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EFFECTIVE NUMBER OF ROUNDS OF THE GIBBS SAMPLER NEEDED FOR ESTIMATION OF PARAMETERS FOR THRESHOLD AND CONTINUOUS TRAITS

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SUMMARY

Reproductive measurements on ewes from 8,489 matings were recorded from 1975 to 1978. The ewes were of five breeds; Dorset (D), Finnsheep (F), Rambouillet(R), Suffolk(S) and Targhee(T) and two composite lines C1, (1/2 F + 1/4 R + 1/4 D) and C2, (1/2 F + 1/4 S + 1/4 T). The Brody model was used to fit sample estimates of variance components from Gibbs sampling after adjusting for breed of ewe as fixed effect. The Brody model has three parameters. The parameters can be interpreted as asymptotic estimate of the variance component, rate of change of estimates of the variance component per round and degree of convergency. Two traits were analyzed as single traits; lamb survival at weaning (LSW) which was analyzed as a threshold trait and total lamb weight at birth (TLWB) which was analyzed as a continuous trait. A two trait analysis included a threshold trait (number of lambs alive at birth) and a continuous trait (total lamb weight at birth). Year, age of ewe, breed of ewe, hormone treatment and season of breeding were fixed effects. Direct genetic and uncorrelated permanent environmental effects of the ewe were considered to be random effects. The Gibbs Sampler for animal models programs that allows analysis of ordered categorical data using a Bayesian threshold model for the threshold trait and a Bayesian linear model for the continuous trait was used (Van Tassell and Van Vleck, 1995).

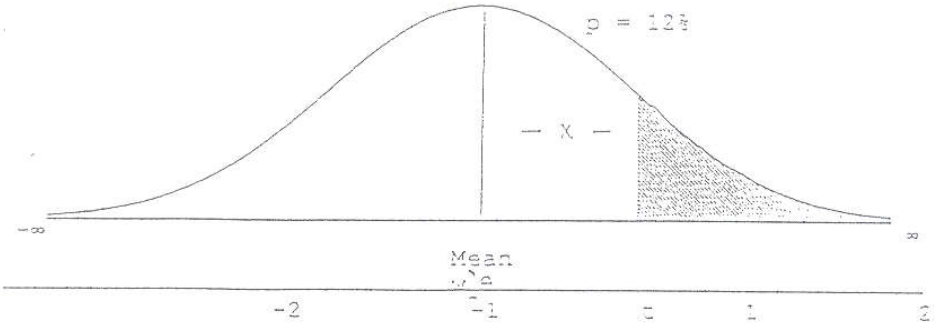
Estimates of the three parameters for the Brody equation using as data sample estimates of genetic variance created by Gibbs sampling were 0.12, -.03 and .0004 for LSW; .53, .24 and .0012 for TLWB and .06, -.01, 0.0001 for the genetic covariance between NLAB and TLWB. The three traits reached the asymptotic estimate after a different number of rounds was 24,610 for genetic variance for LSW, 7,000 for genetic variance for TLWB and 70,910 for the genetic covariance between NLAB and TLWB.

Keywords: Sheep, gibbs sampler, fertility

MATERIALS AND METHODS

Data

The threshold trait, lamb survival at weaning had two phenotypic classes with a single threshold separating them. The two classes will be referred to as alive = 1, or dead = 0. The individual can have only two visible measures. The percentage scale is used as description of mean for each class. Incidence on percentage scale was converted to mean liabilities, with liability being normal distributed. The scale on the unit liability scale is its standard deviation, σ .



For example :

If the propability of lamb alive is 12%, than

x is deviation of T, the threshold from the mean in standard deviation units and,

i is mean deviation of individuals with values exceeding T in standard deviation units from the population mean.

From the normal distribution table (e.g., Falconer 1989), $x = 1.175\ \sigma$, $i = 1.667\ \sigma$. The mean liability is, $- 1.175\sigma$. At the phenotypic level, a Bernoulli random variable y_i is observed for each individual i (i = 1, 2.....n) taking values of 1 or 0 (e.g., alive or dead).

The variable y_i is the expression of an underlying continuous random variable u_i, the liability of individual i. When u_i exceeds an unknown fixed threshold, t (in this example $t = 1.175\ \sigma$), then $y_i = 1$, and $y_i = 0$. The liability is assumed normally distributed with the mean value indexed by a parameter vectr, θ. The unit of liability is its standard deviation σ.

Hence with $\sigma = 1$:

$$(u_i \mid \theta) \sim N (w_i \theta`, 1) \qquad [1]$$

where

$\theta` = (b` a` c`)$ is a vector of parameters with p fixed effects (b), q random additive genetic values (a), and r uncorrelated random effects (c), w_i' is a row incidence vector linking θ, to the i^{th} observation. Then conditional on θ, the u_i

$$p(u \mid \theta) \prod_{i=1}^{P_i} \phi u_i (w_i' \theta, 1) = \phi u (w\theta, I) \qquad [2]$$

where

ϕ (•) is the normal density with parameters as indicated in the argument. In [2], $W\theta = xb + Z_a a + Z_c c$, where W, X, Z_a, Z_c are known incidence matrices of order n by 1 n by p, n by q, and n by r, respectively.

Given the model:

$$p(y_i = 1 \mid \theta, t) = p(u_i > t \mid \theta, t) = \int_{t - w_i'\phi}^{\infty} \phi(x)\, d_x = \Phi[-(t - w_i'\theta)] \qquad [3]$$

where

Φ (•) is the cumulative distribution function of a standardized normal variate. In [3], we can set t to zero to reduce [3] to

$$p(y_i = 1 \mid \theta) = \Phi(w_i' \theta) \qquad [4]$$

Conditionally on θ, u_i follows a truncated distribution than is, for $y_i = 1$.

$$p(u_i \mid \theta, y_i = 1) = \frac{\phi\, u_i (w_i' \theta, 1)}{\Phi(w_i' \theta)} 1 = (u_i > 0) \qquad [5]$$

where

1 ($X \in A$) is the indicator function that takes the value 1 if the random variable x is contained in the set A, and 0 otherwise.

$$p(u_i \mid \theta, y_i = 0) = \frac{\phi\, u_i (w_i' \theta, 1)}{\Phi(-w_i' \theta)} 1 = (u_i \leq 0) \qquad [6]$$

Model

As an example, a univariate mixed model is considered with three variance components: σ_a^2 for additive genetic and σ_c^2 for permanent environmental and σ_e^2 for residual. Extensions to more general mixed models are given by Wang et al. (1993; 1994) and Jensen et al. (1994).

The conditional distribution that pertains to realization of y is assumed to be:

$$(y \mid b, a, c, \sigma_e^2) \sim N(Xb + Z_a a + Z_c c \mid \sigma_e^2) \qquad [7]$$

for the continuous traits and;

$$(u \mid b, a, c, \sigma_e^2, Y) \sim N(Xb + Z_a a + Z_c c \mid \sigma_e^2)$$

for the categorical trait.

I is a known n by n matrix which is assumed here to be the identity, and σ_e^2 is a unknown scalar variance of residuals.

The vector of additive genetic values, a, conditional on additive genetic variance is multivariate normal :

$$(a \mid A, \sigma_a^2) \sim N(0, A\,\sigma_a^2) \qquad [8]$$

where

A is the matrix of additive genetic relationships among animals, and σ_a^2 (a scalar) is the unknown additive genetic variance.

Next the Bayesian inputs of the model are needed. The vector of fixed effects, b, will be assumed to follow a priori a uniform distribution

$$P(b) \propto \text{constant} \qquad [9]$$

The σ_a^2 , σ_c^2 , and σ_e^2 will be assumed to follow a priori, a scaled inverted Wishart distribution.

$$P(\sigma_i^2 \mid \nu_i, s_i^2) \propto (\sigma_i^2)^{-((\nu_i/2)+1)} \exp\left[\frac{\nu_i s_i^2}{2\sigma_i^2}\right] \qquad [10]$$

for

i = a, c, e

where

ν_i and s_i^2 are parameters of distribution. Note that a uniform prior can be obtained by setting $\nu_i = -2$ and $s_i^2 = 0$ in [10].

Posterior distribution

Bayes Theorem provides a way of deriving the posterior distribution of θ conditional on the data:

$$P(\theta \mid y) = \frac{p(y \mid \theta)\, p(\theta)}{P(y)} \qquad [11]$$

The first term in the numerator of the right hand side is the joint distribution of the parameters in the model. The denominator is the marginal distribution of the data that does not depend on è. Applying [11], and assuming the set of priors in [10] for the variance components, the joint posterior distribution of the parameters is:

$$p(b, a, c, u, \Sigma_i \mid y, \nu_i, s_i) \propto p(y \mid b, a, c, u, \Sigma_i)\, p(b, a, c, u, \Sigma_i \mid \nu_i, s_i)$$

$$= p(y \mid b, a, c, u, \Sigma_i)\, p(b) p(a \mid \sigma_a^2)\, p(c \mid \sigma_c^2)\, p(\sigma_a^2 \mid \nu_a, s_a^2)\, p(\sigma_c^2 \mid \nu_c, s_c^2)\, p(\sigma_e^2 \mid \nu_e, s_e^2) \qquad [12]$$

where

$\nu = p(\nu_a, \nu_c, \nu_e)$, $s = (s_a^2, s_c^2, s_e^2)$, and $\Sigma_i = (\sigma_a^2, \sigma_c^2, \sigma_e^2)$.

Using [7], [8], [9], [10] in [12] yields, the joint posterior density:

$$P(b, a, \sigma_a^2, \sigma_c^2, \sigma_e^2 \mid y, \nu, s) \propto (\sigma_e^2)^{-\frac{n + \nu_e}{2} \left[\frac{+1}{x}\right]}$$

$$\exp - \left[\frac{(y - xb - Za - Zc)' (y - xb - Za - Zc)}{2\sigma_e^2}\right] + \nu_e s_e^2$$

$$x\ (\sigma_a^2)^{-\left[\frac{q + \nu_a}{2} + 1\right]} \exp\left[-\frac{a'A^{-1}a + \nu_a s_a^2}{2\sigma_a^2}\right] x$$

$$(\sigma_c^2)^{-\left[\frac{q + \nu_c}{2} + 1\right]} \exp \frac{(y' - xb - Za)(y' - xb - Za) + \nu_c s_c^2}{2\sigma_c^2} \qquad [13]$$

In order to implement the GS, all conditional posterior distributions of the parameters of the model are needed.

The first fixed effect

$$p(b \mid a, c, u, \sigma_a^2, \sigma_c^2, y) \propto p(u \mid b, a, c)$$

which is proportional to $(x_b + Z_a + Z_c, I)$. As shown in Wang et al. (1994), the scalar form of the GS for the i^{th} fixed effect consists of sampling from:

$$(b_i \mid b_{-i}, a, c, u, \sigma_a^2, \sigma_c^2, y) \sim N(\hat{b}_i, (x_i'x_i)^{-1}\ \sigma_e^2) \qquad [14]$$

where x_i is the i^{th} column of matrix x, and $\hat{b}_i$ is the fixed effect under consideration and b_{-i} is all other elements of b without the i^{th} element where $\hat{b}_i$ satisfies:

$$x_i' s_i\ \hat{b}_i = x_i' (y - x_{-i}\, b_{-i} - Za - Zc) \qquad [15]$$

The random effects

$$(a_i \mid b, c, a_{-1}, u, \Sigma_i, y) \sim N(\hat{a}_i,\ (Z_i'Z_i + A_{ii}k^{-1})\ \sigma_e^2 \qquad [16]$$

where $k = \frac{\sigma_e^2}{\sigma_a^2}$, A_{ii} is the element in the row and column of A^{-1} and Z_i is the i^{th} column of Z, and $\hat{a}$ is the random effect and satisfies:

$$(Z_i'Z_i + A_{ii}k)\ \hat{a}_i, = Z_i' (y - xb - Zc) - kA_{i-i}\ a_{-i} \qquad [17]$$

where

A_{i-i} is the row of A^{-1} corresponding to the i^{th} individual with the i^{th} element excluded. a_{-i} is a without its i^{th} element.

Similarly, the permanent environmental effect

$$(c_i \mid b, a, c_{-i}, \Sigma_i, y) \sim N(c_i, (Z_i' Z^{-1})\sigma_e^2 \qquad [18]$$

Implementation of GS.

The GS works as follows:

i) Set arbitrary initial values for b, a, c and Σ_i;
ii) Sample from [14], and update b_i, i = 1, ...p,
iii) Sample from [16] and update a_i,
iv) Sample from [18] and update c_i,
v) Sample from [10] and update $\sigma_a^2, \sigma_c^2, \sigma_e^2$,
vi) Repeat (ii) to (v) k (length of chain) times.
As $k \to \infty$, this creates a Markov chain with an equilibrium distribution.

When the GS reaches convergence, for m samples we have

$(b, a, c, \sigma_a^2, \sigma_c^2, \sigma_e^2)$ .....$(b, a, c, \sigma_a^2, \sigma_c^2, \sigma_e^2)_m$ we have

b_1, ... , $b_m \sim p(b \mid y)$

a_1, ... , $a_m \sim p(a \mid y)$

c_1, ... , $c_m \sim p(c \mid y)$

$(\sigma_a^2)_i$, ... , $(\sigma_a^2)_m \sim p(\sigma_a^2 \mid y)$

$(\sigma_c^2)_i$, ... , $(\sigma_c^2)_m \sim p(\sigma_c^2 \mid y)$

$(\sigma_e^2)_i$, ... , $(\sigma_e^2)_m \sim p(\sigma_c^2 \mid y)$

Non-linear equation. To fit sample estimates the Brody model equation is:

$$y_{im} = A_i (1 - B_i e^{(-r_i m)}) + e_{im},$$

Where:

y_{im} is the predicted estimate for i^{th} component sampled at cycle m, (m = 1, ..., 5,000).

Parameter A_i is the asymptotic estimate of the i^{th} component,

Parameter B_i is related to early changes in estimates of the i^{th} component,

Parameter r_i is the estimate of the ratio of observed estimate to asymptotic estimate as this fraction measures how close the observed estimate is to the asymptotic variance.

The residual e_{im} is the deviation of the m^{th} prediction of component i from observed estimate *ith*.

The Brody equation (1945) had many applications to biological functions such as that by Brown (1970) and Brown et al. (1972), who applied this

equation to the growth pattern of beef cattle.

The estimates of genetic variances as output of the GS were used to estimate parameters A, B and r without discarding estimates from the burn-in period, using Proc NLIN of SAS (SAS Institut Inc., 1989).

RESULTS AND DISCUSSION

Different patterns of sample estimates of variance component by round were obtained from the GS. These patterns depended on the trait under analysis and also the starting value Raftery and Lewis (1992).

Gauss-Seidel iteration using the starting variances (σ_a^2 = .01, σ_c^2 = .003, σ_e^2=.10) for LSW were used to calculate the starting solutions for fixed effects and random effects.

The mean of posterior genetic variance for LSW when 110,000 rounds were sampled with 10,000 discarded as burn-in was .11. The mean of the posterior heritability estimate was .09. Estimate of mean of posterior distribution for (σ_c^2) was .12. Proportional variance due to permanent environmental effects, c^2, was .09.

Estimates from the first 5,000 rounds without discarding any burn-in were used to estimate the parameters for the Brody equation.

The estimates of A, B and r for samples of the genetic variance for LSW were .12, -.03 and .0004, respectively. The estimates of asymptotic variance from the equation as A was (.12), compared with the mean of marginal distribution as a result of 100,000 rounds was (.11) was slightly higher. The asymptotic estimate of the parameters from Brodyevaluation model were generally larger than from other non linear models in the study of Brown et al. (1976). On the other hand, the approach of this paper provides the researcher with an idea about the number of rounds needed to be dropped from the total number of rounds by fitting the Brody equation to a small number of rounds after plotting the samples to see if the Brody equation describes the pattern of sample estimates or not.

From the estimates of parameters of the Brody equation we can predict the estimate at any number of rounds and thus determine when the estimate of variance will be parallel to the horizontal axis by substituting the parameter in the Brody equation with sequences of m until y = A, and $\left(1 - be^{-rm}\right) \approx 1$. No change in y was observed after that when substitute by more round (m). In this case, the estimate of variance reached the asymptote at round number 24,610. This means that the first 24,610 estimates in the chain found must be dropped out before we consider the remaining estimates to obtain the distribution or mean estimate.

For the continuous trait (total lamb weight, TLWB), starting values for the parameters were σ_a^2 = .43, σ_c^2 = .14 and σ_e^2 = 3.93.

Estimates of the mean of marginal distributions for 100,000 rounds after discarding 2000 rounds for burn-in were .45, .21 and 3.90 for σ_a^2, σ_c^2, and σ_e^2, respectively.

Brody parameters A, B, and r estimated from 5,000 samples without burn-in for the genetic variance were .53, .24, and .0012. Using this parameter to predict ? at sequence m, = 1, 2, ... N where N number of rounds until no different happen in ? with increase m, in this case $\hat{y} = A$ and $(1 - be^{-rm}) \approx 1$. We can say the genetic variance be asymptotic at m = 7,000 rounds

The third application was to fit the Brody equation curve for estimates of genetic covariance from a bivariate analysis. Traits were number of lambs alive at birth and total lamb weight at birth. The starting values were .03, .05, .43, .01, .02, .14, .50, .69, and 3.93 for σ_a^2, σ_{a1a2}, σ_{a2}^2, σ_{c1}^2, σ_{c1c2}, σ_{c2}^2, σ_{e1}^2 σ_{e1e2} and σ_{e2}^2, respectively.

The means of the marginal distributions $f(\sigma^2 \mid y)$ from 100,000 rounds with 2,000 rounds of burn-in were .03 for $f(\sigma_{a1}^2 \mid y)$,

.06 for $f(\sigma_{a1a2} \mid y)$, .41 for $f(\sigma^2_{a2} \mid y)$, .02 for $f(\sigma^2_{c1} \mid y)$,

.05 for $f(\sigma_{c1c2} \mid y)$, .20 for $f(\sigma^2_{c2} \mid y)$, .40 for $f(\sigma^2_{e1} \mid y)$,

.85 for $f(\sigma_{e1e2} \mid y)$, and 3.91 for $f(\sigma^2_{e2} \mid y)$.

The estimates of A, B, and r when applied to the samples of the genetic covariance using 5,00samples without burn-in were .06, -.01, .0001, respectively. The effective number of rounds was found to be 70,910. The asymptotic estimate of covariance component from Brody's equation is equal to the mean of f $(\sigma_{a1a2} \mid y)$ from the 100,000 sample estimates. This means that the covariance estimates for samples from rounds 70,910 to 100,000 essentially do not change in any direction. Covariance estimates may take more rounds than estimates of variance components to reach convergence. In this case, the pattern in estimates of variances was different from the pattern in estimates of the covariance.

A linear regression on number of rounds was fit for each of the three previous sets of estimate cases to be sure there was no trend started from the round for which the effective number was determined previously up to round 100,000. The coefficient for regression of estimates of (co)variance on the number of rounds was zero as required for convergence and for averaging of estimates.

Implications

For the examples examined, variance component estimates from Gibbs

sampling for a single continuous trait need an effective number of rounds less than for a threshold trait. For running the Gibbs Sampler on two traits, one a threshold and the other a continuous trait, many rounds may be needed to reach the effective number. In this example, at least 70,000 rounds were needed as burn-in before averaging the subsequent sample estimates of the covariance component. The generality of this method of estimating the length of burn-in needed depends on whether the Brody equation describes the sample estimates. If the sample estimates follow the Brody equation, then the parameters of the Brody equation have a meaning for each parameter which may help to understand the number of rounds needed and to estimate the asymptotic estimate, especially for a researcher who is just starting to use the Gibbs Sampler.

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الدورات اللازمة من عينات الجبس في التقديرات للصفات المتقطعة والصفات المستمرة

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تمت هذه الدراسة على الصفات التناسلية لـ ٨٤٨٩ نعجة من سنة ١٩٧٥ إلى سنة ١٩٧٨ وكانت أنواع النعاج كالتالي : دوست ، فنش ، رامبوابة ، مسفولك ، تارجي وكذلك سلالتين خليطتين أحدهما تكون من ½ فنش مع ¼ رامبوية مع ¼ دورست والأخرى ½ فنش، ¼ سفولك، ½ تارجي.

استخدمت في الدراسة معادلة برودي وذلك لملائمة شكلها مع شكل النموذج الناتج من عينات الجبس لمكونات التباين .

حيث كانت أحد هذه المجاهيل في معادلة برودي موضع الاعتبار تعبر عن حالة الاستقرار في التقدير والتي تأخذ الرمز (A) وهي الجزء من التقدير الذي يوازي محور السينات بعد الاهتزازات التي تسبق استقرار التقدير الناتج من طريقة الجبس وهو يماثل بطريقة الرميل (التقارب) .

تم تطبيق المعادلة على ثلاثة صفات أحدهما منقطعة وهي بقاء الحملان حية حتى الفطام (LSW) والأخرى مستمرة وهي الوزن الكلي للحملان عند الميلاد (TLWB) والصفة الأخيرة هي أدماج (TLWB) عدد الحملان الحية عند الميلاد (NLAB) .

تم أيضا تصحيح البيانات للعوامل الثابتة كالسنة وعمر النعجة ، نوع النعجة، والمعاملة الهرمونية، وموسم التلقيح .

تم تقدير الجزء الوراثي المباشر وكذلك الجزء الغير مرتبط للتأثير البيئي الدائم كتأثيرات عشوائية.

إستخدمت طريقة الجبس في نموذج الحيوان لتحليل الصفة المنقطعة وكذلك المستمر والدمج بينهما متبعين في ذلك طريقة البيزيان .

تقدير الثلاثة مجاهيل لمعادلة برودي باستخدام عينة من عينات الجبس والتي تقدر بحوالي ٥٠٠٠ عينة أو لفة بدون استقطاع للفترة الأولي من عدم استقرار التقدير والمسماه بالـ Burn in أو Warm up (مرحلة عدم الاستقرار) كانت ٠,١٢ ، -٠,٠٣ ، ٠,٠٠٤ لصفة بقاء الحيوانات حية حتى الفطام، ٠,٥٣، ٠,٢٤ ، ٠,٠٠١٢ .

أظهرت الأمثلة للصفات الثلاثة أن مرحلة الاستقرار في التقدير بالنسبة للصفة الأولى المتقطعة (بقاء الحملان حية حتى الفطام) تأتي بعد ٢٤٦١٠ لفة وبالنسبة للصفة الثانية المستمرة كانت تأتي بعد ٧٠٠٠ لفة أيا بالنسبة للصفتين المحللتين معا فكانت مرحلة الإستقرار تأتي بعد ٧٠٩١٠ لفة .