Conjugate Bayes for probit regression via unified skew-normals

BY DANIELE DURANTE

Department of Decision Sciences and Bocconi Institute for Data Science and Analytics,
Bocconi University, Via Röntgen 1, 20136, Milan, Italy
daniele.durante@unibocconi.it

SUMMARY

Regression models for dichotomous data are ubiquitous in statistics. Besides being useful for
inference on binary responses, these methods serve also as building blocks in more complex for-
mulations, such as density regression, nonparametric classification and graphical models. Within
the Bayesian framework, inference proceeds by updating the priors for the coefficients, typically
set to be Gaussians, with the likelihood induced by probit or logit regressions for the responses.
In this updating, the apparent absence of a tractable posterior has motivated a variety of computa-
tional methods, including Markov Chain Monte Carlo routines and algorithms which approximate
the posterior. Despite being routinely implemented, Markov Chain Monte Carlo strategies
face mixing or time-inefficiency issues in large \( p \) and small \( n \) studies, whereas approximate rou-
tines fail to capture the skewness typically observed in the posterior. This article proves that the
posterior distribution for the probit coefficients has a unified skew-normal kernel, under Gaussian
priors. Such a novel result allows efficient Bayesian inference for a wide class of applications,
especially in large \( p \) and small-to-moderate \( n \) studies where state-of-the-art computational meth-
ods face notable issues. These advances are outlined in a genetic study, and further motivate the
development of a wider class of conjugate priors for probit models along with methods to obtain
independent and identically distributed samples from the unified skew-normal posterior.

Some key words: Bayesian inference; Binary data; Conjugacy; Probit regression; Unified skew-normal.

1. INTRODUCTION

There is a relevant interest in several fields towards learning how the probability mass function
of a binary response \( y \in \{0; 1\} \) varies with a set of observed predictors \( x = (x_1, \ldots, x_p)^T \in \mathbb{R}^p \)
(e.g. Agresti, 2013). To address this goal, common formulations assume \( y \) is a Bernoulli variable
whose probability parameter changes with a linear combination of the predictors under a probit
or logit mapping. In the first case \( \Pr(y = 1 \mid x, \beta) = \Phi(x^T \beta) \), whereas in the second \( \Pr(y = 1 \mid x, \beta) = \{1 + \exp(-x^T \beta)\}^{-1} \), and the goal is to provide inference on \( \beta = (\beta_1, \ldots, \beta_p)^T \in \mathbb{R}^p \).

Although frequentist inference for the above class of models is well-established (e.g. Agresti,
2013), the Bayesian approach has attracted an increasing interest since it allows borrowing infor-
mation, uncertainty quantification, shrinkage and tractable inference via the posterior distribution
for the regression coefficients (e.g. Agresti, 2013, §7.2). Besides this, predictor-dependent mod-
els for binary data are also useful building blocks in more complex Bayesian formulations, such
as density regression models (Rodriguez & Dunson, 2011), additive trees (Chipman et al., 2010),
nonparametric classification (Rasmussen & Williams, 2006), graphical models (Spiegelhalter &
Lauritzen, 1990), and others. Although these methods provide popular learning procedures, there
are still computational barriers. Indeed, unlike Bayesian regression with Gaussian data, there are no results on the availability of tractable posteriors for $\beta$ in regression models for Bernoulli data, under the common Gaussian priors on the coefficients (e.g. Chopin & Ridgway, 2017).

Motivated by the above issue, several computational methods have been proposed for Bayesian regression with binary response data. Popular routines consider data augmentation strategies relying on hierarchical representations which provide conjugate full conditionals, within a Markov Chain Monte Carlo (Albert & Chib, 1993; Polson et al., 2013; Holmes & Held, 2006; Frühwirth-Schnatter & Frühwirth, 2007). Although being routinely implemented, these methods face poor convergence and mixing in practice, especially for imbalanced datasets (Johndrow et al., 2018).

A solution is to consider alternative strategies, including carefully tuned or adaptive Metropolis–Hastings (Roberts & Rosenthal, 2001; Haario et al., 2001), as well as more recent generalizations of Hamiltonian Monte Carlo, such as the no u-turn sampler by Hoffman & Gelman (2014). Both procedures guarantee computational advantages in large $n$ and moderate $p$ settings compared to data augmentation Markov Chain Monte Carlo. However, when $p$ is large, Metropolis–Hastings has difficulties in exploring the parametric space, whereas Hamiltonian Monte Carlo tends to be expensive (Chopin & Ridgway, 2017). Laplace approximations, variational Bayes and expectation propagation scale-up computations, but commonly provide Gaussian approximations which affect quality of inference when the posterior is skewed. This is a common situation in regression for binary data (Kuss & Rasmussen, 2005) and, as will be discussed in the rest of this article, a property which is inherent to the posterior. Refer to Chopin & Ridgway (2017) for a thorough discussion and comparison among these methods with a specific focus on probit regression.

Although providing state-of-the-art methods in Bayesian regression for binary response data, the aforementioned strategies are still sub-optimal compared to situations in which the posterior belongs to a known and tractable class of random variables. Indeed, this result could facilitate the calculation of several quantities relevant to posterior inference, without relying on Monte Carlo methods. This article proves that when the focus is on probit regression models under Gaussian priors for the coefficients, the posterior belongs to the class of unified skew-normal distributions (Arellano-Valle & Azzalini, 2006). These variables already appeared in probit models to obtain flexible link functions via skewed latent data, instead of Gaussian ones (e.g. Bazán et al., 2006). However, this is a different contribution compared to the one in the present article.

To the best of the author’s knowledge, the above result is not available in the literature, but can provide important advances. In fact, as discussed in this article, the unified skew-normal posterior guarantees closure properties (Arellano-Valle & Azzalini, 2006) in addition to explicit formulas for the marginal, joint and conditional posteriors along with predictive distributions and marginal likelihoods for model selection. These quantities involve cumulative distribution functions $\Phi_n(\cdot)$ of $n$-variate Gaussians, and hence can be efficiently evaluated for small-to-moderate $n$ studies via recent minimax tilting methods (Botev, 2017). The contribution by Botev (2017) is additionally useful to obtain independent samples from the posterior exploiting a representation of the unified skew-normal via a linear combination of $p$-variate Gaussians and $n$-variate truncated Gaussians. Such results are valid for any dimension and provide, per se, key methodological advances which motivate future theoretical studies and facilitate formal understanding of the skewness typically observed in the posterior. However, the associated inference strategies require evaluation of $\Phi_n(\cdot)$ or sampling from $n$-variate truncated Gaussians, and hence are of practical usefulness in small-to-moderate $n$ studies with, typically, few hundreds of units and any, even huge, $p$. This scenario is the most challenging for current Markov Chain Monte Carlo routines (e.g Chopin & Ridgway, 2017) and, in fact, the methods for posterior inference arising from the new unified skew-normal result significantly improve state-of-the-art algorithms in these situations, thus covering also an important computational gap; refer to §2.4 for a more detailed discussion on these aspects.
Conjugate Bayes for probit regression via unified skew-normals

2. POSTERIOR INFERENCE IN PROBIT REGRESSION VIA UNIFIED SKEW-NORMALS

2.1. The unified skew-normal distribution

Before deriving the unified skew-normal posterior induced by Gaussian priors for the $\beta$ coefficients in a probit regression, let us first introduce the unified skew-normal distribution. Recalling Arellano-Valle & Azzalini (2006), this random variable unifies different generalizations of the multivariate skew-normal $z \sim SN_p(\xi, \Omega, \alpha)$ (Azzalini & Dalla Valle, 1996) whose density $2\phi_p(z - \xi; \Omega)\Phi(\alpha^\top\omega^{-1}(z - \xi))$ is obtained by modifying the one of a $p$-variate Gaussian $N_p(\xi, \Omega)$ with the cumulative distribution function of a standard normal evaluated at $\alpha^\top\omega^{-1}(z - \xi)$, where $\omega$ is a $p \times p$ diagonal matrix containing the square root of the diagonal elements in $\Omega$. This strategy introduces skewness in $N_p(\xi, \Omega)$ controlled by $\alpha = (\alpha_1, \ldots, \alpha_p)^\top \in \mathbb{R}^p$, with $\xi = (\xi_1, \ldots, \xi_p)^\top \in \mathbb{R}^p$ and $\Omega$ driving location and variability, respectively (e.g. Azzalini & Dalla Valle, 1996). Indeed, when $\alpha = 0_p$, the multivariate skew-normal coincides with $N_p(\xi, \Omega)$, whereas, setting $p = 1$, leads to a univariate skew-normal $SN(\xi, \omega^2, \alpha)$ (Azzalini, 1985).

Motivated by the success of the above formulation in different studies (e.g. Azzalini & Capitanio, 1999), several extensions have been proposed to incorporate additional properties. Two important generalizations are obtained by adding an additional parameter $\gamma$ in $\Phi\{\alpha^\top\omega^{-1}(z - \xi)\}$ to develop the multivariate extended skew-normal (Arnold & Beaver, 2000; Arnold et al., 2002), and by allowing the skewness-inducing mechanism to be multivariate, thus providing the closed skew-normal family (Gupta et al., 2004; González-Farías et al., 2004) which includes a skewness to develop the multivariate extended skew-normal (Arnold & Beaver, 2000; Arnold et al., 2002), and extensions allow closure properties for marginals, conditionals and joint distributions, thus providing a general class. Azzalini & Capitanio (2013, §7.1.2) for details.

It shall be noticed that Arellano-Valle & Azzalini (2006) add a further condition which restricts the $(n + p) \times (n + p)$ matrix $\Omega^*$, having blocks $\Omega^*_{[11]} = \Gamma$, $\Omega^*_{[22]} = \Omega$ and $\Omega^*_{[21]} = \Omega^*_{[12]} = \Delta$, to be a full-rank correlation matrix. As will be clarified in §2.2, this identifiability restriction is not required in the Bayesian setting. In fact, the parameters of the unified skew-normal posterior for the coefficients $\beta$ are functions of the observed data and the pre-specified hyperparameters of the Gaussian prior, thus avoiding identifiability issues. Nonetheless, such a parameterization will be maintained in the article to inherit the classical results of the unified skew-normal distribution and to ensure identifiability of the prior, when the findings for the Gaussian case will be generalized to the entire class of unified skew-normals priors. Sections 2.2-2.3 prove that the posterior for the $\beta$ coefficients in a probit model with Gaussian priors is a unified skew-normal and study the consequences of this novel finding in posterior inference.
2-2. Unified skew-normal posterior for Bayesian probit regression with Gaussian priors

To introduce the reader to the general case consisting of n observations from a probit model with Gaussian prior \( \pi(\beta) = \phi_p(\beta - \xi; \Omega) \), let us first consider a simple setting with a single data point \( y \) and one covariate \( x \), such that \((y \mid x, \beta) \sim \text{Bern}(\Phi(x\beta))\) and \( \beta \sim N(0, 1) \). Although this scenario is uncommon in practice, it provides key intuitions on the role of \( y \) with Gaussian prior \( \pi(\beta) = \phi_p(\beta - \xi; \Omega) \) in driving departures from normality in the posterior distribution. Indeed, consistent with Lemma 1, \((\beta \mid y, x)\) has a unified skew-normal posterior when \( \pi(\beta) = \phi(\beta) \). See Appendix A for proofs.

**Lemma 1.** Let \((y \mid x, \beta) \sim \text{Bern}(\Phi(x\beta))\) and set \( \pi(\beta) = \phi(\beta; 1) = \phi(\beta) \), then \((\beta \mid y, x) \sim \text{SN}_1(0, \text{SN}(0,1))\), for every \( x \in \mathbb{R} \) and \( y \in \{0, 1\} \).

Figure 1 provides the density function of the unified skew-normal posterior for \( \beta \) in the illustrative example, under different combinations of \( x \) and \( y \). As expected, \((2y - 1)x(x^2 + 1)^{-1/2}\) controls skewness. Indeed, the higher \(|x|\) the more skewness is observed in the posterior. This skewness is either positive or negative depending on the sign of \((2y - 1)x\). To better understand this result, note that the unified skew-normal in Lemma 1 coincides with a basic SN\{0, 1, (2y - 1)x\}.

The above results apply more generally to independent response data \( y_1, \ldots, y_n \) from a probit model \((y_i \mid x_i, \beta) \sim \text{Bern}(\Phi(x_i^\top \beta))\), for \( i = 1, \ldots, n \), where \( x_i = (x_{i1}, \ldots, x_{ip})^\top \in \mathbb{R}^p \) denotes the vector of covariates for unit \( i \) and \( \beta = (\beta_1, \ldots, \beta_p)^\top \in \mathbb{R}^p \) the associated coefficients. Indeed, based on Theorem 1, when \( \beta \) has a Gaussian prior \( \beta \sim N_p(\xi, \Omega) \) with mean \( \xi \in \mathbb{R}^p \) and full-rank variance-covariance matrix \( \Omega = \omega \Omega \omega \), the posterior coincides with a unified skew-normal.

**Theorem 1.** If \( y = (y_1, \ldots, y_n)^\top \) comprises conditionally independent binary response data from a probit model \((y_i \mid x_i, \beta) \sim \text{Bern}(\Phi(x_i^\top \beta))\), for \( i = 1, \ldots, n \), and \( \beta \sim N_p(\xi, \Omega) \), then

\[
(\beta \mid y, X) \sim \text{SN}_{n,p}(\xi_{\text{post}}, \Omega_{\text{post}}, \Delta_{\text{post}}, \gamma_{\text{post}}, \Gamma_{\text{post}}),
\]

with the posterior parameters defined as a function of the data and the prior parameters via

\[
\begin{align*}
\xi_{\text{post}} &= \xi, & \Omega_{\text{post}} &= \Omega, & \Delta_{\text{post}} &= \Omega D - D \xi, & \gamma_{\text{post}} &= \Omega - D \xi, & \Gamma_{\text{post}} &= \Omega D + D \xi - D, \\
\end{align*}
\]

for every \( n \times p \) data matrix \( D = \text{diag}(2y_1 - 1, \ldots, 2y_n - 1)X \) and any \( n \times n \) positive diagonal matrix \( s = \text{diag}\{(d_1^\top \Omega d_1 + 1)^{1/2}, \ldots, (d_n^\top \Omega d_n + 1)^{1/2}\} \). The generic vector \( d_i^\top \) denotes instead the \( i \)-th row of \( D \), whereas \( X \) is the design matrix and \( I_n \) the \( n \times n \) identity matrix.

![Figure 1: Density of a $\text{SN}_{1,1}(0, 1, (2y - 1)x(x^2 + 1)^{-1/2}, 0, 1)$ posterior for $\beta$, under varying $x$ and $y$. Colors range from light grey to dark grey as $x \in (-3, -1.5, 0, 1.5, 3)$ goes from $-3$ to $3$.](image-url)
Conjugate Bayes for probit regression via unified skew-normals

Adapting equation (1) to the results in Theorem 1, it can be immediately noticed, after minor mathematical simplifications, that the density function of the unified skew-normal posterior is

\[
\pi(\beta \mid y, X) = \phi_p(\beta - \xi; \Omega) \frac{\Phi_n\{s^{-1}D\beta; (ss^T)^{-1}\}}{\Phi_n\{s^{-1}D\xi; s^{-1}(D\Omega D^T + I_n)s^{-1}\}},
\]

where \(\Phi_n\{s^{-1}D\xi; s^{-1}(D\Omega D^T + I_n)s^{-1}\}\) defines the normalizing constant. To clarify the role of the prior parameters \(\xi\) and \(\Omega\), along with that of the data \(y\) and \(X\), let us consider a constructive representation of the posterior. In particular, adapting known results from unified skew-normals (Azzalini & Capitanio, 2013, §7.1.2) to the specific posterior in Theorem 1, it can be shown that \((\beta \mid y, X)\) has the stochastic representation in Corollary 1.

**Corollary 1.** If \((\beta \mid y, X)\) has the unified skew-normal distribution from Theorem 1, then

\[
(\beta \mid y, X) \overset{d}{=} \xi + \omega\{V_0 + \bar{\Omega}\omega D^T(D\Omega D^T + I_n)^{-1}sV_1\}, \quad (V_0 \perp V_1),
\]

with \(V_0 \sim N_p(0_p, \bar{\Omega} - \bar{\Omega}\omega D^T(D\Omega D^T + I_n)^{-1}D\omega\bar{\Omega})\) and \(V_1\) from a zero mean \(n\)-variate truncated normal with covariance matrix \(s^{-1}(D\Omega D^T + I_n)s^{-1}\) and truncation below \(-s^{-1}D\xi\).

Based on (4), \(\xi\) has a main role on the location, but has also an effect in controlling departures from normality since it appears in the truncation \(-s^{-1}D\xi\). Instead, the prior variance-covariance matrix \(\Omega\) mainly affects scale, via \(\omega\), and posterior dependence among the \(\beta\) parameters, while contributing also to the weight matrix assigned to the multivariate truncated Gaussian \(V_1\), along with its variability. Finally, the data in \(D\) play a major role in controlling departures from normality. Indeed, if \(D\) has elements close to \(0\), the multivariate truncated Gaussian \(V_1\) has a negligible importance compared to the multivariate Gaussian \(V_0\) in (4).

### 2.3 Inference, prediction and variable selection under unified skew-normal posteriors

A general primary focus in Bayesian regression studies is on marginal posteriors \((\beta_j \mid y, X)\), for \(j = 1, \ldots, p\), their associated moments and more complex functionals including measures of posterior dependence along with credible intervals or regions. A fundamental property of unified skew-normals, which potentially facilitates this type of inference, is that such a class of variables is closed under marginalization, linear combinations and conditioning (Arellano-Valle & Azzalini, 2006; Azzalini & Capitanio, 2013). In particular, adapting the derivations in Arellano-Valle & Azzalini (2006) to Theorem 1, each marginal posterior is still from a unified skew-normal for every \(\beta_j\), \(j = 1, \ldots, p\). More specifically, \((\beta_j \mid y, X) \sim \text{SUN}_{1,n}(\xi_{\text{post}j}, \Omega_{\text{post}jj}, \Delta_{\text{post}j}, \gamma_{\text{post}}, \Gamma_{\text{post}})\) with \(\Delta_{\text{post}j}\) denoting the \(j\)-th row of \(\Omega\omega D^T s^{-1}\), \(\xi_{\text{post}j}\) the \(j\)-th element of the prior mean vector \(\xi\), \(\Omega_{\text{post}jj}\) the entry \([jj]\) in \(\Omega\), whereas \(\gamma_{\text{post}}\) and \(\Gamma_{\text{post}}\) coincide with those already defined in Theorem 1. A similar result holds also for sub-vectors of coefficients \((\beta_J \mid y, X)\), with \(J \subset \{1; \ldots; p\}\), linear combinations \((a + A^T\beta \mid y, X)\), and conditional posteriors \((\beta_J \mid y, X, \beta_{J^*})\), with \(J \subset \{1; \ldots; p\}\), \(J^* \subset \{1; \ldots; p\}\), and \(J \cap J^* = \emptyset\). Refer to Azzalini & Capitanio (2013) for details to obtain the parameters of these unified skew-normals from simple transformations of those in Theorem 1. Note that some linear combinations of \(\beta\), such as \(x^T\beta\), are of particular interest.

The aforementioned results facilitate graphical representation of marginal or joint posteriors, along with calculation of posterior moments and credible intervals for the probit coefficients via one-dimensional integrals involving marginal posterior densities. This can be done via numerical integration (e.g. Quarteroni et al., 2010, §9) whenever it is possible to evaluate \(\Phi_n(\cdot)\) with efficiency and accuracy. When the focus is on posterior moments, another solution is to obtain such quantities via direct derivation of the moment generating function. Indeed, adapting the result in Arellano-Valle & Azzalini (2006) to (2) a similar strategy can be considered when studying the functionals of the unified skew-normal posterior, provided that \((\beta \mid y, X)\) has moment generating
function

\[ M(t) = \exp(\xi^T t + 0.5t^T \Omega t) \frac{\Phi_n\{s^{-1}D\xi + s^{-1}D\Omega t; s^{-1}(D\Omega D^T + I_n)s^{-1}\}}{\Phi_n\{s^{-1}D\xi; s^{-1}(D\Omega D^T + I_n)s^{-1}\}}, \quad (t \in \mathbb{R}^p). \]  

Exploiting (5) and adapting the derivations in Azzalini & Bacchieri (2010) to the unified skew-normal in Theorem 1, the posterior expectation of \( \beta \) can be explicitly calculated as

\[ E(\beta \mid y, X) = \xi + \frac{1}{\Phi_n\{s^{-1}D\xi; s^{-1}(D\Omega D^T + I_n)s^{-1}\}} \Omega D^T s^{-1} \eta, \]

where \( \eta \) represents an \( n \times 1 \) vector whose generic \( i \)-th component is equal to \( \phi(\gamma_i)\Phi_n(\gamma_i - \Gamma_{-i}^\gamma, \Gamma_{-i} - \Gamma_{-i}^\gamma) \), with \( \gamma_i \) and \( \gamma_{-i} \) denoting the \( i \)-th element of \( s^{-1}D\xi = \gamma_{\text{post}} \) and the \((n-1) \times 1 \) vector obtained by removing the \( i \)-th entry in \( \gamma_{\text{post}} \), respectively. Similarly, \( \Gamma_{-i} \) defines the sub-matrix of \( s^{-1}(D\Omega D^T + I_n)s^{-1} = \Gamma_{\text{post}} \) without the \( i \)-th row and column, whereas \( \Gamma_{-i} \) is the \( i \)-th column of \( \Gamma_{\text{post}} \) with the \( i \)-th row element removed. Computing the expectation via (6) is more efficient than numerical integration since it requires calculation of \( n + 1 \) cumulative distribution functions, which is typically much less than the number of evaluations of \( \Phi_n(\cdot) \) required in numerical integration of marginal posteriors. However, as noticed in Gupta et al. (2013), obtaining expressions for higher-order marginal and joint moments via direct derivation of (5) requires tedious calculations, thus motivating Monte Carlo methods based on samples from the posterior, as discussed in §2.4. Refer also to Gupta et al. (2013) and Azzalini & Bacchieri (2010) for an expression of the variance-covariance matrix and the cumulative distribution function of a generic unified skew-normal. Both quantities, appropriately computed under the parameters in Theorem 1, are useful in posterior inference, especially for credible intervals or regions.

Although inference on the posterior distribution of \( \beta \) is often of interest, prediction of a future response \( y_{\text{new}} \in \{0; 1\} \) given the associated covariates \( x_{\text{new}} \in \mathbb{R}^p \) and the current data \( (y, X) \) is a primary goal in applications of probit models to classification. Within the Bayesian framework, this task requires the derivation of the posterior predictive distribution \( (y_{\text{new}} \mid y, X, x_{\text{new}}, \beta) \), which is simply a Bernoulli having parameter \( \Pr(y_{\text{new}} = 1 \mid y, X, x_{\text{new}}) = \int \Phi(x_{\text{new}}^TX\beta)\pi(\beta \mid y, X)d\beta \), in the binary case. According to Corollary 2, this probability parameter is available in explicit form.

**Corollary 2.** If \( (y_i, x_i, \beta) \sim \text{Bern}(\Phi(x_i^T\beta)) \), for \( i = 1, \ldots, n \), and \( \beta \sim N_p(\xi, \Omega) \), then

\[ \Pr(y_{\text{new}} = 1 \mid y, X, x_{\text{new}}) = \frac{\Phi_{n+1}\{s_{\text{new}}^{-1}D_{\text{new}}\xi; s_{\text{new}}^{-1}(D_{\text{new}}^T\Omega D_{\text{new}} + I_{n+1})s_{\text{new}}^{-1}\}}{\Phi_n\{s^{-1}D\xi; s^{-1}(D\Omega D^T + I_n)s^{-1}\}}, \]

with \( D_{\text{new}} \) representing the \((n+1) \times p \) matrix obtained by adding a last row \( d_{\text{new}}^T \) to \( D \), whereas \( s_{\text{new}} = \text{diag}\{(d_1^T\Omega d_1 + 1)^{1/2}, \ldots, (d_{n}^T\Omega d_n + 1)^{1/2}\} \).

An advantage of (7), compared to Markov Chain Monte Carlo strategies (e.g. Albert & Chib, 1993; Holmes & Held, 2006; Frühwirth-Schnatter & Frühwirth, 2007; Polson et al., 2013), is that prediction does not require Monte Carlo integration for \( \int \Phi(x_{\text{new}}^T\beta)\pi(\beta \mid y, X)d\beta \) via sampling of \( \beta \) from the posterior, and hence the computational burden does not depend on \( p \). As will be discussed in §2.4, this result is especially useful in large \( p \) and small-to-moderate \( n \) studies.

The above derivations are further helpful in obtaining explicit methods to perform Bayesian selection among models \( M_1, \ldots, M_K \) characterizing, in general, different subsets \( J_1, \ldots, J_K \) of covariates entering the linear predictor. Although there are different strategies for model selection (e.g. O’Hara & Sillanpää, 2009), the general approach formally defines prior probabilities \( \Pr(M_1), \ldots, \Pr(M_K) \) for the set of models, and subsequently ranks them via the posterior probabilities \( \Pr(M_k \mid y, X) \propto \Pr(M_k) \int \Pr(y \mid M_k, X, \beta_{J_k}) \pi(\beta_{J_k} \mid M_k)d\beta_{J_k}, k = 1, \ldots, K \) (e.g. Forte et al., 2018; Chipman et al., 2001). Clearly, the major issue in this task is the calculation of
Conjugate Bayes for probit regression via unified skew-normals

\[ \int \Pr(y \mid \mathcal{M}_k, X, \beta_{\mathcal{J}_k}) \pi(\beta_{\mathcal{J}_k} \mid \mathcal{M}_k) d\beta_{\mathcal{J}_k} \] which may be intractable in the absence of conjugacy, thus requiring Monte Carlo integration or approximations (e.g. Kass & Raftery, 1995). This procedure can be implemented also in probit models leveraging the methods in §1, but inference and computational performance face the issues previously discussed. Corollary 3 provides instead an explicit formula for the marginal likelihood in probit models with Gaussian priors, which can be easily evaluated, especially in large \( p \) and small-to-moderate \( n \) settings of interest in such studies.

**Corollary 3.** Let \( \mathcal{M}_k \) denote the probit regression model for \( y_1, \ldots, y_n \) including only the covariates with indices in the subset \( \mathcal{J}_k \subset \{1; \ldots; p\} \) and assume \( (\beta_{\mathcal{J}_k} \mid \mathcal{M}_k) \sim N_{p_k}(\xi_k, \Omega_k) \), with \( p_k = |\mathcal{J}_k| \) and \( \beta_{\mathcal{J}_k} \in \mathbb{R}^{p_k} \), the probit coefficients for the covariates in model \( \mathcal{M}_k \), then

\[ \int \Pr(y \mid \mathcal{M}_k, X, \beta_{\mathcal{J}_k}) \pi(\beta_{\mathcal{J}_k} \mid \mathcal{M}_k) d\beta_{\mathcal{J}_k} = \Phi_n\{s_k^{-1}D_k\xi_k; s_k^{-1}(D_k\Omega_kD_k^T + I_n)s_k^{-1}\}, \tag{8} \]

for every model \( \mathcal{M}_k \), \( k = 1, \ldots, K \), where \( D_k = \text{diag}(2y_1 - 1, \ldots, 2y_n - 1)X_k \in \mathbb{R}^{n \times p_k} \), \( s_k = \text{diag}\{(d_{kk}^T\Omega_kd_{kk} + 1)^{1/2}, \ldots, (d_{kk}^T\Omega_kd_{kk} + 1)^{1/2}\} \in \mathbb{R}_+^{n \times n} \), and \( X_k \in \mathbb{R}^{n \times p_k} \) denoting the \( n \times p_k \) design matrix of covariates with indices in \( \mathcal{J}_k \).

Equation (8) is additionally useful to compute Bayes factors (e.g. Kass & Raftery, 1995) and to perform Bayesian model averaging (Hoeting et al., 1999) without sampling from the posterior.

### 2.4. Computational considerations and sampling procedures

All the inference methods outlined in §2-3 can, in principle, proceed via direct strategies without sampling from the posterior, thus improving the available procedures in large \( p \) applications. The only barrier, which is relevant for a large \( n \), is evaluation of \( \Phi_n(\cdot) \). Quasi-randomized Monte Carlo (Genz, 1992; Genz & Bretz, 2009) allows, in fact, accurate calculation of \( \Phi_n(\cdot) \) for small \( n \), and have been recently improved via minimax tilting (Botev, 2017) to ensure effective evaluation of \( \Phi_n(\cdot) \) in moderate \( n \) studies. This procedure, available in the \( \mathbb{R} \) library TruncatedNormal, has a rare vanishing asymptotic relative error, thus allowing tractable inference without sampling from the posterior in studies having, typically, few hundreds of units. This strategy is also useful in larger \( n \) applications when few evaluations of \( \Phi_n(\cdot) \) are required, as in prediction of not many outcomes and in selection among few models. However, for general inferential tasks requiring a plenty of evaluations of \( \Phi_n(\cdot) \), such as in numerical integration, moments calculation and high-dimensional prediction or model selection, inference without sampling from the posterior might face non-negligible increments in computational time when \( n \) is large; refer to Botev (2017, §5) for details on scalability in the evaluation of \( \Phi_n(\cdot) \). In this situation, sampling from the posterior provides a tractable and common strategy to obtain numerical evaluations of generic functionals via Monte Carlo integration approximating

\[ E\{g(\beta) \mid y, X\} = \int g(\beta)\pi(\beta \mid y, X)d\beta. \]

Indeed, the availability of a large number \( R \) of replicates from the unified skew-normal posterior, allows fast and accurate approximation of \( E\{g(\beta) \mid y, X\} \) via \( \sum_{r=1}^{R} g(\beta^{(r)})/R \).

Popular routines addressing the above goal require data augmentation Markov Chain Monte Carlo (e.g. Albert & Chib, 1993; Holmes & Held, 2006; Frühwirth-Schnatter & Frühwirth, 2007; Polson et al., 2013), which provide poor performance, especially in imbalanced high-dimensional studies (Johndrow et al., 2018). This issue can be addressed via Algorithm 1, which combines the stochastic representation of the unified skew-normal posterior in Corollary 1 with a new scheme proposed by Botev (2017) to obtain independent samples from multivariate truncated Gaussians. This routine relies on minimax tilting and accept-reject methods to improve the acceptance rate of classical rejection sampling, while avoiding convergence and mixing issues of Markov Chain Monte Carlo methods. By combining this sampler with classical routines for multivariate Gaussians, Algorithm 1 inherits these properties, thus improving the computational methods discussed.
Algorithm 1. Exact scheme to draw independent samples from the posterior in Theorem 1

\begin{verbatim}
for r from 1 to R do
    [1] Sample $V_0^{(r)}$ from $N_p\{0_p, \Omega - \Omega_0^T(D\Omega_0^T + I_n)^{-1}D\Omega^T\}$, [in R use rnorm]
    [2] Sample $V_1^{(r)}$ from an n-variate truncated Gaussian with mean vector $0_n$, correlation matrix $s^{-1}(D\Omega_0^T + I_n)s^{-1}$ and truncation below $-s^{-1}D\xi$, using the accept-reject algorithm of Botev (2017), [in R use mvnorm]
    [3] Compute $\beta^{(r)}$ via $\beta^{(r)} = \xi + \omega\{V_0^{(r)} + \tilde{\Omega}_0^T(D\Omega_0^T + I_n)^{-1}sV_1^{(r)}\}$

output: $\beta^{(1)}, \ldots, \beta^{(R)}$
\end{verbatim}

in §1, especially in large $p$ and small-to-moderate $n$ applications. Clearly, when $n$ increases and $p$ decreases, sampling from the $n$-variate truncated Gaussian progressively affects computational time in favor of more efficient Markov Chain Monte Carlo strategies which directly explore the $p$-dimensional parametric space (e.g. Chopin & Ridgway, 2017). In this situation, a possibility to scale-up the computations is to exploit the structure of Algorithm 1 to perform parallel computing. Another alternative is to leverage the closure properties of multivariate truncated Gaussians under conditioning (Horrace, 2005) and iteratively block-update sub-vectors of $V_1$ whose dimension still allows efficient sampling via Botev (2017). Although this hybrid strategy could induce some auto-correlation in the posterior samples of $\beta$, the blocking approach typically guarantees improvements in mixing and convergence (e.g. Roberts & Sahu, 1997).

It is also worth noticing that Botev (2017) applied his accept-reject method to Bayesian probit regression. However, unlike Algorithm 1, the proposed strategy requires sampling from the $(n+p)$-variate truncated Gaussians. Separating these two blocks, as in Algorithm 1, reduces computational complexity and allows parallel computing. A more similar representation can be found in Holmes & Held (2006, §2.1) and in the documentation of the R library TruncatedNormal by Botev (2017). In fact, the resulting routines are closely related to Algorithm 1. However, Holmes & Held (2006, §2.1) and Botev (2017, §5.4) base their derivations on different arguments without noticing that the posterior is indeed a unified skew-normal. This last result and its broader implications are arguably the most important contribution of the present article.

Finally, Algorithm 1 can be also adapted to sample from a generic unified skew-normal. This can be broadly useful much beyond Bayesian inference. An example is parametric bootstrap (e.g. Efron & Tibshirani, 1994) for frequentist inference on the unified skew-normal parameters.

2.5. A class of conjugate unified skew-normal priors for Bayesian probit regression

The derivations in §2-2 suggest the more general result outlined in Corollary 4, thereby allowing tractable inference in Bayesian probit regression under more flexible priors for $\beta$.

**Corollary 4.** If $(y_i \mid x_i, \beta) \sim \text{Bern}\{\Phi(x_i^T \beta)\}$ independently for $i = 1, \ldots, n$, and $\beta$ is assigned a $\text{SUN}_{p,m}(\xi, \Omega, \Delta, \gamma, \Gamma)$ prior (Arellano-Valle & Azzalini, 2006), then

\[(\beta \mid y, X) \sim \text{SUN}_{p,m+n}(\xi_{\text{post}}, \Omega_{\text{post}}, \Delta_{\text{post}}, \gamma_{\text{post}}, \Gamma_{\text{post}}), \quad (9)\]

with posterior parameters $\xi_{\text{post}} = \xi$, $\Omega_{\text{post}} = \Omega$, $\Delta_{\text{post}} = (\Delta \Omega_0^T D^T s^{-1})$, $\gamma_{\text{post}} = (\gamma^T \xi^T D^T s^{-1})^T$ and $\Gamma_{\text{post}}$ characterizing an $(m+n) \times (m+n)$ full-rank correlation matrix having block entries $\Gamma_{\text{post}[1]} = \Gamma$, $\Gamma_{\text{post}[2]} = s^{-1}(D\Omega_0^T + I_n) s^{-1}$, $\Gamma_{\text{post}[1]} = \Gamma^T_{\text{post}[1]} = s^{-1}D\omega\Delta$.

According to Corollary 4, tractable inference in Bayesian probit regression is possible under a broader class of priors. Indeed, all the methods in §2-2–§2-4 also apply to this more general case, since the posterior in (9) is still a unified skew-normal. This ensures increased flexibility in
prior specification, thus allowing departures from normality. Although the general unified skew-normal choice may be uncommon in applied contexts, it shall be noticed that this class incorporates several priors of interest, including multivariate Gaussians, independent skew-normals for each $\beta_1, \ldots, \beta_p$, and multivariate skew-normals for $\beta$ (Arellano-Valle & Azzalini, 2006).

3. EMPIRICAL STUDIES

To evaluate the methods developed in §2 and compare performance with the popular strategies for Bayesian inference in probit regression discussed in §1, let us consider an online available dataset on the gene expression of $n = 74$ normal and cancerous biological tissues at $p - 1 = 516$ different tags (Martinez et al., 2005). An overarching focus in these applications is quantifying the effects of gene expression on the probability of a cancerous tissue and predicting the status of new tissues as a function of the gene expression (e.g. Tzanis & Vlahavas, 2007). Consistent with this goal, let us focus on studying the location of the posterior for $\beta$ and the predictive distribution in the Bayesian model $(y_i \mid x_i, \beta) \sim \text{Bern}(\Phi(x_i^T \beta))$, for $i = 1, \ldots, n$, with $\beta \sim N_{517}(0_{517}, 16 \cdot I_{517})$ prior. In this probit regression, $x_i$ denotes the vector having an intercept term and the gene expressions for tissue $i$, whereas $y_i$ is either 1 or 0 if the tissue is cancerous or not, respectively.

The choice of a weakly informative prior for the $\beta$ coefficients is motivated by the guidelines in Gelman et al. (2008) and by similar implementations from Botev (2017) and Chopin & Ridgway (2017). In line with these contributions, the gene expressions at the 516 different tags have been also standardized to have mean 0 and standard deviation 0.5. To assess predictive performance, the prior for $\beta$ is updated with the information of 50 randomly chosen observations, and out-of-sample classification via the posterior predictive distribution is made on the 24 held-out units.

Although other datasets could be considered, it shall be emphasized that state-of-the-art computational methods for probit regression provide valuable strategies in a variety of applications, but face mixing and time-inefficiency issues in large $p$ and small $n$ studies (e.g Chopin & Ridgway, 2017). As shown in Figs. 2–3 and in Table 1, the novel results outlined in §2 allow notable improvements in these large $p$ and small $n$ studies, thus providing straightforward Bayesian inference in relevant applications where this task was previously impractical. To clarify these results, the strategies in §2 are compared with state-of-the-art procedures, covering the data augmentation Gibbs sampler by Albert & Chib (1993), the Hamiltonian no u-turn sampler in Hoffman & Gelman (2014) and the adaptive Metropolis–Hastings from Haario et al. (2001). To increase acceptance rate and efficiency, the starting Gaussian proposal for the Metropolis–Hastings routine has been initialized with the mean and the rescaled variance-covariance matrix provided by an expectation propagation approximation. Consistent with Chopin & Ridgway (2017) and Roberts & Rosenthal (2001), the scaling factor has been set to $2^{38^2}/p$.

| Samples of $\beta$ per second | Minimum | First quartile | Median |
|--------------------------------|---------|---------------|--------|
| Unified skew-normal sampler    | 886-64  | 20000-00      | 20000-00 |
| Gibbs sampler                  | 13-48   | 55-46         | 2417-38 |
| Hamiltonian no u-turn sampler  | 15-95   | 20000-00      | 20000-00 |
| Adaptive Metropolis–Hastings sampler | 19-34  | 28-55         | 49-22  |

Table 1: Assessment on computational efficiency. For each sampling scheme under analysis, total number of samples from $(\beta \mid y, X)$ per second and statistics summarizing the effective sample sizes computed from the produced chains for the coefficients $\beta_1, \ldots, \beta_{517}$.
Quality in posterior mean calculation via Monte Carlo methods

Unified skew-normal sampler  Gibbs sampler  Hamiltonian no-u-turn sampler  Adaptive Metropolis-Hastings sampler

Fig. 2: Moments calculation performance. For each sampling scheme under study, boxplot of the differences between the posterior means for the coefficients based on the samples from $(\beta \mid y, X)$ and those calculated via (6). The jittered dots represent the values of the differences from which each boxplot is derived.

Quality in posterior predictive probability calculation via Monte Carlo methods

Unified skew-normal sampler  Gibbs sampler  Hamiltonian no-u-turn sampler  Adaptive Metropolis-Hastings sampler

Fig. 3: Predictive performance. For each sampling scheme under study, boxplot of the differences between the posterior predictive probabilities for the 24 held-out units based on the samples from $(\beta \mid y, X)$ and those calculated via (7). The jittered dots represent the values of the differences from which each boxplot is derived.

The above Markov Chain Monte Carlo routines were run for 20000 iterations after a burn-in of 5000, and can been easily implemented in R, leveraging the libraries bayesm, rstan, and a combination of LaplacesDemon and EPGLM, respectively. Although certain routines converged rapidly than others and with excellent mixing, the same settings were considered for all the algorithms to facilitate comparison. The sampling scheme proposed in Algorithm 1 provides instead independent samples from the exact posterior and hence requires no burn-in or convergence checks. Refer to the Supplementary Materials for details on code and implementation.

According to Table 1, the Hamiltonian no u-turn sampler has the same mixing of Algorithm 1 which displays, however, a significantly faster sampling speed. This could be due to the number of leap-frog steps required at each iteration of the no u-turn sampler (Chopin & Ridgway, 2017). As expected, the data augmentation Gibbs sampler and Metropolis–Hastings display lower mixing, but provide similar or improved running time compared to Hamiltonian no u-turn samplers. However, as is clear from Figs. 2–3, this reduction in mixing has a direct effect on the accuracy of posterior inference and prediction. There is instead an almost perfect match between Monte Carlo and direct estimates of posterior means and posterior predictive probabilities for the proposed Algorithm 1 and the Hamiltonian no u-turn sampler. However, as already discussed, such a
Conjugate Bayes for probit regression via unified skew-normals

routine is significantly slower than Algorithm 1 in this application. These computational gaps further increased when focusing on larger $p$ studies, with the competing methods becoming rapidly impractical. Conversely, the inference and sampling methods relying on the unified skew-normal results have difficulties in scaling with $n$. This claim is confirmed by a voice rehabilitation study presented at the online repository in the Supplementary Materials. However, also in this application having doubled $n$ and almost halved $p$, Algorithm 1 remains still competitive.

4. Final considerations and future directions of research

This article shows that the posterior for the coefficients in a probit regression having Gaussian priors is a unified skew-normal (Arellano-Valle & Azzalini, 2006), thus allowing key advances in Bayesian modeling of binary response data, especially for large $p$ and small-to-moderate $n$ studies. Indeed, unified skew-normals have moment generating functions involving known quantities, tractable additive representations, and are closed under marginalization, conditioning and linear transformations, thus facilitating derivations of marginal likelihoods for model selection and posterior predictive distributions. As shown in the empirical assessments in §3, in small-to-moderate $n$ settings with large or even huge $p$, posterior inference can proceed via direct methods or via an efficient sampler from the posterior, which notably improves available computational methods.

The above results could lead to computational gains also in more complex formulations relying on predictor-dependent observed or latent binary data, such as in mixture models for density regression (Rodriguez & Dunson, 2011). For instance, leveraging results in §2-3, binary classification via Gaussian processes (Rasmussen & Williams, 2006) could avoid sampling or approximations by exploiting closure properties of unified skew-normals, especially under conditioning. Moreover, when binary regression serves as a latent dictionary function, sampling the binary data via (7), instead of conditioning on $\beta$, could speed-up computations. Finally, the novel conjugacy results in §2-5, open new avenues for incorporation of skewness in prior specification.

There are also different directions for future advances. For instance, improved studies on the moment generating function of the unified skew-normal could facilitate direct calculation of relevant functionals without the need to sample from $(\beta \mid y, X)$. On the same line, improving the methods for efficient evaluation of $\Phi_n(\cdot)$ in large $n$ applications, either via data transformations, blocking methods (Chopin, 2011) or recent algorithms (Genton et al., 2018), could enlarge the range of applications which allow direct inference, prediction and model selection, without sampling from $(\beta \mid y, X)$. Also approximations of the exact posterior, which preserve the skewness but allow analytical inference provide an interesting direction. Finally, more detailed studies on particular forms of the prior variance-covariance matrix $\Omega$, such as those associated with $g$-priors or generalized $g$-priors (Maruyama & George, 2011) and limiting cases arising from flat priors, could provide novel insights on the effect of these specific choices and, potentially, lead to simplifications in the unified skew-normal parameters which may ease posterior inference. It is also possible to consider hyper-priors for $(\xi, \Omega)$ such as the normal-inverse-Wishart. With this choice, Theorem 1 holds only for the full conditional $(\beta \mid y, X, \xi, \Omega)$. Moreover, it is straightforward to notice that $(\xi, \Omega \mid y, X, \beta)$ has still a normal-inverse-Wishart kernel, since $(\xi, \Omega)$ only enter the Gaussian prior for $\beta$. Hence, although an hierarchical prior would not allow direct sampling from a unified skew-normal posterior, Gibbs sampling methods can be easily applied to this situation.

As discussed in §1, the availability of an exact posterior with tractable stochastic representations and closure properties can also motivate novel finite-sample and asymptotic theory. Finally, although the studies in §3 and the discussion in §2-4 provide the general guidelines on the practical usefulness of the unified-skew results in §2, additional quantitative assessments on scalability and its relations with specific prior settings or dataset structures, are certainly interesting.
SUPPLEMENTARY MATERIALS

Codes and tutorial implementations for the methods associated with this article are available at https://github.com/danieledurante/ProbitSUN.

APPENDIX A

Proof of Lemma 1. Let $\Phi(x;\beta)^{\tilde{y}(1 - \Phi(x;\beta))^{1 - y}} = \Phi((2y - 1)x;\beta)$ denote the probability mass function of $y$ in Lemma 1. Direct application of the Bayes rule provides

$$\pi(\beta \mid y, x) \propto \phi(\beta)\Phi((2y - 1)x;\beta) = \phi(\beta)\Phi((2y - 1)x(x^2 + 1)^{-1/2};(x^2 + 1)^{-1}).$$

Hence, letting $\xi_{\text{post}} = 0$, $\Omega_{\text{post}} = 1$, $\Delta_{\text{post}} = (2y - 1)x(x^2 + 1)^{-1/2}$, $\gamma_{\text{post}} = 0$, and $\Gamma_{\text{post}} = (x^2 + 1)^{-1} + \Delta_{\text{post}}^2\Delta_{\text{post}} = 1$, the kernel of the unified skew-normal in Lemma 1, with correlation matrix $\Omega_{\text{post}}$, having block entries $\Omega_{\text{post}[11]}^* = \Omega^*_{\text{post}[12]} = 1$ and $\Omega_{\text{post}[21]} = \Omega^*_{\text{post}[22]} = \Delta_{\text{post}}$. □

Proof of Theorem 1. Adapting the proof of Lemma 1, it is possible to write the joint probability mass function of the responses $y$ as $\prod_{i=1}^n \Phi((2y_i - 1)x_i;\beta) = \Phi_n(D\beta;I_n) = \Phi_n(s^{-1}D\beta;(ss^T)^{-1})$, with $D$ and $s$ defined as in Theorem 1. Combining this likelihood for $y$ with the Gaussian prior for $\beta$ provides

$$\pi(\beta \mid y, X) \propto \phi_p(\beta - \xi;\Omega)\Phi_n(s^{-1}D\beta;(ss^T)^{-1}) = \phi_p(\beta - \xi;\Omega)\Phi_n(s^{-1}D\xi + s^{-1}D(\beta - \xi);(ss^T)^{-1}).$$

To establish the relation among the above kernel and the unified skew-normal density in (3), note that $(\beta - \xi) = \omega\omega^{-1}\omega^{-1} - 1(\beta - \xi)$. Therefore, letting $\xi_{\text{post}} = \xi$, $\Omega_{\text{post}} = \Omega$, $\Delta_{\text{post}} = \omega\omega^{-1}\omega^{-1}$, $\gamma_{\text{post}} = s^{-1}D\xi$, and $\Gamma_{\text{post}} = (ss^T)^{-1} + \Delta_{\text{post}}^{1}\Gamma_{\text{post}}^{1}\Delta_{\text{post}}^{1} = s^{-1}D\omega^{-1}\omega^{-1}D\omega^{-1}Dss^{-1} = s^{-1}(D\omega\omega^{T} + I_n)s^{-1}$, provides the kernel of a unified skew-normal whose parameters coincide with those presented in Theorem 1.

To conclude the proof it is also necessary to guarantee that

$$\Omega_{\text{post}}^* = \begin{bmatrix} s^{-1}(D\omega\omega^{T} + I_n)s^{-1} & s^{-1}D\omega\omega^{-1} \\ \omega\omega^{-1}s^{-1}D\omega\omega^{-1} & \omega\omega^{-1} \end{bmatrix} = \begin{bmatrix} s^{-1} & 0 \\ 0 & \omega^{-1} \end{bmatrix} \times \begin{bmatrix} D\omega\omega^{T} + I_n & \omega\omega^{-1} \\ \omega\omega^{-1}D\omega\omega^{-1} & \omega\omega^{-1} \end{bmatrix} \times \begin{bmatrix} s^{-1} & 0 \\ 0 & \omega^{-1} \end{bmatrix}$$

is a full-rank correlation matrix. This last result can be easily proved by noticing that $\Omega_{\text{post}}^*$ coincides with the correlation matrix of the random vector $(z_1^*, z_2^*)^T$ where $z_1 = Dz_2 + \epsilon$ with $E(\epsilon) = 0_n$, $E(\epsilon^T) = I_n$, and $z_2$ is a $p$-variate random variable having zero mean and positive definite variance-covariance matrix $E(z_2^*z_2^*) = \Omega = \omega\omega$. Finally, $s = \text{diag}(\{d_1^2\Omega d_1 + 1\}^{1/2}, \ldots, (d_n^2\Omega d_n + 1)^{1/2})$ is the diagonal matrix with the square root of the diagonal elements of $E(z_2^*z_2^*) = D\omega\omega^{T} + I_n$. □

Proof of Corollary 1. The proof is a simple adaptation of equation (7.4) in Azzalini & Capitano (2013, §7.1.2) to the unified skew-normal posterior in Theorem 1. In particular, according to Azzalini & Capitano (2013, §7.1.2) the posterior in equation (2) has the same distribution of the random variable

$$\xi_{\text{post}} + \omega_{\text{post}}(V_0 + \Delta_{\text{post}}\Gamma_{\text{post}}^{-1}V_1)$$

with $V_0 \sim N_p(0_p, \Omega_{\text{post}} - \Delta_{\text{post}}\Gamma_{\text{post}}^{-1}\Delta_{\text{post}}^T)$ and $V_1$ from an $n$-variate truncated normal with mean $0_n$, covariance matrix $\Gamma_{\text{post}}$ and truncation below $\gamma_{\text{post}}$. Substituting the posterior parameters in this stochastic representation with their expressions in Theorem 1 concludes the proof. To clarify this final claim, note that $\Delta_{\text{post}}\Gamma_{\text{post}}^{-1}\Delta_{\text{post}}^T = \omega\omega^{-1}s^{-1}(D\omega\omega^{T} + I_n)^{-1}s = \omega\omega^{-1}s^{-1}(D\omega\omega^{T} + I_n)^{-1}s$ and that $\Delta_{\text{post}}\Gamma_{\text{post}}^{-1}\Delta_{\text{post}}^T$ coincides with the matrix $\omega\omega^{-1}s^{-1}(D\omega\omega^{T} + I_n)^{-1}s^{-1}D\omega\omega^{T} = \omega\omega^{-1}(D\omega\omega^{T} + I_n)^{-1}D\omega\omega^{T}$. □
Conjugate Bayes for probit regression via unified skew-normals

Proof of Corollary 2. Recalling the expression for $\pi(\beta \mid y, X)$ outlined in equation (3), the posterior predictive probability $\text{pr}(y_{\text{new}} = 1 \mid y, X, x_{\text{new}})$ can be expressed as

$$
\Phi_n\{s^{-1}D\xi; s^{-1}(D\Omega D^T + I_n)s^{-1}\}^{-1} \int \phi_p(\beta - \xi; \Omega) \Phi(x^T_{\text{new}}\beta) \Phi_n\{s^{-1}D\beta; (ss^T)^{-1}\} d\beta.
$$

Exploiting the proof of Theorem 1, the quantity inside the above integral can be re-expressed as $\phi_p(\beta - \xi; \Omega) \Phi(x^T_{\text{new}}\beta) \Phi_n\{s^{-1}D\beta; (ss^T)^{-1}\}$, with $D_{\text{new}}$ and $s_{\text{new}}$ defined as in Corollary 2. Comparing, now, this function with the density of the unified skew-normal posterior in (3) it can be immediately noticed that $\phi_p(\beta - \xi; \Omega) \Phi(x^T_{\text{new}}\beta) \Phi_n\{s^{-1}D\beta; (ss^T)^{-1}\}$ is the kernel of a unified skew-normal with normalizing constant $\int \phi_p(\beta - \xi; \Omega) \Phi(x^T_{\text{new}}\beta) \Phi_n\{s^{-1}D\beta; (ss^T)^{-1}\} d\beta = \Phi_n\{s^{-1}D_{\text{new}}\xi; s^{-1}_{\text{new}}(D_{\text{new}}D_{\text{new}}^T + I_{n+1})s^{-1}_{\text{new}}\}$. To conclude the proof, substitute this quantity in the above formula for the posterior predictive probability $\text{pr}(y_{\text{new}} = 1 \mid y, X, x_{\text{new}})$.

Proof of Corollary 3. To prove Corollary 3 simply notice that $\int \text{pr}(y \mid M_k, X, \beta_{\mathcal{J}_k}) \pi(\beta_{\mathcal{J}_k} \mid M_k) d\beta_{\mathcal{J}_k}$ is the normalizing constant of the posterior for $\beta_{\mathcal{J}_k}$ in model $M_k$. Hence, adapting equation (3) to model $M_k$, leads to $\text{pr}(y \mid M_k, X, \beta_{\mathcal{J}_k}) \pi(\beta_{\mathcal{J}_k} \mid M_k) d\beta_{\mathcal{J}_k} = \Phi_n\{s^{-1}_{\mathcal{J}_k}D\xi_k; s^{-1}_{\mathcal{J}_k}(D_k\Omega_k D_k^T + I_n)s^{-1}_{\mathcal{J}_k}\}$. □

Proof of Corollary 4. To prove Corollary 4 it suffices to generalize Theorem 1. In particular, adapting the proof of Theorem 1 to the case in which $\beta \sim \text{SUN}_{p,m}(\xi, \Omega, \Delta, \gamma, \Gamma)$, provides

$$
\pi(\beta \mid y, X) \propto \phi_p(\beta - \xi; \Omega) \Phi_n\{s^{-1}D\beta; (ss^T)^{-1}\} \Phi_m\{\gamma + \Delta^T\Omega^{-1}\omega^{-1}(\beta - \xi); \Gamma - \Delta^T\Omega^{-1}\Delta\}.
$$

To proceed with the proof, note that exploiting Theorem 1, it is possible to re-write $\Phi_n\{s^{-1}D\beta; (ss^T)^{-1}\}$ as $\Phi_n\{s^{-1}D\xi + (\Omega\omega D^T s^{-1})^T\Omega^{-1}\omega^{-1}(\beta - \xi); s^{-1}(D\Omega D^T + I_n)s^{-1} - s^{-1}D\omega\Omega^{-1}\Omega\omega D^T s^{-1}\}$. Consistent with this result, let us define the appropriate parameters for which the above kernel coincides with the one of the unified skew-normal posterior in Corollary 4. This goal is easily accomplished by setting $\xi_{\text{post}} = \xi, \Omega_{\text{post}} = \Omega, \Delta_{\text{post}} = (\Delta \Omega\omega D^T s^{-1})^T \gamma_{\text{post}} = (\gamma^T \Omega\omega D^T s^{-1})^T$ and $\Gamma_{\text{post}}$ a full-rank correlation matrix with blocks $\Gamma_{\text{post}[11]} = \Gamma, \Gamma_{\text{post}[22]} = s^{-1}(D\Omega D^T + I_n)s^{-1}, \Gamma_{\text{post}[21]} = \Gamma_{\text{post}[12]} = s^{-1}D\omega\Delta$. As in Theorem 1, it is also necessary to ensure that

$$
\begin{bmatrix}
\Gamma & \Delta^T \\
\Delta & \Omega\omega D^T s^{-1}
\end{bmatrix}
\begin{bmatrix}
\Delta^T \\
\Omega\omega D^T s^{-1}
\end{bmatrix} = \Gamma \\
\Delta
\begin{bmatrix}
\Omega\omega D^T s^{-1} & -1 \\
-1 & (D\Omega D^T + I_n)s^{-1} - s^{-1}D\omega\Omega
\end{bmatrix}.
$$

is a full-rank correlation matrix. This result follows under minor modifications of the proof in Theorem 1, after noticing that by definition the $(m + p) \times (m + p)$ unified skew-normal prior matrix $\Omega^*$ having block entries $\Omega^*_{[11]} = \Gamma, \Omega^*_{[22]} = \Omega = \omega^{-1}\Omega\omega^{-1}, \Omega^*_{[21]} = \Omega^*_{[12]} = \Delta$, is a full-rank correlation matrix. □

References

Agresti, A. (2013). Categorical Data Analysis (Third Edition). Wiley.

Albert, J. H. & Chib, S. (1993). Bayesian analysis of binary and polychotomous response data. J. Am. Statist. Assoc. 88, 669–679.

Arellano-Valle, R. B. & Azzalini, A. (2006). On the unification of families of skew-normal distributions. Scand. J. Statist. 33, 561–574.

Arnold, B. C. & Beaver, R. J. (2000). Hidden truncation models. Sankhya 62, 23–35.

Arnold, B. C., Beaver, R. J., Azzalini, A., Balakrishnan, N., Bhaumik, A., Dey, D., Cuadras, C. & Sarabia, J. M. (2002). Skewed multivariate models related to hidden truncation and/or selective reporting. Test 11, 7–54.

Azzalini, A. (1985). A class of distributions which includes the normal ones. Scand. J. Statist. 12, 171–178.

Azzalini, A. & Bacci, M. & Marrel, A. & Del Castillo, E. (2010). A prospective combination of phase II and phase III in drug development. Metron 68, 347–369.

Azzalini, A. & Capitanio, A. (1999). Statistical applications of the multivariate skew normal distribution. J. R. Statist. Soc. B. 61, 579–602.

Azzalini, A. & Capitanio, A. (2013). The Skew-normal and Related Families. Cambridge University Press.

Azzalini, A. & Dallal, V. A. (1996). The multivariate skew-normal distribution. Biometrika 83, 715–726.

Bazán, J. L., Branco, M. D. & Bolfarine, H. (2006). A skew item response model. Bayesian Anal. 1, 861–892.
BOTEV, Z. (2017). The normal law under linear restrictions: simulation and estimation via minimax tilting. *J. R. Statist. Soc. B.* **79**, 125–148.

CHIPMAN, H., GEORGE, E. I., MCCulloch, R. E., CLYDE, M., FOSTER, D. P. & STINE, R. A. (2001). The practical implementation of Bayesian model selection. In *Model Selection*. Lecture Notes-Monograph Series, vol. 38. Hayward, CA: Inst. Math. Statist, pp. 65–116.

CHIPMAN, H. A., GEORGE, E. I. & MCCulloch, R. E. (2010). BART: Bayesian additive regression trees. *Ann. Appl. Statist.* **4**, 266–298.

CHOPIN, N. (2011). Fast simulation of truncated Gaussian distributions. *Statist. Comp.* **21**, 275–288.

CHOPIN, N. & RIDGWAY, J. (2017). Leave Pima indians alone: Binary regression as a benchmark for Bayesian computation. *Statist. Sci.* **32**, 64–87.

EFRON, B. & TIBSHIRANI, R. J. (1994). *An Introduction to the Bootstrap*. CRC press.

FORT, A., GARCIA-DONATO, G. & STEEL, M. (2018). Methods and tools for Bayesian variable selection and model averaging in normal linear regression. *Int. Statist. Rev.* **86**, 237–258.

FRÜHWIRTH-SCHNATTER, S. & FRÜHWIRTH, R. (2007). Auxiliary mixture sampling with applications to logistic models. *Comp. Statist. Data Anal.* **51**, 3509–3528.

GELMAN, A., JAKULIN, A., PITTAU, M. G. & SU, Y.-S. (2008). A weakly informative default prior distribution for logistic and other regression models. *Ann. Appl. Statist.* **2**, 1360–1383.

GENTON, M. G., KEYES, D. E. & TURKIYYAH, G. (2018). Hierarchical decompositions for the computation of high-dimensional multivariate normal probabilities. *J. Comp. Graph. Statist.* **27**, 268–277.

GENZ, A. (1992). Numerical computation of multivariate normal probabilities. *J. Comp. Graph. Statist.* **1**, 141–149.

GENZ, A. & BRETZ, F. (2009). *Computation of Multivariate Normal and t Probabilities*. Springer.

GONZÁLEZ-FARIAS, G., DOMÍNGUEZ-MOLINA, A. & GUPTA, A. K. (2004). Additive properties of skew normal random vectors. *J. Statist. Plan. Infer.* **126**, 521–534.

GUPTA, A. K., AZIZ, M. A. & NING, W. (2013). On some properties of the unified skew-normal distribution. *J. Statist. Theory Pract.* **7**, 480–495.

GUPTA, A. K., GONZÁLEZ-FARIAS, G. & DOMÍNGUEZ-MOLINA, J. A. (2004). A multivariate skew normal distribution. *J. Mult. Anal.* **89**, 181–190.

HAARIO, H., SAKSMAN, E. & TAMMINEN, J. (2001). An adaptive Metropolis algorithm. *Bernoulli* **7**, 223–242.

HOETING, J. A., MADIGAN, D., RAFTERY, A. E. & VOLINSKY, C. T. (1999). Bayesian model averaging: A tutorial. *Statist. Sci.* **14**, 382–401.

HOFFMAN, M. D. & GELMAN, A. (2014). The No-U-turn sampler: Adaptively setting path lengths in Hamiltonian Monte Carlo. *J. Mach. Learn. Res.* **15**, 1593–1623.

HOLMES, C. C. & HELD, L. (2006). Bayesian auxiliary variable models for binary and multinomial regression. *Bayesian Anal.* **1**, 145–168.

HORRACE, W. C. (2005). Some results on the multivariate truncated normal distribution. *J. Mult. Anal.* **94**, 209–221.

JOHNDROW, J. E., SMITH, A., PILLAI, N. & DUNSON, D. B. (2018). MCMC for imbalanced categorical data. *J. Am. Statist. Assoc.* , in press.

KASS, R. E. & RAFTERY, A. E. (1995). Bayes factors. *J. Am. Statist. Assoc.* **90**, 773–795.

KUSS, M. & RASMUSSEN, C. E. (2005). Assessing approximate inference for binary Gaussian process classification. *J. Mach. Learn. Res.* **6**, 1679–1704.

MARTINEZ, R., CHRISTEN, R., PASQUIER, C. & PASQUIER, N. (2005). Exploratory analysis of cancer SAGE data. In *Proceedings of the ECML–PKDD Discovery Challenge Workshop*, pp. 72–77.

MARUYAMA, Y. & GEORGE, E. (2011). Fully Bayes factors with a generalized g-prior. *Ann. Statist.* **39**, 2740–2765.

O’HARA, R. B. & SILLANPÄÄ, M. J. (2009). A review of Bayesian variable selection methods: What, how and which. *Bayesian Anal.* **4**, 85–117.

POLSON, N. G., SCOTT, J. G. & WINDLE, J. (2013). Bayesian inference for logistic models using Pólya–Gamma latent variables. *J. Am. Statist. Assoc.* **108**, 1339–1349.

QUARTERONI, A., SACCO, R. & SALeri, F. (2010). *Numerical Mathematics (Second Edition)*. Springer.

RASMUSSEN, C. E. & WILLIAMS, C. K. I. (2006). *Gaussian Processes for Machine Learning*. MIT Press.

ROBERTS, G. O. & ROSENTHAL, J. S. (2001). Optimal scaling for various Metropolis-Hastings algorithms. *Statist. Sci.* **16**, 351–367.

ROBERTS, G. O. & SAHU, S. K. (1997). Updating schemes, correlation structure, blocking and parameterization for the Gibbs sampler. *J. R. Statist. Soc. B.* **59**, 291–317.

RODRIGUEZ, A. & DUNSON, D. B. (2011). Nonparametric Bayesian models through probit stick-breaking processes. *Bayesian Anal.* **6**, 145–178.

SPIEGELHALTER, D. J. & LAURITZEN, S. L. (1990). Sequential updating of conditional probabilities on directed graphical structures. *Networks* **20**, 579–605.

TZANIS, G. & VLAHAVAS, I. (2007). Accurate classification of SAGE data based on frequent patterns of gene expression. In *19th IEEE International Conference on Tools with Artificial Intelligence*. pp. 96–100.