A new Monte Carlo sampling in Bayesian probit regression

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Abstract: We study probit regression from a Bayesian perspective and give an alternative form for the posterior distribution when the prior distribution for the regression parameters is the uniform distribution. This new form allows simple Monte Carlo simulation of the posterior as opposed to MCMC simulation studied in much of the literature and may therefore be more efficient computationally. We also provide alternative explicit expression for the first and second moments. Additionally we provide analogous results for Gaussian priors.

AMS 2000 subject classifications: Primary 62J12; secondary 62F15.

Keywords and phrases: Bayesian approach, probit regression, noninformative prior, Monte Carlo sampling.

1. Introduction

The analysis of binary response data is important in statistics and related areas including econometrics and biometrics. The classical maximum likelihood method and inferences based on the associated asymptotic theory is often not accurate for small sample sizes. A Bayesian approach with respect to the non-informative or flat prior is a worthy natural competitor.

We study this problem with the aim of providing an alternative expression for the posterior distribution that allows simple Monte Carlo simulation as opposed to the somewhat more involved MCMC methods in much of the literature. (See e.g. Albert and Chib (1993)) We also give explicit expressions for the first and second moments of the regression parameters. Additionally we provide analogous results for Gaussian priors.

Suppose that \( n \) independent binary random variables \( Y_1, \ldots, Y_n \) are observed, where \( Y_i = 1 \) with probability of success \( p_i \). The \( p_i \) are related to a set of covariates that may be continuous or discrete. Define the probit

*This work was partially supported by KAKENHI #23740067.
†This work was partially supported by a grant from the Simons Foundation (#209035 to William Strawderman).
regression model as \( p_i = \Phi(x_i' \beta), \ i = 1, \ldots, n \), where \( \beta \) is a \( p \times 1 \) vector of unknown parameters, \( x_i \) is a vector of known covariates, and \( \Phi \) is the standard Gaussian cumulative distribution function. Let \( Y = (Y_1, \ldots, Y_n)' \), \( y = (y_1, \ldots, y_n)' \) and \( X = (x_1, \ldots, x_n)' \) with full rank \( p \). Then the joint probability distribution of \( y \) is given by

\[
\text{Pr}(Y = y | \beta) = \prod_{i=1}^{n} \Phi(x_i' \beta)^{y_i} [1 - \Phi(x_i' \beta)]^{1-y_i}.
\]

(1.1)

The posterior density with respect to the flat prior \( \pi(\beta) = 1 \) is proportional to the joint density (1.1). Because this posterior is somewhat intractable theoretically, instead of pursuing analytic results, a variety of simulation algorithms have been proposed for obtaining samples from the posterior distribution \( \pi(\beta | y) \). To our knowledge, the default choice is the so-called Albert and Chib’s (1993) sampler, which we now describe.

The computational scheme proceeds by introducing \( n \) independent latent variables \( Z_1, \ldots, Z_n \), where \( Z_i \sim N(x_i' \beta, 1) \). If we let \( Y_i = I(Z_i > 0) \), then \( Y_1, \ldots, Y_n \) are independent Bernoulli with \( p_i = P(Y_i = 1) = \Phi(x_i' \beta) \). Under the flat prior, the posterior density of \( \beta \) and \( Z = (Z_1, \ldots, Z_n) \) given \( y = (y_1, \ldots, y_n) \) is

\[
\pi(\beta, Z | y) = \prod_{i=1}^{n} \Phi(x_i' \beta)^{y_i} [1 - \Phi(x_i' \beta)]^{1-y_i} \phi(Z_i - x_i' \beta),
\]

where \( \phi \) is the standard Gaussian probability density function. Since \( \pi(\beta | \{y, z\}) \) is proportional to

\[
\prod_{i=1}^{n} \phi(z_i - x_i' \beta),
\]

we have

\[
\beta | \{y, z\} \sim N_p((X' X)^{-1} X' z, (X' X)^{-1}).
\]

(1.2)

Further it is clear that

\[
z_i | \{y_i, \beta\} \sim \begin{cases} N_+(x_i' \beta, 1, 0) & \text{if } y_i = 1, \\ N_-(x_i' \beta, 1, 0) & \text{if } y_i = 0, \end{cases}
\]

(1.3)

where \( N_+(\nu, 1, 0) \) and \( N_-(\nu, 1, 0) \) are the Gaussian distributions with mean \( \nu \) and variance 1 that are left-truncated and right-truncated at 0, respectively.
Based on (1.2) and (1.3), the corresponding Gibbs sampler is derived and $\pi(\beta|y)$ is approximated. For discussions of related computational techniques for probit regression, see Marin and Robert (2007).

In this paper, we push the theoretical analysis somewhat further to provide an expression for the posterior that allows more direct simulation and thereby, a more efficient random sampler. Let

$$X_y = \{2\text{diag}(y) - I_n\} X,$$

where $\text{diag}(y)$ is the $n \times n$ matrix with $y_i$ as the $i$-th diagonal entry, and which will be seen to be sufficient for the joint probability. Also let $\Psi[X_y]$ be the projection matrix onto the orthogonal complement of the column space of $X_y$, which is

$$\Psi[X_y] = I - X_y(X'_yX_y)^{-1}X'_y.,$$

Then under the mild condition on $\Psi[X_y]$, $\pi(\beta|y)$ is shown to be

$$\pi(\beta|y) = \int\int \pi(\beta|s,u,y)\pi(s|u,y)\pi(u|y)dsdu$$

(1.6)

where the elements of this hierarchical structure are given by

$$\pi(\beta|s,u,y) = N_p((X'X)^{-1}X'_ys^{1/2}u, (X'X)^{-1}),$$

$$\pi(s|u,y) = \|\Psi[X_y]u\|^{-2}\chi^2_n,$$

$$\pi(u|y) \propto \|\Psi[X_y]u\|^{-n} \text{ on } S^n_+,$$

(1.7)

and $S^n_+$ is the unit hyper-sphere restricted to the positive orthant given by

$$S^n_+ = \{h : \|h\|^2 = h^2_1 + \cdots + h^2_n = 1, \text{ and } h_i \geq 0, (i = 1, \ldots, n)\}.$$

(1.8)

As seen in Remark 3.1, the hierarchical structure of the posterior distribution given by (1.7) enables direct Monte Carlo sample generation essentially based on Gaussian random samplers. Further, the posterior mean of $\beta$ has the closed form

$$\begin{align*}
2^{1/2}\Gamma(\{n+1\}/2)
\Gamma(n/2)\
\frac{(X'_yX_y)^{-1}X'_y}{E_h\left[\|\Psi[X_y]h\|^{-(n+1)}\right]}
\frac{E_h\left[\|\Psi[X_y]h\|^{-n}\right]}{E_h\left[\|\Psi[X_y]h\|^{-n}\right]}.\end{align*}$$

(1.9)

where $E_h$ refers to the expectation with respect to the uniform distribution on $S^n_+$. More generally, a closed form of any moment of the posterior distribution, including the posterior variance, can also be expressed similarly.

This paper is organized as follows. In Section 2, we give a polar coordinate representation of the joint probability given by (1.1). Using this representation, we develop an alternative representation of the posterior distribution in Section 3, which leads to more efficient direct simulation based analyses.
2. The polar coordinate representation of the joint probability

The probability that \( Y_i = 1 \) is given by

\[
Pr(Y_i = 1|\beta) = \Phi(x_i^T \beta) = \int_{-\infty}^{\infty} \frac{1}{(2\pi)^{1/2}} \exp(-t^2/2) dt = \int_{0}^{\infty} \frac{1}{(2\pi)^{1/2}} \exp\left(-\frac{(t - x_i^T \beta)^2}{2}\right) dt. \tag{2.1}
\]

Similarly we have

\[
Pr(Y_i = 0|\beta) = \Phi(-x_i^T \beta) = \int_{0}^{\infty} \frac{1}{(2\pi)^{1/2}} \exp\left(-\frac{(t + x_i^T \beta)^2}{2}\right) dt. \tag{2.2}
\]

By (2.1) and (2.2),

\[
Pr(Y_i = y_i|\beta) = \int_{0}^{\infty} \frac{1}{(2\pi)^{n/2}} \exp\left(-\frac{\|t - X_{y_i} \beta\|^2}{2}\right) dt. \tag{2.3}
\]

where \( X_{y_i} = \{2\text{diag}(y_i) - I_n\} X, \) \( t = (t_1, \ldots, t_n)' \) and the range of integration is the positive orthant of \( \mathbb{R}^n \) given by

\[
\mathcal{R}_+^n = \{t|0 < t_i < \infty \ (1 \leq i \leq n)\}. \tag{2.4}
\]

Note that by the presentation of (2.3), \( X_{y_i} \) is sufficient for the joint probability.

A polar coordinate representation of (2.3) for \( t_1, \ldots, t_n \) is given by

\[
t_1 = s^{1/2} \cos \varphi_1, \ t_i = s^{1/2} \prod_{j=1}^{i-1} \sin \varphi_j \cos \varphi_i, \ (i = 2, \ldots, n - 1),
\]

\[
t_n = s^{1/2} \prod_{j=1}^{n-1} \sin \varphi_j, \ t = s^{1/2} h(\varphi) \tag{2.5}
\]

where \( \varphi = (\varphi_1, \ldots, \varphi_{n-1})' \). The Jacobian is

\[
\text{Jacobian}[t \to (s, \varphi)'] = 2^{-1} s^{n/2 - 1} \prod_{j=1}^{n-2} \{\sin \varphi_j\}^{n-1-j}. \tag{2.6}
\]

From (2.4), the range of \( \varphi, \mathcal{R}(\varphi) \), is given by

\[
0 < \varphi_i < \pi/2 \ (i = 1, \ldots, n - 1).
\]
Therefore we have

$$
\Pr(Y = y|\beta) = \frac{1}{2(2\pi)^{n/2}} \int_{R(\varphi)} m(y|\beta, h(\varphi)) \prod_{j=1}^{n-2} \{\sin \varphi_j\}^{n-1-j} d\varphi
$$

(2.7)

where

$$
m(y|\beta, h(\varphi)) = \int_0^\infty s^{n/2-1} \exp \left( -\frac{s^{1/2}h(\varphi) - X_y\beta}{2} \right) ds.
$$

Note that

$$
\int_0^{\pi/2} \{\sin \varphi_j\}^{n-1-j} d\varphi = \frac{B(1/2, \{n-j\}/2)}{2} = \frac{\pi^{1/2}\Gamma(\{n-j\}/2)}{2\Gamma(\{n-j+1\}/2)},
$$

and that

$$
\int_{R(\varphi)} \prod_{j=1}^{n-2} \{\sin \varphi_j\}^{n-1-j} d\varphi = \frac{\pi^{n/2}}{2^n\Gamma(n/2)} = c_1(n).
$$

Therefore the joint probability is given by

$$
\Pr(Y = y|\beta) = \frac{c_1(n)}{2(2\pi)^{n/2}} E_h [m(y|\beta, h)].
$$

(2.8)

In (2.8), $E_h$ refers to the expectation with respect to the distribution of $h = (h_1, \ldots, h_n)'$, which is uniformly distributed on $S^n$, given in (1.8), the unit hyper-sphere restricted to the positive orthants.

3. Posterior inference with respect to the flat prior

In this section, we consider posterior inference with respect to the flat prior. The posterior distribution is given by

$$
\pi(\beta|y) = \frac{E_h [m(y|\beta, h)]}{E_h [\int_{R(\varphi)} m(y|\beta, h) d\beta]}.
$$

(3.1)

First we give a hierarchical structure for the posterior distribution which enables simple and efficient Monte Carlo sample generation. Recall that $\Psi[X_y]$ given in (1.5) is the projection matrix to the orthogonal complement of the column space of $X_y$.

For posterior inference, propriety of posteriors has been studied by many. 

Speckman, Lee and Sun (2009) showed that the posterior distribution with
respect to the flat prior is proper if and only if there does not exist \( \beta \) such that
\[
(2\text{diag}(y) - I_n)X\beta = X_y\beta \in \mathcal{R}_+^n. \tag{3.2}
\]
As seen in Lemma 3.1 below, this is equivalent to the non-existence of \( u \in S_+^n \) such that \( \Psi[X_y]u = 0 \). So \( \pi(s|u,y) \) and \( \pi(u|y) \) below are well-defined.

**Theorem 3.1.** Assume there does not exist \( u \in S_+^n \) such that \( \Psi[X_y]u = 0 \). Then \( \pi(\beta|y) \) is given by
\[
\pi(\beta|y) = \int \int \pi(\beta|s,u,y)\pi(s|u,y)\pi(u|y)dsdu \tag{3.3}
\]
where the elements of this hierarchical structure are given by
\[
\begin{align*}
\pi(\beta|s,u,y) &= N_p((X'X)^{-1}X'_y s^{1/2}u, (X'X)^{-1}), \\
\pi(s|u,y) &= \|\Psi[X_y]u\|^{-2} \chi^2_n, \\
\pi(u|y) &\propto \|\Psi[X_y]u\|^{-n} \text{ on } S_+^n.
\end{align*} \tag{3.4}
\]

**Proof.** Note \( X'_y X_y = X'X \). Since
\[
\|s^{1/2}h - X_y\beta\|^2 = s\|\Psi[X_y]h\|^2 + (\beta - \hat{\beta})'X'X(\beta - \hat{\beta}), \tag{3.5}
\]
where
\[
\hat{\beta} = s^{1/2}(X'X)^{-1}X'_yh,
\]
we have
\[
E_h[m(y|\beta,h)] = E_h \left[ \int_0^\infty s^{n/2-1} \exp \left( -s\frac{\|\Psi[X_y]h\|^2}{2} \right) \right.
\]
\[
\times \exp \left( -\frac{(\beta - \hat{\beta})'X'X(\beta - \hat{\beta})}{2} \right) ds \bigg] \tag{3.6}
\]
\[
= \frac{(2\pi)^{n/2}}{|X'X|^{1/2}2^{n/2}\Gamma(n/2)}E_h \left[ \frac{1}{\|\Psi[X_y]h\|^n} \right. \times \int_0^\infty \frac{\|\Psi[X_y]h\|^n}{2^{n/2}\Gamma(n/2)} s^{n/2-1} \exp \left( -s\frac{\|\Psi[X_y]h\|^2}{2} \right)
\]
\[
\times \left. \frac{|X'X|^{1/2}}{(2\pi)^{n/2}} \exp \left( -\frac{(\beta - \hat{\beta})'X'X(\beta - \hat{\beta})}{2} \right) ds \right] \]
\]
provided all integrals exist. Let
\[
\pi(u|y) = \frac{\|\Psi[X_y]u\|^{-n}}{\int_{u \in S_+^n} \|\Psi[X_y]u\|^{-n} du}. \tag{3.7}
\]
Then
\[
E_{h}[m(y|\beta, h)] = \frac{(2\pi)^{p/2}2^{n/2}\Gamma(n/2)}{|X'X|^{1/2}} \int_{u \in S^n_+} \|\Psi[Xy]u\|^{-n} du \\
\quad \times \int_0^\infty \int_{S^n_+} \pi(\beta|s, u, y)\pi(s|u, y)\pi(u|y) ds du.
\]
(3.8)

Hence the theorem follows.

Remark 3.1. Let \(Z_1, \ldots, Z_n\) be independently distributed \(N(0, 1)\). Then \(t = \sum_{i=1}^n Z_i^2 \sim \chi^2_n\) and \(h = (|Z_1|/t^{1/2}, \ldots, |Z_n|/t^{1/2})'\) is uniformly distributed on \(S^n_+\) which is independent of \(t\). Using this property, we can propose the following algorithm. The so-called SIR (Sampling/Importance Resampling) method, described in part 2 and 3 below, enables to obtain samples from \(\pi(u|y)\) based on samples from the uniform distribution on \(S^n_+\).

Algorithm 3.1 (sampling from the posterior distribution \(\pi(\beta|y)\)).

1. For \(i = 1, \ldots, N\)
   (a) Generate \(n\) standard Normal random samples \(z^{(i)}_1, \ldots, z^{(i)}_n\).
   (b) Compute \(t^{(i)} = \sum_{j=1}^n \{z^{(i)}_j\}^2\) and \(h^{(i)} = \{t^{(i)}\}^{-1/2}(|z^{(i)}_1|, \ldots, |z^{(i)}_n|)'\).
   (c) Compute \(v^{(i)} = 1/\|\Psi[Xy]h^{(i)}\|\).

2. Re-sample \(i_1, \ldots, i_M\) with replacement from the multinomial distribution with probabilities
   \[
   \Pr(J = i) = \frac{\{v^{(i)}\}^n}{\sum_{i=1}^N \{v^{(i)}\}^n}, i = 1, \ldots, N.
   \]

3. Let \(u^{(k)} = h^{(i_k)}\) and \(w^{(k)} = v^{(i_k)}\) for \(k = 1, \ldots, M\).

4. For \(k = 1, \ldots, M\)
   (a) Generate \(p\) standard Normal random samples \(z^{(k)}_1, \ldots, z^{(k)}_p\).
   (b) Compute
   \[
   \beta^{(k)} = w^{(k)}\sqrt{t^{(k)}}(X'X)^{-1}X'_y u^{(k)} + (X'X)^{-1/2}(z^{(k)}_1, \ldots, z^{(k)}_p)'.
   \]

Therefore, in order to obtain samples from (3.4), it suffices to generate the Gaussian random samples. The simplicity and directness of this method gives an advantage over the methods in much of the literature. In addition to the simple structure described above, we note that, generally speaking, Monte Carlo sampling is more efficient than MCMC sampling which has been utilized in this area.
Remark 3.2. When interest lies primary in the posterior moments, a closed form of any posterior moments with respect to the flat prior is available. For example, the posterior mean is given by

\[
E[\beta|y] = \int \beta \pi(\beta|y) d\beta = (X'X)^{-1}X'_y E_{s,u}[s^{1/2}u|y] \tag{3.9}
\]

where \(E[s^{1/2}u|y]\) may be written as

\[
E_u\left[E_{s,u}[s^{1/2}|u,y]u\right] = \frac{2^{1/2}\Gamma((n+1)/2)}{\Gamma(n/2)} \frac{E_h\left[h\|\Psi[X_y]h\|^{-(n+1)}\right]}{E_h\left[\|\Psi[X_y]h\|^{-n}\right]} \tag{3.10}
\]

The posterior variance is

\[
\text{Var}[\beta|y] = E\left[(\beta - E[\beta|y])(\beta - E[\beta|y])'|y\right]
\]

\[
= E\left[\beta\beta'|y\right] - E[\beta|y]E[\beta|y]'
\]

\[
= E_{s,u}\left[E[\beta|s,u,y]\right] - E[\beta|y]E[\beta|y]'
\]

\[
= (X'X)^{-1} + E_{s,u}\left[E[\beta|s,u,y]\right] - E[\beta|y]E[\beta|y]'
\]

where the second term of the right-hand side of (3.11) is re-expressed as

\[
E_{s,u}\left[E[\beta|s,u,y]\right] - E[\beta|y]E[\beta|y]'
\]

\[
= n(X'X)^{-1}X'_y \frac{E_h\left[hh'\|\Psi[X_y]h\|^{-(n+2)}\right]}{E_h\left[\|\Psi[X_y]h\|^{-n}\right]} X_y (X'X)^{-1}. \tag{3.12}
\]

Compared to the sample mean and sample variance of simulated samples by Algorithm 3.1, these expressions with closed forms given in (3.9),(3.10), (3.11) and (3.12) should be more useful and efficient, where samples \(h^{(i)}\) for \(i = 1, \ldots, N\) in Algorithm 3.1 are sufficient.

In order to give an explicit expression of higher order moments, the first step is to take the expectation of the functions of \(\beta\) given \(s\) and \(u\), as in the third equation of the right-hand side of (3.11). These are the moments of multivariate Normal distribution. The second step is take the expectation of the function of \(s\) given \(u\). These are the moments of \(\chi^2\) distribution. As a result, the expression of the moments while complicated, are still exact.

Further we note that the posterior moments in the above have a kind of equivariant property. Suppose that the scale of each covariate changes as
$XD$ with a $p \times p$ positive diagonal matrix $D$. Since
\[
\Psi[[XD]_y] = \Psi[X_y],
\]
\[
([XD]_y X D_y)^{-1} [XD]_y' = D^{-1}(X'X)^{-1}X'_y, \tag{3.13}
\]
the posterior means satisfy the desirable property
\[
E[\beta|{XD}_y] = D^{-1}E[\beta|X_y]. \tag{3.14}
\]
In the same way, the posterior variances satisfy
\[
Var[\beta|{XD}_y] = D^{-1}Var[\beta|X_y]D^{-1}. \tag{3.15}
\]
Remark 3.3. We briefly remark that a similar direct MC sampler is possible
for Normal priors for $\beta$. Let $\beta \sim N_p(0, Q)$. The main difference comes from
completing squares corresponding to (3.5) as
\[
\beta'Q^{-1}\beta + \|s^{1/2}h - X_y\beta\|^2
\]
\[
= sh'\Psi[X_y,Q]h + (\beta - \hat{\beta})'(X'X + Q^{-1})(\beta - \hat{\beta}), \tag{3.16}
\]
where
\[
\Psi[X_y,Q] = I_n - X_y(X'X + Q^{-1})^{-1}X'_y
\]
\[
\hat{\beta} = s^{1/2}(X'X + Q^{-1})^{-1}X'_yh.
\]
Hence there is a corresponding hierarchical structure to (3.4) of Theorem
3.1, which is given by
\[
\pi(\beta|s,u,y) = N_p((X'X + Q^{-1})^{-1}X'_ys^{1/2}u, (X'X + Q^{-1})^{-1}),
\]
\[
\pi(s|u,y) = (u'\Psi[X_y,Q]u)^{-1/2} \times \chi^2_n,
\]
\[
\pi(u|y) \propto (u'\Psi[X_y,Q]u)^{-n/2} \text{ on } S^+_n.
\]
Since the prior is proper, the posterior is always proper even if there exists
$\alpha \in \mathcal{R}^p$ such that $X_y\alpha \in \mathcal{R}^n_+.
\]

The lemma below is related to the regularity condition of Theorem 3.1.

Lemma 3.1. The necessary and sufficient condition for the existence of
$\alpha \in \mathcal{R}^p$ such that $X_y\alpha \in \mathcal{R}^n_+$ is that the existence of $u \in S^+_n$ such that
$\Psi[X_y]u = 0$.

Proof. Suppose there exists $\alpha \in \mathcal{R}^p$ such that $X\alpha \in \mathcal{R}^n_+$. Let $u = X\alpha$.
Then $u$ satisfies $\Psi[X_y]u = 0$.
Suppose there exists $u \in S^+_n$ such that $\Psi[X_y]u = 0$. Let $\alpha = (X'X)^{-1}X'_yu$.
Then $X\alpha = X_y(X'X)^{-1}X'_yu = u$ is in $\mathcal{R}^n_+$. \qed
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