{z})$ (under proper identifiability constraints; see Celeux *et al.* (2000)). The *integrated* DIC is then

$$\mathrm{DIC}_1 = \sum_{\mathbf{z} \in Z} [\mathrm{DIC}|\mathbf{z}] \Pr(\mathbf{z}|\mathbf{x}),$$

where $\Pr(\mathbf{z}|\mathbf{x})$ can be approximated (Casella *et al.*, 1999).

A second possibility is the *observed* DIC, $\mathrm{DIC}_2$, based on the observed likelihood, which does not use the latent variables $\mathbf{z}$. (We note the strong dependence of DIC on the choice of the saturated function $f$ and the corresponding lack of clear guidance outside exponential families. For instance, if $f(x_i)$ goes from the marginal density to the extreme alternative where both $\theta_1$ and $\theta_2$ are set equal to $x_i$, $\mathrm{DIC}_2$ goes from $-31.71$ to 166.6 in the following example.)



**Table 6.** Comparison of the three different criteria $\mathrm{DIC}_1$, $\mathrm{DIC}_2$ and $\mathrm{DIC}_3$ for a simulated sample of 100 observations from $0.5\mathcal{N}(5, 1.5) + 0.5\mathcal{N}(7.5, 8)$ with a conjugate prior $\theta_1 \sim \mathcal{N}(4, 5)$ and $\theta_2 \sim \mathcal{N}(8, 5)$, and of DIC based on the true complete sample ($\mathbf{x}$, $\mathbf{z}$) and DIC for the single-component normal model (with an $\mathcal{N}(6, 5)$ prior and a variance set of 6.07)

| | *Results for the following models:* | | | | |
|---|---|---|---|---|---|
| | *Normal ($k = 1$)* | *Complete, $[DIC\,|\,\mathbf{z}]$* | *Integrated, $DIC_1$* | *Observed, $DIC_2$* | *Full, $DIC_3$* |
| DIC | 465.1 | 413.5 | 462.6 | 457.6 | 447.4 |
| $\Delta$DIC | — | −51.6 | −2.5 | −7.5 | −17.6 |
| $p_D$ | 0.99 | 1.96 | 2.27 | 1.98 | 28.06 |

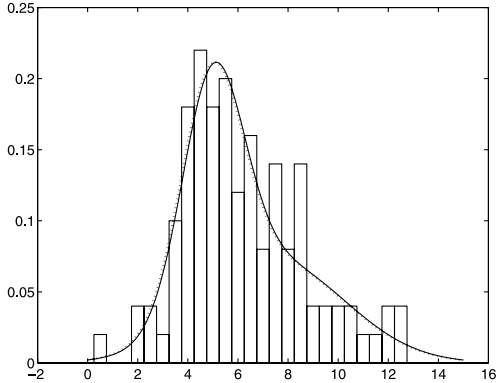


**Fig. 9.** Histogram of the simulated data set and true density

A third possibility is the *full* DIC, $\mathrm{DIC}_3$, based on the completed likelihood (45) when it incorporates $\mathbf{z}$ as an additional parameter, in which case the saturated deviance could be the normal standardized deviance, although we still use $f(x) = 1$ for comparison.

The three possibilities above lead to rather different figures, as shown by Table 6 for the simulated data set in Fig. 9; Table 6 exhibits in addition a lack of clear domination of the mixture ($k = 2$) *versus* the normal distribution ($k = 1$) (second column), except when $\mathbf{z}$ is set to its true value (third column) or estimated (last column). Note that, for the full DIC, $p_D$ is far from 102; this may be because, for some combinations of $\mathbf{z}$, the likelihood is the same. (This also relates to the fact that $\mathbf{z}$ is not a parameter in the classical sense.)

**David Draper** (*University of California, Santa Cruz*)

The authors of this interesting paper talk about Bayesian model assessment, comparison and fit, but—if their work is to be put seriously to practical use—the real point of the paper is Bayesian model choice: we are encouraged to pick the model with the smallest deviance information criterion DIC among the class of 'good' models (those which are 'adequate candidates for explaining the observations'). (It is implicit that somehow this class has been previously specified by means that are not addressed here—would the

authors comment on how this set of models is to be identified in general?) However, in the case of model selection it would seem self-evident that *to choose a model you have to say to what purpose the model will be put*, for how else will you know whether your model is sufficiently good? We can, perhaps, use DIC to say that model 2 is better than model 1, and we can, perhaps, compare $\bar{D}$ with 'the number of free parameters in $\theta$' to 'check the overall goodness of fit' of model 2, but we cannot use the authors' methods to say whether model 2 is sufficiently good, because the real world definition of this concept has not been incorporated into their methods. It seems hard to escape the fact that specifying the purpose to which a model will be put demands a decision theoretic basis for model choice; thus (Draper, 1999) I am firmly in the camp of Key *et al.* (1999).

See Draper and Fouskakis (2000) and Fouskakis and Draper (2002) for an example from health policy that puts this approach into practice, as follows. Most attempts at variable selection in generalized linear models conduct what might be termed a benefit-only analysis, in which a subset of the available predictors is chosen solely on the basis of predictive accuracy. However, if the purpose of the modelling is to create a scale that will be used—in an environment of constrained costs, which is frequently the case—to make predictions of outcome values for future observations, then the model selection process must seek a subset of predictors which trades off predictive accuracy against data collection cost. We use stochastic optimization methods to maximize the expected utility in a decision theoretic framework in the space of all $2^p$ possible subsets (for $p$ of the order of 100), and because our predictors vary widely in how much they cost to collect (which will also often be true in practice) we obtain subsets which are sharply different from (and much better than) those identified by benefit-only methods for performing 'optimal' variable selection in regression, including DIC.

**Alan E. Gelfand** (*Duke University, Durham*) **and Matilde Trevisani** (*University of Trieste*)
The authors' generally informal approach motivates several remarks which we can only briefly develop here. First, in Section 2.1, we think that better terminology would be 'focused on $p(y|\theta)$' with 'interest in the models for $\theta$', as in, for example, the example in Section 8.1 where there is no $\theta$ in the likelihood for any of the given models. Even the example in Section 8.2, where $\theta$ does not change across models, emphasizes the focus on $p(y|\theta)$ since $f(y)$ depends on the choice of $p$. So, here, a relative comparison of the models depends on the choices made for the $f$s. Without a clear prescription for $f$ (once we leave the exponential family), the opportunity exists to fiddle the support for a model.

Though the functional form of the Bayesian deviance does not depend on $p(\theta)$, DIC and $p_D$ will. With the authors' hierarchical specification,

$$p(y, \theta, \psi) = p(y|\theta)\ p(\theta|\psi)\ p(\psi),$$

the effective degrees of freedom will depend on $p(\psi)$. But, also, under this specification, rather than $p(y|\theta)$, we can put a different distribution, $p(y|\psi)$, in focus. Again, it seems preferable not to speak in terms of 'parameters in focus'.

Moreover, since $p(y|\theta)$ and $p(y|\psi)$ have the same marginal distribution $p(y)$, a coherent model choice criterion must provide the same value under either focus. Otherwise, a particular hierarchical specification could be given more or less support according to which distribution we focus on. But let $\mathrm{DIC}_1$, $p_{D_1}$ and $f_1(y)$ be associated with $p(y|\theta)$ and $\mathrm{DIC}_2$, $p_{D_2}$ and $f_2(y)$ with $p(y|\psi)$. To have $\mathrm{DIC}_1 = \mathrm{DIC}_2$ requires, after some algebra, that

$$\ln\{f_2(y)\} - \ln\{f_1(y)\} = p_{D_1} - p_{D_2} + E[\ln\{p(y|\psi)|y\}] - E[\ln\{p(y|\theta)|y\}].$$

Just as the functional form of $f_1(y)$ depends only on the form of $p(y|\theta)$, the form for $f_2(y)$ should depend only on $p(y|\psi)$. Evidently this is not so. For instance, under the authors' example in expression (2), $f_1(y) = 0$. The above expression yields the non-intuitive choice

$$\ln\{f_2(y)\} = \sum w_i + \frac{1}{2}\sum \ln(1 - w_i) - \lambda\ \mathrm{var}(\psi|y)\ \sum w_i^2 - \frac{\lambda}{2}\ \sum w_i^2\{y_i - E(\psi|y)\}^2$$

where $w_i = \tau_i/(\tau_i + \lambda)$. This issue is discussed further in Gelfand and Trevisani (2002).

**Jim Hodges** (*University of Minnesota, Minneapolis*)
This is a most interesting paper, presenting a method of tremendous generality and, as a bonus, a fine survey of related methods. I can think of a dozen models for which I would like to see $p_D$, but I shall ask for just one: a balanced one-way random-effects model with unknown between-group precision, in which each group has its own unknown error precision, these latter precisions being modelled as draws from, say, a common gamma distribution with unknown parameters. Thus the precisions will be shrunk as well as the means, and presumably the two kinds of shrinkage will affect each other. The focus could be either the means or the precisions, or preferably both at once.



One thing is troubling: the possibility of a negative measure of complexity (Section 2.6, comment (d)). Hodges and Sargent (2001) is linked (shackled?) to linear model theory, in which complexity is defined as the dimension of the subspace of $\Re^n$ in which the fitted values lie. In our generalization, the fitted values may be restricted to 'using' only part of a basis vector's dimension, because they are stochastically constrained by higher levels of the model's hierarchy. (Basing complexity on fitted values may remove the need to specify a focus, although, if true, this is not obvious.) In this context, zero complexity makes sense: the fitted values lie in a space of dimension 0 specified entirely by a degenerate prior. Negative complexity, however, is uninterpretable in these terms. The authors attribute negative complexity to a poor model fit, which suggests that $p_D$ describes something more than the fitted values' complexity *per se*. Perhaps the authors could comment further on this.

**Youngjo Lee** (*Seoul National University*)
It is very interesting to see the Bayesian view of Section 4.2 of Lee and Nelder (1996), which used extended or $h$-likelihood and in which we introduced various test statistics. For a lack of fit of the model we proposed using the scaled deviance

$$D_r = -2(\log\{p(y|\tilde{\theta}^{\mathrm{t}})\} - \log[p\{y|\mu(\theta) = y\}])$$

with degrees of freedom $E(D_r)$, estimated by $n - \mathrm{tr}(-L''_{\tilde{\theta}}V)$ where $-L''_{\tilde{\theta}} = V^*$ as in Sections 4.3 and 5.4 of this paper. We considered a wider class of models, which we called hierarchical generalized linear models (HGLMs) (see also Lee and Nelder (2001a, b)), but some of our proofs hold more widely than this, so that, for example, Section 3.1 of this paper is summarized in our Appendix D, etc. For model complexity the authors define in equation (9) the scaled deviance

$$D_m = -2[\log\{p(y|\theta)\} - \log\{p(y|\tilde{\theta}^{\mathrm{t}})\}].$$

$D_r$ and $D_m$ are the scaled deviances for the residual and model respectively, whose degrees of freedom add up to the sample size $n$. We are very glad that the authors have pointed out the importance of the parameterization of $\theta$ in forming deviances. We extended the canonical parameters of Section 5 to arbitrary links by defining the $h$-likelihood on a particular scale of the random parameters, namely one in which they occur linearly in the linear predictor. In HGLMs the degrees of freedom for fixed effects are integers whereas those for random effects are fractions. Thus, a GLM has integer degrees of freedom $p_m = \mathrm{rank}(X)$ because $C_2^{-1}\delta$ is 0 in Section 5, whereas the estimated degrees of freedom of $D_m$ in HGLMs are fractions. Lee and Nelder (1996) introduced the adjusted profile $h$-likelihood eliminating $\theta$, and this can be used to test various structures of the dispersion parameters $\lambda$ discussed in the examples of Section 8: see the model checking plots for the lip cancer data in Lee and Nelder (2001b). Lee and Nelder (2001a) justified the simultaneous elimination of fixed and random nuisance parameters. It will be interesting to have the Bayesian view of the adjusted profile $h$-likelihood.

**Xavier de Luna** (*Umeå University*)
This interesting paper presents Bayesian measures of model complexity and fit which are useful at different stages of a data analysis. My comments will focus on their use for model selection. In this respect, one of the noticeable contributions of the paper is to propose a Bayesian analogue, the deviance information criterion DIC, to the Akaike information criterion AIC and TIC. Both DIC and TIC are generalizations of AIC. The former may be useful in a Bayesian data analysis, whereas the frequentist criterion TIC has the advantage of not requiring the 'good model' assumption discussed by the authors.

Such 'information-based' criteria use measures of model complexity (denoted $p^*$ or $p_D$ in the paper). It should, however, be emphasized that models can be compared without having to define and compute their complexity. Instead, out-of-sample validation methods, such as cross-validation (Stone, 1974) or prequential tests (Dawid, 1984) can be used in wide generality. Moreover, to use an estimate of $p^*$ in a model selection criterion, some characteristics of the data-generating mechanism (DGM)—'true model' in the paper—must be known. For instance, depending on the DGM either AIC-type or Bayes information type criteria are asymptotically optimal (see Shao (1997) for a formal treatment of linear models). Thus, when little is known about the DGM, out-of-sample validation provides a *formal* and general framework to perform model selection as was presented in de Luna and Skouras (2003), in which accumulated prediction errors (defined with a loss function chosen in accordance with the purpose of the data analysis)

were advocated to compare and choose between different model selection strategies. When many models are under scrutiny, out-of-sample validation may be computationally prohibitive and generally yields high variability in the selection of a model. In such cases, different model selection strategies based on $p^*$ (making—implicitly or explicitly—diverse DGM assumptions) can be applied to reduce the dimension of the selection problem. Accumulated prediction errors can then be used to identify the best strategy while making very few assumptions on the DGM.

**Xiao-Li Meng** (*Harvard University, Cambridge, and University of Chicago*)

The summary made me smile, for the 'mean of the deviance − deviance of the mean' theme once injected a small dose of excitement into my student life. I was rather intrigued by the 'cuteness' of expressions (3.4) and (3.8) of Meng and Rubin (1992), and seeing a Bayesian analogue of our likelihood ratio version certainly brought back fond memories. My excitement back then was short lived as I quickly realized that all I was deriving was just a masked version of a well-known variance formula. Let $D(x, \mu) = (x - \mu)^2$ be the deviance, a case of *realized discrepancy* of Gelman *et al.* (1996); then

$$\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \overline{D(x_i, \mu)} - D(\bar{x}, \mu). \tag{46}$$

Although equation (46) is typically mentioned (with $\mu$ set to 0) for computational convenience, it is the back-bone of the theme under quadratic or normal approximations, or more generally with log-concave likelihoods, beyond which assumptions become much harder to justify or derive. (Obviously, equation (46) is applicable for posterior or likelihood averaging by switching $x$ and $\mu$.)

Section 1 contained a small puzzle. I wondered why Ye (1998) was omitted from the list of 'the most ambitious attempts', because Ye's 'data derivative' perspective goes far beyond the independent normal model cited in Section 4.2 (for example, it addresses data mining). It also provides a more original and insightful justification than normal approximations, especially considering that Markov chain Monte Carlo sampling is most needed in cases where such approximations are deemed unacceptable.

Section 2.1 presented a bigger puzzle. The authors undoubtedly would agree that a statement like 'In hierarchical modelling we cannot uniquely define a "posterior" or "model complexity" without specifying the level of the hierarchy that is the focus of the modelling exercise' is tautological. Surely the 'posterior' and thus the corresponding 'model complexity' depend on the level or parameter(s) of interest. So why does the statement become a meaningful motivation when the word posterior is replaced by 'likelihood'? There is even some irony here, because hierarchical models are models where there are unambiguous and uncontroversial *marginal* likelihoods—both $L(\theta|y) = p(y|\theta)$ and $L(\phi|y) = p(y|\phi)$ in Section 2.1 are *likelihoods* in the original sense.

Although limitations on space prevent me from describing my reactions when reading the rest, I do wish that DIC would stick out in the dazzling AIC—TIC alphabet contest, so we would all be less compelled to look for UIC (*unified or useful information criterion*?) ....

The **authors** replied later, in writing, as follows.

We thank all the contributors for their wide-ranging and provocative discussion. Our reply is organized according to a number of recurring themes, but constraints on space mean that it is impossible to address all the points raised. Echoing Brooks's opening remarks, our hope is that discussants and readers will be sufficiently inspired to pursue the ideas proposed in this paper and to address some of the unresolved issues highlighted in the discussion.

*Model focus and definition of deviance*

Our notion of the 'focus' of a model and its relationship to the prediction problem of interest provoked some controversy. The crucial role of the model focus is to define the (parameterization of the) likelihood, and we appreciate Gelfand and Trevisani's suggestion of the term 'focus on $p(y|\theta)$', with interest in the structure of $\theta$, rather than models 'focused on $\theta$'. In all our examples the likelihood has been taken to be $p(y|\theta)$ (using the notation of Section 2.1) leading to models with a closed form likelihood but an unknown number of effective parameters that we propose to estimate by $p_D$. However, as Brooks points out, if the focus is on $p(y|\psi)$ (i.e. integrating over the random effects $\theta$), then in general the likelihood will no longer be available in closed form, and other methods must be sought to evaluate $p(y|\psi)$: in this circumstance the number of parameters will be the dimension of $\psi$ or less, depending on the strength of the prior information on $\psi$.



Smith and others ask how the model focus should be chosen in practice. We argue that the focus is operationalized by the prediction problem of interest. For example, if the random effects $\theta$ in a hierarchical model relate to observation units such as schools or hospitals or geographical areas, where we might reasonably want to make future predictions for those same units, then taking $p(y|\theta)$ as the focus is sensible. The prediction problem is then to predict a new $Y_{i,\mathrm{rep}}$ conditional on the posterior estimate of $\theta_i$ for that unit. However, if the random effects relate to individual people, say, then we are often interested in population-average inference rather than subject-specific inference, so we may want to predict responses for a new or 'typical' individual rather than an individual who is already in the data set. In this case, it is appropriate to integrate over the $\theta$s and to predict $Y_{\mathrm{rep}}$ for a new individual conditional on $\psi$, leading to a model focused on $p(y|\psi)$. A crucial insight is that a predictive probability statement such as $p(Y_{\mathrm{rep}}|y)$ is not uniquely defined without specifying the level of the hierarchy that is kept fixed in the prediction—this defines the focus of the model. In summary, we feel that the issue of focus with respect to predictive model assessment and selection is an issue in hierarchical modelling and not specifically Bayesian.

When the forms of the likelihoods differ between models being compared, it is clearly vital to be careful that any standardizing terms that are used in the deviance are common. As observed by Smith, a comparison of models with focus at different levels of the hierarchy may not be meaningful as they correspond to different prediction problems.

*Features of $p_D$*

Several discussants questioned the definition or performance of $p_D$. As to the definition we maintain our claim (in spite of Dawid's comment) that it is in our models that there is a genuine Bayesian interest in quantifying the interaction between $Y$ and $\Theta$ in probabilistic terms. One can indeed often think of $p_D$ in terms of dimensionality as Hodges suggests, but in general we prefer to think of it as a feature of the *joint* distribution of $Y$ and $\Theta$. This frees it from the shackles imposed by normal linear model theory. Such a measure of interaction or model complexity may, for example, be used to reparameterize hyperparameters $\psi$ to facilitate an intuitively interpretable specification of model priors on $\psi$ (Holmes and Denison, 1999). Still, as suggested by Brooks, $p_D$ may turn out to be only a step towards a (better) definition of model complexity such as that suggested by Plummer: we feel that the quantity that he proposes is intuitively intriguing and that it may be particularly appropriate in exponential families, but we wonder about its general validation and justification.

Our uncertainty about whether to recommend $p_D$ as a definition or as an estimate of a quantity still to be defined makes it difficult to judge proposals for an 'improvement'. For example, using an invariant estimator such as that proposed by Robert and Titterington or Bernardo instead of $\bar{\theta}$ is tempting as part of a definition, but it takes into account only one feature of $p_D$ while destroying others such as the trace approximation. Similarly the occurrence of a negative value of $p_D$, typically observed if the model fits poorly, might resemble a negative estimate for a positive parameter. We take a pragmatic point of view and look forward to theoretical progress that provides insight into why $p_D$ generally appears to work well. Green provides a valuable insight into the interpretation of $p_D$ in the normal case, using an attractive decomposition of the total predictive variance of the observables.

Replying to those discussants who were concerned about observing $p_D < n$ under 'flat' priors, we re-emphasize that $p_D = n$ was obtained theoretically only in the normal case or under normal approximations. There is no proof that $p_D = n$ for general distributions. In the case of Brooks's illustration using the Scottish lip cancer data, in which he shows that $p_D$ appears to 'lose' two or three (modulo Monte Carlo error) parameters under such priors, we point out that two of the 56 observations in this data set are 0 with small expected values and so contribute negligibly to the Poisson deviance. We have replicated his analysis replacing these two observations by non-zero counts, and we found that $p_D$ increases by about 2 to around 55.5.

We certainly do not recommend the unthinking use of default priors, a concern of Smith and Bernardo: on the contrary, one of our main aims is to demonstrate how an informative prior reduces model complexity. Typically a large number of parameters $p$ relative to a small sample size $n$ is compensated by using an informative prior, and the deviance information criterion DIC and $p_D$ adjust accordingly without any need for additional adjustment for small sample size (see Burnham, and Lawson and Clark's comment on the example in Section 8.1).

There is evidence (Daniels and Kass, 1999, 2001) that, in the absence of missing data, the use of default priors for variance components typically has little effect on the posteriors for the main effects in a model. Still, Smith and Bernardo observe that the flat priors that may maximize $p_D$ are not necessarily weakly informative, and we agree. Reference priors that are least informative in an information theoretical sense can

be easily studied in some of our examples. For example, Fig. 1 displays the performance of the beta($\frac{1}{2}$, $\frac{1}{2}$) reference prior (corresponding to a prior sample size of $n_i = a + b = 1$) for the binomial likelihood, and the approximation (31) indicates that $p_{D_i}^{\Theta}$ based on the reference prior is greater than $p_{D_i}^{\Theta}$ based on the uniform beta(1, 1) prior (which has prior sample size $n_i = 2$). Similarly for a Poisson likelihood the reference prior $\pi(\mu_i) \propto \sqrt{\mu_i}$ yields a $\Gamma(y_i + \frac{1}{2}, n_i)$ posterior distribution corresponding to $a = \frac{1}{2}, b \to 0$. Hence $p_{D_i}^{\mu} \approx y_i/(y_i + \frac{1}{2})$ and $p_{D_i}^{\Theta} \approx n_i/n_i = 1$ might be compared with the values shown in Fig. 2.

*Properties of DIC*

Another main part of the discussion focused on the properties and performance of DIC. Plummer doubted the usefulness of the expected loss that DIC approximates, but he has included a standardizing constant in the loss function which should not be present (we have made this clearer in the paper). The expected loss in the (independent) normal linear case is then $p + p_D + n \log(2\pi\sigma^2)$: this says that when comparing 'good' models with the same $\sigma^2$s the expected loss is minimized with a degenerate prior in which no parameters are estimated. This seems entirely reasonable, as all the models have equivalent fit, and so distinction is based on complexity alone. Of course in practice either $\sigma^2$ will be estimated or $\sigma^2$ will vary between models, and hence the appropriate trade-off between fit and complexity will naturally arise. A practical aspect, related to the need for 'good' models in the derivation of DIC, is that the term $\mathcal{L}_2$ ignored by DIC will tend to be negative with poorly fitting models and hence to inflate DIC: the approximation of DIC to expected loss will thus tend automatically to penalize models that are not 'good'.

Though we agree with Brooks that owing to its heuristic derivation DIC may be considered as a 'broad brush technique', we do not regard it to be as arbitrary as the alternatives that he suggests. In particular we do not feel that terms of 'fit' and 'complexity' can be arbitrarily combined, but we re-emphasize that a measure of model complexity results from correcting overfit due to an approximation of the expected loss that 'uses the observations twice'. Similarly we would like to see a justification of Vehtari's estimates of expected utilities as valid approximations generalizing DIC.

Bernardo asks for the application of DIC to nested models and hypothesis testing, in particular the occurrence of Lindley's paradox. This is an interesting question partially answered by the example discussed in Section 8.1 where some of the competing models are nested. The key point is that DIC is designed to take into account priors that are concentrated on parameters which are specified in a model, thus effectively assigning prior probability 0 to hypothetically omitted parameters (if there are remaining parameters). Let us consider Lindley's paradox in the following version: when comparing using the Bayes factor $\bar{X} \sim N(\mu_0, \sigma^2/n)$ with $\bar{X} \sim N(\mu, \sigma^2/n)$ where $\mu \sim N(\mu_1, \tau^2)$, evidence in favour of $H_0 : \mu = \mu_0$ becomes overwhelming as $\tau^2 \to \infty$ even if $\bar{x}$ would cause the rejection of $H_0$ at any arbitrary significance level. If $\sigma^2$ is known $\mu$ is the only parameter in the model. To apply DIC we compare the model $\bar{X} \sim N(\mu, \sigma^2/n)$ with prior $\mu \sim N(\mu_0, \tau^2)$, $\tau^2 \to 0$, corresponding to $H_0$ with the same likelihood but prior $\mu \sim N(\mu_1, \tau^2)$, $\tau^2 \to \infty$. Then $D(\mu) = n(\bar{x} - \mu)^2/\sigma^2$, $\overline{D(\mu)} = (n/\sigma^2)\{D(\bar{\mu}) + \mathrm{var}(\mu|\bar{x})\}$ and $p_D = n/\sigma^2 \,\mathrm{var}(\mu|\bar{x})$. For $\tau^2 \to 0$, $p_D \to 0$, $\bar{\mu} \to \mu_0$ and DIC $\to D(\mu_0)$. Similarly, for $\tau^2 \to \infty$, $p_D \to 1$, $\bar{\mu} \to \bar{x}$ and DIC $\to D(\bar{x}) + 2 = 2$. Hence the model with the flat prior—the 'alternative hypothesis'—is favoured if $D(\mu_0) > 2$ or $|\sqrt{n}(\bar{x} - \mu_0)/\sigma| > 1.414$ which corresponds to a rejection of $H_0$ at a significance level $\alpha \approx 0.16$—exactly the behaviour of the Akaike information criterion. Thus Lindley's paradox is not observed. Similarly Sahu contrasts the prior concentrated on $\mu_0 = 0$ with an informative prior $N(0, \tau^2)$ which is centered at $\mu_0$, also. Thus it is reasonable to reject $H_0$ using DIC if the data are suitably compatible with the 'alternative' prior. However, we do not accept an assessment of DIC that uses Bayes factors as a 'gold standard', since they are dealing with different prediction problems (see below).

Several discussants (Brooks, Bernardo, Burnham and Smith) were concerned with the lack of calibration of DIC. However, unlike the Bayesian reference criterion (Bernardo, 1999), which is based on a Kullback–Leibler distance and therefore a relative measure, DIC is an approximation to an absolute expected loss, and we cannot calibrate it (externally). Correspondingly, 'coherence' of model choice cannot be required in terms of equal DIC-values as Gelfand and Trevisani or Smith claim but can only be discussed in terms of model ranking by DIC. Note, by the way, that Plummer's alternative measure of model complexity, as well as our $p_D$, are defined relatively, indicating that these measures might be calibrated.

Finally, we certainly do not claim that applying DIC is an exhaustive tool for model assessment. Although we feel that our Fig. 4 is a step in the right direction, additional techniques such as those discussed by Nelder and Atkinson are certainly needed for refined analyses.

*Applications*

There were various comments on the interpretation of $p_D$ in the Scottish lip cancer analysis (Lawson and Clark, and Richardson) and in mixture models (Richardson, and DeIorio and Robert). Here we tend to think of $p_D$ as the estimable dimension of the parameter space or, alternatively, as the size of the parameter space that is identifiable by the data. We repeat that the spatial model 3 in the lip cancer example (Section 8.1) provides stronger prior information than the exchangeable model 2 leading to a smaller $p_D$. Only the sum of the spatial and exchangeable random effects is uniquely identifiable in model 4 and so $p_D$ remains virtually unchanged compared with the spatial-only model 3, thus justifying the lack of an additional 'penalty' for the apparently more complex model. The same is true for mixture models, where increasing the number of components does not necessarily increase the identifiable parameter space. We do appreciate the discussion of DIC in mixture models introduced by DeIorio and Robert, and by Richardson (though Richardson does not appear to have calculated DIC as we have defined it, but a different criterion based on predictive deviances). DeIorio and Robert's example nicely illustrates a range of possibilities for defining DIC in this case, although we re-emphasize that a comparison of models with different focus (e.g. their $\mathrm{DIC}_2$ *versus* $\mathrm{DIC}_3$) may not be meaningful, and we further note that their integrated DIC ($\mathrm{DIC}_1$) does not correspond to our definition of DIC.

In response to Lawson and Clark's query about averaging 'location' parameters, we point to Green's comment concerning the calculation of $p_D$ and DIC for models with discrete parameters, and his suggestion that marginal posterior modes could be used for $\tilde{\theta}$ in this case.

We thank Nelder and Atkinson for their refinements to the analysis of the stack loss data (Section 8.2). We disagree with Smith that our models 4 and 5 for these data are predictively identical since, as already discussed, the prediction problem addressed by model 4 integrates over the random effects and corresponds to predicting stack loss for a new chimney, whereas model 5 conditions on the random effects and corresponds to predicting future stack loss for the 21 chimneys in the data set.

*Alternatives to DIC*

Several discussants (Brooks, Dawid and Sahu) feel that DIC suffers in comparison with more traditional Bayesian model selection criteria based on posterior model probabilities and Bayes factors. Here we can only repeat that our deliberate intention was to offer an alternative to Bayes factors, which are most suitable when the entire collection of candidate models can be specified ahead of time (the '$\mathcal{M}$ closed' case of Bernardo and Smith (1994)). In our practical experience, the model-building, criticism and rebuilding process is typically an iterative '$\mathcal{M}$ open' one in which the ultimate model collection is rarely known ahead of time, and here DIC may emerge as more appropriate. Moreover, Bayes factors address how well the prior has predicted the observed data; this prior predictive emphasis ultimately leads to the Lindley paradox. DIC instead addresses how well the *posterior* might predict future data generated by the same mechanism that gave rise to the observed data; this posterior predictive outlook might be considered intuitively more appealing in many practical contexts. We emphasize that these techniques are intended to answer different questions and cannot be expected to give the same conclusions: in any case, posterior model probabilities may be highly dependent on within- and between-model priors, so their comparison with DIC is not straightforward. On a related point, several discussants (Brooks, Burnham and Draper) mention the possible alternative of model averaging. We do not, however, see any justification for transforming DIC-values to relative probabilities, and in any case the prior on the model space may be difficult to develop, and might even reasonably be related to model complexity!

Dawid wishes for a better definition of $p \log(n)$ (instead of just $p$) for use in the Bayesian information criterion (BIC) but previous work has shown that many such definitions are justifiable asymptotically (e.g. Volinsky and Raftery (2000)), so this line of research does not appear promising. Regarding the suggestion by Lawson and Clark of using $\bar{p} \log(n)$ as a penalty for the BIC, this of course assumes that the number of parameters $p$ is a suitable measure of model complexity. But most spatial models of the type that they refer to will involve random effects, where such use of the raw parameter count $p$ would be inappropriate; indeed, this is precisely the situation that $p_D$ was designed to address.

Vehtari and de Luna argue persuasively on behalf of cross-validation as an alternative to our posterior predictive approach that avoids a definition of complexity. Whereas no knowledge of the data-generating mechanism is required for cross-validation, the data-generating mechanism *is* necessary in a fully Bayesian analysis. Still, cross-validation as an alternative estimation method was also used to estimate model complexity by Efron (1986). We certainly acknowledge the potential of this approach, particularly in comparisons of different model selection strategies. We agree with Stone concerning further investigation of model assessment procedures in which the model is not assumed to be correct, and we refer to Konishi and Kitagawa (1996) (whose GIC adds yet further to the alphabet).

In conclusion, it is clear that several of the discussants feel that our pragmatic aims are muddying otherwise pure Bayesian waters. We feel, however, that the huge increase in the use of Bayesian methods in complex practical problems means that full elicitation of informative priors and utilities is simply not feasible in most situations, and that reasonably simple and robust methods for prior specification, model criticism and model comparison are necessary. We hope that we have made a positive contribution to the final concern.

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