Implicit copula variational inference

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Abstract

Key to effective generic, or “black-box”, variational inference is the selection of an approximation to the target density that balances accuracy and calibration speed. Copula models are promising options, but calibration of the approximation can be slow for some choices. Smith et al. (2020) suggest using “implicit copula” models that are formed by element-wise transformation of the target parameters. We show here why these are a tractable and scalable choice, and propose adjustments to increase their accuracy. We also show how a sub-class of elliptical copulas have a generative representation that allows easy application of the re-parameterization trick and efficient first order optimization methods. We demonstrate the estimation methodology using two statistical models as examples. The first is a mixed effects logistic regression, and the second is a regularized correlation matrix. For the latter, standard Markov chain Monte Carlo estimation methods can be slow or difficult to implement, yet our proposed variational approach provides an effective and scalable estimator. We illustrate by estimating a regularized Gaussian copula model for income inequality in U.S. states between 1917 and 2018.

Keywords: Elliptical copula; Factor approximation; Re-parameterization trick; Spherical coordinates; Stochastic gradient ascent; Variational Bayes.
1 Introduction

Variational inference (VI) methods are increasingly used for the Bayesian estimation of big or complex statistical models (Blei et al., 2017). They require the selection of a variational approximation (VA) to the posterior distribution and an optimization approach for its calibration. Recent focus is on so-called “black box” VI methods (Ranganath et al., 2014) that combine generic VAs and optimization methods that require little or no tailoring to the statistical model being estimated.

One promising black box approach is “copula VI” (Tran et al., 2015, Han et al., 2016, Smith et al., 2020, Gunawan et al., 2021), where copula models are used as generic VAs. Copula models are multivariate distributions constructed from marginals and a copula function; see Nelsen (2006) and Joe (2014) for introductions. However, for many choices of copula function and/or marginals, the resulting copula VAs can be computationally expensive to calibrate. To address this problem, Smith et al. (2020) show that “implicit copula” models can be flexible, scalable and fast to calibrate.

The objective of this paper is to refine, extend and demonstrate the efficacy of this approach.

An implicit copula is constructed from a known continuous multivariate distribution \( \psi \sim F \) by inverting Sklar’s theorem; e.g. see Nelsen (2006, Sec. 3.1). An attractive feature for VI is that implicit copula models can be represented as a one-to-one element-wise transformation between \( \psi \) and the target parameter \( \theta \). Smith et al. (2020) show that selecting tractable parametric forms for this transformation and the distributional family of \( F \), allows ready application of the “re-parameterization trick” (Salimans et al., 2013, Kingma and Welling, 2014, Rezende et al., 2014, Titsias and Lázaro-Gredilla, 2014). This then facilitates efficient implementation of stochastic gradient optimization algorithms for calibration of the resulting implicit copula VA. We extend this idea here in three ways. First, the transformations suggested by these authors are shown to produce VAs that have a level of accuracy that varies with the location and scale of \( \theta \), which is a poor property. An adjustment to the transformations are proposed to correct for this. Second, for \( F \) we consider the sub-class of elliptical distributions that can be expressed as a scale mixture

\footnote{These are the statistical model parameters (or a transformation of them) which are also often called “latent variables” in the machine learning literature.}
of normals (Kano, 1994). These have a generative representation that is amenable to the re-parameterization trick. The resulting implicit copulas are a sub-class of elliptical copulas studied by Fang et al. (2002). Third, we follow Miller et al. (2017), Ong et al. (2018), Mishkin et al. (2018) and others by adopting a sparse factor (also called a “low rank plus diagonal”) decomposition for the positive definite scale matrix \( \Sigma \) of distribution \( F \). However, to identify the elliptical copula \( \Sigma \) should have a leading diagonal of ones, and we show how to use spherical co-ordinates to impose this bound efficiently. The end result is a class of black-box elliptical copula VAs that is scalable and fast to calibrate.

Other copula VI methods include that suggested by Tran et al. (2015) who use vine copulas. Calibration in high dimensions is typically slow because in general vine copulas lack the computationally advantageous transformation representation of implicit copulas. Chi et al. (2021) suggest speeding up Monte Carlo gradient estimates in vine copula VI using draws under a mean field simplification. However, such estimates are still typically more noisy than those computed using an effective re-parameterization gradient. The simplest implicit copula is the Gaussian copula, which was first employed as a VA by Han et al. (2016). Smith et al. (2020) extend this to the skew-normal copula and exploit sparse factorizations of the form in Ong et al. (2018) for the scale matrix and the re-parameterization trick. Gunawan et al. (2021) generalize the VI method of Smith et al. (2020) to a copula formed from a mixture of normals. Each mixture component is calibrated sequentially using a variational boosting algorithm, although the re-parameterization gradients can remain noisy in this case (Miller et al., 2017) and more computationally demanding estimates are necessary. The transformations suggested in our paper can also be used to make the VA of Gunawan et al. (2021) invariant to changes in the location and scale of \( \theta \).

To illustrate the implicit copula VI approach we use it to estimate a correlation matrix \( \Omega \) which is neither sparse nor patterned. In this circumstance, it is well known that regularization can increase estimation accuracy (Rothman et al., 2008). Following Rebonato and Jäckel (1999), Creal and Tsay (2015) and others, we re-parameterize \( \Omega = LL^T \) using spherical co-ordinates for the Cholesky factor \( L \). We then then use a horseshoe prior (Carvalho et al., 2010) for a monotonic
transformation of these angles that corresponds to adaptive shrinkage of partial correlations towards zero. Estimation of the joint posterior of $\Omega$ and the shrinkage hyper-parameters using standard MCMC methods can be prohibitively slow. However, implicit copula VI can be employed to successfully estimate $\Omega$ in higher dimensions than MCMC. We show how to do so for a regularized Gaussian copula correlation matrix for annual income inequality in 49 U.S. states between 1917 and 2018. A rich pattern of interstate dependence that mirrors geographical and socio-economic commonalities between states is observed. A t-copula VA is shown to capture the posterior more accurately than either a t-distribution or mean field approximations.

The rest of the paper is organized as follows. Section 2 gives a brief introduction to copula VI, with a focus on implicit copula VI in Section 2.3. Section 3 details our extension and refinement of the methodology of Smith et al. (2020), along with empirical illustration of the improvements that can result. Section 4 demonstrates the efficacy of the copula VI approach when estimating the regularized Gaussian copula correlation matrix, while Section 5 concludes. Appendix A contains the closed form gradients required to implement the method, and additional details for the example in Section 4 are given in an Online Appendix.

2 Copula variational inference

2.1 Variational inference

Consider a statistical model with continuous parameters $\theta = (\theta_1, \ldots, \theta_m)^\top$, data $y$, and Bayesian posterior density $p(\theta|y) \propto p(y|\theta)p(\theta) = g(\theta)$. Variational inference approximates $p(\theta|y)$ with a density $q(\theta)$ that is called a “variational approximation” (VA). The approximation is obtained by minimizing a divergence measure between $q$ and the posterior, with the Kullback-Leibler (KL) divergence the most common choice. In this case, the optimal approximating density in a family $\mathcal{F}$ is

$$ q^* = \arg\min_{q \in \mathcal{F}} \left\{ \int \frac{q(\theta)}{p(\theta|y)} q(\theta) d\theta \right\}. $$
It is straightforward to show (e.g. Ormerod and Wand (2010)) that

\[ q^* = \arg\max_{q \in \mathcal{F}} L(q), \]

where \( L(q) = \int \log \frac{g(\theta)}{q(\theta)} q(\theta) d\theta = E_q [\log g(\theta) - \log q(\theta)] \) is the evidence lower bound (ELBO) function; see Ormerod and Wand (2010) and Blei et al. (2017) for overviews of variational inference.

In many applications, the variational family \( \mathcal{F} \) is specific to the statistical model being estimated. However, generic fixed form approximations that can be employed to estimate a wide range of statistical models are also used. These have densities \( q_\lambda(\theta) \) with variational parameters \( \lambda \) that fully specify the density, so that \( q^*(\theta) = q^*_\lambda(\theta) \) with \( \lambda^* = \arg\max_\lambda L(q_\lambda) \). When combined with generic optimization algorithms, the resulting approaches are often called “black box” VI (Ranganath et al., 2014).

The most common optimization approaches used are stochastic gradient ascent (SGA) methods (Bottou, 2010). In SGA, given an initial value \( \lambda^{(0)} \), the variational parameters are updated recursively as

\[ \lambda^{(s+1)} = \lambda^{(s)} + \delta^{(s)} \circ \nabla_\lambda \widehat{L}(q_\lambda), \quad s = 0, 1, 2, \ldots. \]

Here, \( \delta^{(s)} \) is a vector of adaptive step sizes determined using an algorithm such as ADADELTA (Zeiler, 2012), the operator “\( \circ \)” is the element-wise product, and \( \nabla_\lambda \widehat{L}(q_\lambda) \) is an unbiased estimator of the gradient evaluated at \( \lambda = \lambda^{(s)} \).

A low variance gradient estimator is the main requirement of effective SGA methods, and using the “re-parameterization trick” (Salimans et al., 2013, Kingma and Welling, 2014, Rezende et al., 2014, Titsias and Lázaro-Gredilla, 2014) is a particularly effective means of obtaining one. Here, the model parameters are re-parameterized as \( \theta = h(\varepsilon, \lambda) \sim q_\lambda \), where \( h \) is a deterministic function and \( \varepsilon \) is distributed with density \( f_\varepsilon \) that is invariant to \( \lambda \). Then the ELBO is \( L(q_\lambda) = E_{f_\varepsilon} [\log g(h(\varepsilon, \lambda)) - \log q_\lambda(h(\varepsilon, \lambda))] \) and its gradient is

\[
\nabla_\lambda L(q_\lambda) = E_{f_\varepsilon} \left[ \nabla_\lambda \log g(h(\varepsilon, \lambda)) - \nabla_\lambda \log q_\lambda(h(\varepsilon, \lambda)) \right]
\]

\[
= E_{f_\varepsilon} \left[ \frac{dh(\varepsilon, \lambda)}{d\lambda} \top \left( \nabla_\theta \log g(\theta) - \nabla_\theta \log q_\lambda(\theta) \right) \right].
\]

(1)
Equation (1) is widely called a “re-parameterization gradient” and a low variance unbiased estimate of it is obtained by generating draws $\varepsilon \sim f_{\varepsilon}$, computing $\theta = h(\varepsilon, \lambda)$ and then evaluating the terms in the parentheses at these values. It is often the case that only a single draw of $\varepsilon$ is sufficient to produce a low noise gradient estimator.

Thus, to use SGA with the re-parameterization trick requires selecting a VA with density $q_{\lambda}$ that admits a re-parameterization $\{f_{\varepsilon}, h\}$ from which it is both fast to generate and for which the two derivatives $\frac{dh(\varepsilon, \lambda)}{d\lambda}$, and $\nabla_{\theta} \log q_{\lambda}(\theta)$ are fast to compute. The latter typically requires closed form expressions.

### 2.2 Copula model variational approximations

Copula models are scalable and tractable representations of multivariate distributions (Nelsen, 2006, Joe, 2014), and have been explored previously as VAs by Han et al. (2016), Tran et al. (2015), Smith et al. (2020), Gunawan et al. (2021) and Chi et al. (2021). A copula model VA has density

$$q_{\lambda}(\theta) = c(u|\tilde{\pi}) \prod_{i=1}^{m} q_{\lambda_i}(\theta_i),$$

where $u = (u_1, \ldots, u_m)^T$, $q_{\lambda_i}(\theta_i)$ is the marginal density of $\theta_i$ that is selected arbitrarily, and $u_i = Q_{\lambda_i}(\theta_i) = \int_{-\infty}^{\theta_i} q_{\lambda_i}(s)ds$. The function $c(u|\tilde{\pi})$ is called the “copula density” and is a well-defined density function on the unit cube $[0,1]^m$ with uniform marginals and parameters $\tilde{\pi}$. Typically, the copula is selected from a list, with vine (Czado, 2019) or elliptical (Fang et al., 2002) copulas the most popular in high dimensions. Thus, a copula model VA is usually specified by choices for $q_{\lambda_1}, \ldots, q_{\lambda_m}$ and $c(\cdot|\tilde{\pi})$, with variational parameters $\{\tilde{\pi}, \lambda_1, \ldots, \lambda_m\}$.

However, two problems can arise when using copula models as high-dimensional VAs. First, an efficient re-parameterization $\{f_{\varepsilon}, h\}$ may be difficult to identify. Second, the derivative $\nabla_{\theta} \log q_{\lambda}(\theta)$ is required to evaluate the re-parameterization gradient at (1). By application of the chain rule, this is

$$\nabla_{\theta} \log q_{\lambda}(\theta) = \left( \frac{\partial u}{\partial \theta} \right)^T \left( \frac{\partial}{\partial u} \log c(u|\tilde{\pi}) \right)^T + \left( \nabla_{\theta_1} \log q_{\lambda_1}(\theta_1), \ldots, \nabla_{\theta_m} \log q_{\lambda_m}(\theta_m) \right)^T,$$
where we write gradients as column vectors throughout the paper. Here, the terms $\frac{\partial}{\partial \theta}$ and $\frac{\partial}{\partial u} \log c(u|\pi)$ may be prohibitively slow to compute; for example, Chi et al. (2021) note this problem for a vine copula. However, “implicit copulas” defined through transformation are one class of copulas that can avoid both problems, as now discussed.

### 2.3 Implicit copula model variational approximations

**Implicit copula definition**

Consider a continuous random vector $\psi = (\psi_1, \ldots, \psi_m)^T$ with known parametric distribution $F(\psi; \pi)$, marginals $F_1(\psi_1; \pi_1), \ldots, F_m(\psi_m; \pi_m)$, and parameters $\pi = \bigcup_{i=1}^m \pi_i$. Then the copula of this distribution is unique and has density

$$c(u; \pi) = \frac{p(\psi; \pi)}{\prod_{i=1}^m p_i(\psi_i; \pi_i)},$$

(3)

where $p(\psi; \pi) = \frac{\partial}{\partial \psi} F(\psi; \pi)$, $p_i(\psi_i; \pi_i) = \frac{d}{d\psi_i} F_i(\psi_i; \pi_i)$, and $\psi_i = F_i^{-1}(u_i; \pi_i)$. The copula parameters $\pi$ are constrained to ensure they are identified in the copula density at (3), which is called an implicit copula. Different choices for $F(\psi; \pi)$ produce different copula families. These include Gaussian copulas, t copulas, elliptical copulas, skew t copulas, factor copulas and copula processes; Smith (2021) provides an overview of the broad class of implicit copulas.

**Transformation representation**

An implicit copula can also be defined through the element-wise transformations

$$\psi_i = F_i^{-1}(Q_{\lambda_i}(\theta_i); \pi_i) \equiv k_i(\theta_i), \text{ for } i = 1, \ldots, m.$$

These functions are strictly increasing functions because the distribution functions $F_i$ and $Q_{\lambda_i}$ are also. If $k'_i(\theta_i) = \frac{d}{d\theta_i} k_i(\theta_i)$, then by a change of variables the marginal density of the VA is simply

$$q_{\lambda_i}(\theta_i) = p_i(\psi_i; \pi_i) k'_i(\theta_i).$$

(4)
Thus, from (2)–(4) the joint density of the implicit copula model VA is

\[
q_{\lambda}(\theta) = c(u|\pi) \prod_{i=1}^{m} q_{\lambda_i}(\theta_i) = \frac{p(\psi; \pi)}{\prod_{i=1}^{m} p_i(\psi_i; \pi_i)} \prod_{i=1}^{m} p_i(\psi_i; \pi_i) k'_i(\theta_i) = p(\psi; \pi) \prod_{i=1}^{m} k'_i(\theta_i) .
\]

(5)

Computing the re-parameterization gradient using the expression at (5) can be much simpler than that at (2) because it avoids evaluation of the terms \(\frac{\partial u}{\partial \theta}\) and \(\frac{\partial}{\partial u} \log c(u|\pi)\). To see this, if \(k''_i(\theta_i) = \frac{d^2}{d\theta^2} k_i(\theta)\), then the derivative

\[
\nabla_{\theta} \log q_{\lambda}(\theta) = \left( \frac{\partial}{\partial \psi} \log p(\psi; \pi) \right)^\top + \left( k''_1(\theta_1) \cdots k''_m(\theta_m) \right)^\top ,
\]

(6)

where \(\frac{\partial \psi}{\partial \theta} = \text{diag}(k'_1(\theta_1), \ldots, k'_m(\theta_m))\) is a diagonal matrix. This expression, and thus the re-parameterization gradient, is fast to compute whenever \(k'_i, k''_i\) and \(\frac{\partial}{\partial \psi} \log p(\psi; \pi)\) are also.

A copula model is usually defined from (2) by selecting the marginals \(q_{\lambda_1}, \ldots, q_{\lambda_m}\) and copula \(c\). However, the transformation representation motivates another way to define an implicit copula model by selecting \(k_1, \ldots, k_m\) and \(p(\psi; \pi)\) instead. These can be chosen so that (6) and the re-parameterization gradient at (1) are fast to compute in high dimensions. In particular, picking each transformation \(k_i\) directly avoids the need to evaluate either \(F_i\) or \(Q_{\lambda_i}\), which can be slow or difficult. In principle, any tractable distribution can be adopted for \(\psi\), with Smith (2021) outlining a wide range of choices and their respective implicit copulas. In the next section we detail how to implement variational inference with a sub-class of elliptical copulas, but discuss the potential of other choices in Section 5.

3 Learnable elliptical copula VA

3.1 Definition

In this paper, for each \(k_i\) we select a parametric monotonically increasing function denoted as \(k_{\tilde{\gamma}_i}\) with parameter vector \(\tilde{\gamma}_i\), so that \(\lambda = \{\pi, \tilde{\gamma}_1, \ldots, \tilde{\gamma}_m\}\). Smith et al. (2020) suggest using the Yeo-Johnson (YJ) and the inverse G-and-H (iGH) transformations for \(k_{\tilde{\gamma}_i}\), because they are popular
in data analysis as transformations from asymmetric to symmetric distributions. (The G-and-H transformation is from symmetry, which is why its inverse is used.) However, both transformations produce marginals \( q_\lambda_i(\theta_i) \) that are not invariant to changes in location and scale, as demonstrated in Section 3.4. We therefore introduce location and scale parameters \( \mu_i \) and \( \sigma_i \) directly for \( \theta_i \), so that

\[
\psi_i = k_{\tilde{\gamma}_i}(\theta_i) = t_{\gamma_i} \left( \frac{\theta_i - \mu_i}{\sigma_i} \right),
\]

(7)

where \( t_{\gamma_i} \) is either the YJ or iGH transformation, or compositions of the two. The transformation \( k_{\tilde{\gamma}_i} \) has parameters \( \tilde{\gamma}_i = (\gamma_i^\top, \mu_i, \sigma_i)^\top \) and is fast to implement within SGA methods.

An elliptical distribution is employed for \( \psi \), in which case (3) is the density of an elliptical copula studied by Fang et al. (2002). We consider the sub-class of elliptical distributions that can be written as scale mixture of normals with stochastic representation

\[
\psi = \sqrt{W} X,
\]

(8)

where \( X \sim N_m(0, \Sigma) \) and \( W \sim F_W(\cdot; \omega) \) are distributed independently. This provides a generative representation for implementing the SGA algorithm with the re-parameterization trick efficiently as discussed in Section 3.3. The density of an elliptical distribution with location zero and scale matrix \( \Sigma \) is

\[
p(\psi; \pi) = |\Sigma|^{-1/2} \tilde{g}_{m, \omega} \left( \psi^\top \Sigma^{-1} \psi \right),
\]

where \( \tilde{g}_{m, \omega}(x) = K_{m, \omega} g_\omega(x) \), the function \( g_\omega : [0, \infty) \rightarrow (0, \infty) \) with parameters \( \omega, \pi = (\omega^\top, \text{vech}(\Sigma)^\top)^\top \), and \( K_{m, \omega} = \Gamma(m) / (\pi^m \int_0^\infty t^{m-1} g_\omega(t) dt) \) is a constant. We set the location to zero and \( \Sigma \) to be a correlation matrix to identify their values, which is necessary because \( \mu_i, \sigma_i \) are introduced in the transformation at (7).

While all elliptical distributions are closed under marginalization (i.e. the marginal of an elliptical distribution is also an elliptical distribution), only a sub-class have marginals of the same parametric family, which is a property called “consistency” by Kano (1994). This author shows that elliptical distributions with the stochastic representation at (8) are consistent whenever the
distribution of $W$ is not a function of $m$. In this case the marginal has density $p_i(\psi_i | \pi_i) = \tilde{g}_{1,\omega}(\psi_i^2)$ with $\pi_i = \omega$, which can be used to define the implicit copula density at (3). Inconsistent elliptical distributions can also be used in our framework, but $\psi_i = \sqrt{WX_i}$ has density of a different parametric form.

Table 1 gives four elliptical distributions that are scale mixtures of normals. They are the consistent Gaussian, t and Laplace distributions, and the inconsistent exponential power distribution. For each, the function $\tilde{g}_{m,\omega}$, its derivative, $\omega$ and the distribution of $W$ are given. These are necessary to implement variational inference using their implicit copula models as VAs.

From (3) our proposed learnable VA has density

$$q_{\Lambda}(\theta) = |\Sigma|^{-1/2}g_{m,\omega}(\psi^T \Sigma^{-1} \psi) \prod_{i=1}^{m} \psi_i^T \left( \frac{\theta_i - \mu_i}{\sigma_i} \right) \frac{1}{\sigma_i},$$

with marginal

$$q_{\Lambda}(\theta_i) = p_i(\psi_i; \pi_i) \psi_i^T \left( \frac{\theta_i - \mu_i}{\sigma_i} \right) \frac{1}{\sigma_i},$$

where $p_i(\psi_i; \pi_i) = \tilde{g}_{1,\omega}(\psi_i^2)$ if the distribution for $\psi$ is consistent. Notice that by introducing $\mu_i$ and $\sigma_i$, the marginal density for $\theta_i$ is flexible in terms of its location and scale. In contrast, Smith et al. (2020) and Gunawan et al. (2021) instead include a location and scale for $\psi_i$ (and not for $\theta_i$) which restricts the flexibility of the marginal approximation as illustrated in Section 3.4 below.

### 3.2 Factor correlation matrix

If $\Sigma$ is unrestricted, then the number of elements increases quadratically with $m$, prohibiting usage of the VA in high dimensions. A popular solution for Gaussian VAs is to adopt a factor decomposition (also called a “low rank plus diagonal” decomposition in the machine learning literature) see Miller et al. (2017), Ong et al. (2018), Mishkin et al. (2018) and Zhou et al. (2021) for recent examples. We follow this approach for the elliptical copula and set $\Sigma = BB^T + D^2$, where $B = \{b_{i,j}\}$ is an $(m \times K)$ factor loading matrix, $D = \text{diag}(d)$ and $d = (d_1, \ldots, d_m)^T$. To aid identification we set the upper triangle of $B$ to zeros, and bound $d$ and the leading edge of $B$ to be positive. Alternative identifying restrictions may also be used as discussed in Zhou et al. (2021) for Gaussian VAs. However, unlike
Table 1: Four Elliptical Distributions with Scale Mixture of Normals Generative Representations

| Distribution          | $\tilde{g}_{m,\omega}(x)$ | $\tilde{g}_{m,\omega}'(x)$ | $\omega$ | $W$ Distribution or Density |
|-----------------------|-----------------------------|----------------------------|----------|-----------------------------|
| Gaussian              | $(2\pi)^{-m/2} \exp\left(-\frac{x^2}{2}\right)$ | $-\frac{1}{2}\tilde{g}_{m,\omega}(x)$ | $\emptyset$ | Point Mass at 1             |
| $\psi \sim N_m(0, \Sigma)$ |                             |                             |          |                             |
| Symmetric Laplace     | $\frac{2}{(2\pi)^{m/2}} \left(\frac{x}{2}\right)^{\nu/2} K_\nu(\sqrt{2x})$ | $c_1 \left[\left(\frac{x}{2}\right)^{\nu/2} K_\nu'(\sqrt{2x}) + \frac{c_1}{2} \left(\frac{x}{2}\right)^{\nu/2} K_\nu(\sqrt{2x})\right]$ | $\emptyset$ | $W \sim \text{Exp}(1)$ |
| $\psi \sim SL_m(0, \Sigma)$ |                             |                             |          |                             |
| Multivariate t        | $\frac{\Gamma\left(\frac{\nu+m}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right) \left(\pi \nu\right)^{m/2}} \frac{-(\nu+m)}{2\nu} \left(1 + \frac{x^2}{\nu}\right)^{-\frac{\nu+m}{2}} \tilde{g}_{m,\omega}(x)$ | $\nu > 0$ | $W \sim \nu/\chi^2(\nu)$ |
| $\psi \sim t_m(0, \Sigma, \nu)$ |                             |                             |          |                             |
| Exponential Power     | $\frac{m\Gamma\left(\frac{m}{2}\right)}{\Gamma\left(\frac{m}{1+2\beta}\right) x^{\frac{m}{2}+\frac{m}{2}}} \exp\left(-\frac{1}{2}x^\beta\right) - \frac{\beta}{2} x^\beta \tilde{g}_{m,\omega}(x)$ | $0 < \beta \leq 1$ | $f_W(w) = \frac{2^{1+\frac{m}{2}} \pi^m \Gamma\left(1+\frac{m}{2}\right)}{\Gamma\left(1+\frac{m}{2}\beta\right)} \times w^{m-3} f_{S,\beta}(w^{-2}; 2^{1-\beta})$ |
| $\psi \sim EP_m(0, \Sigma, \beta)$ |                             |                             |          |                             |

The distributions have density $p(\psi; \pi) = |\Sigma|^{-1/2} \tilde{g}_{m,\omega}(\psi^T \Sigma^{-1} \psi)$, where dim($\psi$) = $m$ and $\pi = (\text{vech}(\Sigma)^T, \omega^T)^T$, and stochastic representation as a scale mixture of normals. In the table, $K_\nu$ denotes the modified Bessel function of the third kind, $\Gamma$ the gamma function, $\text{Exp}(1)$ an exponential distribution with parameter 1, $\chi^2(\nu)$ a chi-squared distribution with parameter $\nu$, $f_{S,\alpha}(\cdot; \sigma)$ is the density of the positive stable distribution, and the constant $c_1 = \frac{2}{(2\pi)^{m/2}}$. For details on the Symmetric Laplace distribution see [Kotz et al. (2001), Ch.5] and on the Exponential Power distribution see [Gómez-Sánchez-Manzano et al. (2008)].
in Smith et al. (2020), a complicating factor is that the positive definite matrix $\Sigma$ has a leading diagonal of ones, so the constraints $d_j^2 + \sum_{k=1}^{K} b_{j,k}^2 = 1$, for $j = 1, \ldots, m$ hold. A popular way of imposing such a constraint is to employ spherical co-ordinates; e.g. see Rebonato and Jäckel (1999) and Creal and Tsay (2015). Here, this is equivalent to restricting $a_j = (a_{j,1}, \ldots, a_{j,K+1})^\top = (d_j, b_{j,1}, \ldots, b_{j,K})^\top$ to lie on the surface of the $(K+1)$-dimensional spherical space $S^n = \{a_j : \sum_{k=1}^{K+1} a_{j,k}^2 = 1\}$. We impose this spherical restriction by writing $a_j$ in terms of the angles $\kappa_j = (\kappa_{j,1}, \ldots, \kappa_{j,K})^\top$, such that

$$a_{j,k} = \begin{cases} 
\cos \kappa_{j,1} & \text{for } k = 1, \\
\cos \kappa_{j,k} \prod_{i=1}^{k-1} \sin \kappa_{j,i} & \text{for } 1 < k < K+1, \\
\prod_{i=1}^{k-1} \sin \kappa_{j,i} & \text{for } k = K+1,
\end{cases} \tag{11}$$

where $\kappa_{j,k} \in (0, \pi)$ if $k < K$ and $\kappa_{j,K} \in (0, 2\pi)$. There is a one-to-one relationship between the angles and $(B, d)$.

One last complication is that our SGA optimization method is applicable to unconstrained variational parameters. To address this, the angles are expressed using a further monotonic transformation to the vectors $\tau_j = (\tau_{j,1}, \ldots, \tau_{j,K})^\top \in \mathbb{R}^K$, with elements $\tau_{j,k} = \Phi^{-1}_1(\kappa_{j,k}/\pi)$ for $k < K$ and $\tau_{j,K} = \Phi^{-1}_1(\kappa_{j,K}/2\pi)$. Finally, the complete variational parameter vector is $\lambda = (\mu^\top, \sigma^\top, \gamma^\top, \tau^\top, \omega^\top)^\top$, with $\mu = (\mu_1, \ldots, \mu_m)^\top$, $\tau = (\tau_1^\top, \ldots, \tau_m^\top)^\top$, $\sigma = (\sigma_1, \ldots, \sigma_m)^\top$, $\gamma = (\gamma_1^\top, \ldots, \gamma_m^\top)^\top$ and $\omega$ is dependent on the choice of elliptical distribution (which is simply $\omega = \emptyset$ for the Gaussian and Laplace distributions). Using this parameterization, the derivative of (6) is fast to compute; see Appendix A.

### 3.3 Re-parametrization trick

For our transformation-based implicit copula

$$\theta = h(\varepsilon, \lambda) = (\mu_1 + \sigma_1 t_{\gamma_1}^{-1}(\psi_1), \ldots, \mu_m + \sigma_m t_{\gamma_m}^{-1}(\psi_m))^\top. \tag{12}$$
To employ the re-parameterization trick, $p(\psi; \pi)$ must have a generative representation based on a random vector $\varepsilon$ that is unrelated to $\lambda$. The scale mixture of normals at (8) provides this representation, as detailed in Algorithm 1. In this algorithm, Step 2 is unnecessary for the Gaussian distribution for $\phi$, while for other elliptical distributions $F_W^{-1}$ can be evaluated either analytically or numerically. Because $W$ is a scalar, the computational burden of this step does not increase with the dimension $m$ of the target distribution. All other steps are computationally inexpensive.

Algorithm 1 (Generating $\theta$ from the elliptical copula VA)

1. Generate independently $z \sim N_m(0, I)$, $\varepsilon \sim N_m(0, I)$, $u \sim \text{Uniform}(0, 1)$ and set $\varepsilon = (z^\top, \varepsilon^\top, u)^\top$
2. Set $w = F_W^{-1}(u; \omega)$ where $F_W^{-1}$ is the quantile function of $W$
3. Set $\psi = \sqrt{w} (Bz + D\varepsilon)$
4. Set $\theta = h(\varepsilon, \lambda)$

3.4 Invariance of the marginal approximation

The marginal of the Gaussian copula VA in Smith et al. (2020) has density

$$q_{SLN2020}^{i}(\theta_i) = \frac{1}{\sigma_{\psi_i}} \phi \left( \frac{\psi_i - \mu_{\psi_i}}{\sigma_{\psi_i}} \right) t_{\gamma_i}(\theta_i),$$

where $\phi(x)$ is a $N(0,1)$ density. The accuracy of this approximation varies with the location and scale of $\theta_i$, which is a poor property for a VA. The same issue arises for other choices of $p(\psi; \pi)$, including elliptical or mixture distributions. In contrast, the marginal approximation at (10) is invariant to the location and scale of $\theta_i$ by definition.

To demonstrate the impact on approximation accuracy, we measure the ability of the marginal of the Gaussian copula VA in Smith et al. (2020) and that at (10) with $p_i(\psi_i; \pi_i) = \phi(\psi_i)$ to approximate the skew normal (SN) distribution of Azzalini and Dalla Valle (1996) for $\theta_i$. Both VAs are constructed using the YJ transformation for $t_{\gamma_i}$. The SN parameters are set so that the Pearson skew coefficient is 0.8553, but the mean $\mu_{SN}$ and standard deviation $\sigma_{SN}$ vary. Figure 1 plots the two optimal VAs (i.e. those with the minimum KL divergence) when (a) $\mu_{SN} = 15$, $\sigma_{SN} = 1$, and (b) $\mu_{SN} = 0$, $\sigma_{SN} = 1$. Simply changing the location $\mu_{SN}$ of the target distribution increases the KL divergence from 0.013 to 0.105 for $q_{SLN2020}^{i}$, but does not affect the accuracy of the approximation.
3.5 Example: mixed logistic regression

To illustrate the improvement that adopting the VA at (9) can provide, we use it to re-estimate the mixed logistic regression example outlined in Smith et al. (2020). This uses a polypharmacy longitudinal dataset on 500 subjects over 7 years. There are 8 fixed effects (including an intercept) and one subject-based $N(0, \exp(2\zeta))$ random effect. The exact posterior can be computed using MCMC methods, so that the accuracy of any VA can be judged. The posterior of random effect values are typically skewed, which is the case for this example. There are 9 model parameters and 500 random effect values, so that a VA to the augmented posterior has $m = 509$.

We employ the t-copula at (2) where $\psi \sim t_m(0, \Sigma, \nu)$, $\tilde{g}_{m,\omega}$ is specified in Table 1 and the location and scale invariant transformation at (7) is used to form the implicit copula. The Gaussian copula VA outlined in Smith et al. (2020) (labeled SLN2020), which is without location and scale correction of the transformation, is used as a comparison. In both cases, we set $K = 5$ factors and considered three transformations for $t_{\gamma_i}$: YJ, iGH and a composition of two YJ transforms (Double-YJ). We also consider fitting t and Gaussian distributions directly, which corresponds assuming identity transformations $t_{\gamma_i}(\theta_i) = \theta_i$ for $i = 1, \ldots, m$ at (7). When calibrating each of the three t-copulas and the t distribution using SGA, we found the variational parameter $\nu^* > 29$, which indicates that a Gaussian copula structure is optimal here. Figure 3 plots the first three posterior moments of the VAs (vertical axes) against their true values (horizontal axes). All approximations identify the posterior means and standard deviations well, but SLN2020 does a poor job of estimating the...
posterior skew in panel (f) in comparison to our proposed VA in panel (c). To further visualize, Figure 4 plots the exact and variational marginal posteriors of three random effect values. The increased accuracy of the VA at (9) compared to SLN2020 is clear.

4 Regularized Correlation Matrix

To illustrate our approach we apply it to estimate a regularized correlation matrix. This problem occurs in various models, including those with random effects (Danaher et al., 2020), multivariate probit models (Zhang et al., 2021) and elliptical copula models (Fang et al., 2002). Bayesian regularization is provided by shrinkage priors that typically make the posterior slow to evaluate using standard MCMC methods. Variational inference provides a faster alternative.

4.1 Gaussian regularized copula model

We consider estimation of a Gaussian copula model for multivariate data (not to be confused with the copula VA) with parameter correlation matrix Ω. In high dimensions either Ω or Ω^{-1} is often assumed to be sparse or patterned; e.g. see Oh and Patton (2017). However, in some applications this may be unreasonable, so that Ω is a full matrix and a regularized estimator is used. Below we suggest an effective form of regularization for Ω based on a spherical coordinate parameterization and then apply our VI approach for its estimation.

Denote as \( y_i = (y_{i,1}, \ldots, y_{i,r})^\top \) the i-th observation of an \( r \)-dimensional vector of data, and \( y = (y_1^\top, \ldots, y_N^\top)^\top \). The Gaussian copula model for this data has likelihood

\[
p(y|\theta) = \frac{1}{|\Omega|^{N/2}} \prod_{i=1}^{N} \exp \left[-\frac{1}{2} x_i^\top (\Omega^{-1} - I_r) x_i\right],
\]

where \( x_i = (\Phi^{-1}(u_{i,1}), \ldots, \Phi^{-1}(u_{i,r}))^\top \), \( u_{i,j} = G_j(y_{i,j}) \) and \( G_j(\cdot) \) denotes the marginal distribution function of \( y_{i,j} \). We follow Pinheiro and Bates (1996), Rebonato and Jäckel (1999), Creal and Tsay (2015) and others, and set \( \Omega = LL^\top \), where \( L = \{l_{i,j}\} \) is a lower triangular Cholesky factor with
elements written in terms of spherical co-ordinates \( \vartheta_{i,j} \) as

\[
 l_{i,j} = \begin{cases} 
 1 & \text{if } i = j = 1 \\
 \sin (\vartheta_{i,i-1}) \prod_{s=1}^{i-2} \sin (\vartheta_{i,s}) & \text{if } i = j > 1 \\
 \cos (\vartheta_{i,j}) \prod_{s=1}^{i-1} \sin (\vartheta_{i,s}) & \text{if } i > j \text{ and } i > 1 \\
 0 & \text{otherwise},
\end{cases}
\]

where \( \prod_{s=1}^{0} \sin (\vartheta_{i,s}) = 1 \) and \( \vartheta_{i,j} \in [0, \pi) \). Denote \( \vartheta_i = (\vartheta_{i,1}, \ldots, \vartheta_{i,i-1})^\top \), then the angles \( \vartheta = (\vartheta_2^\top, \ldots, \vartheta_r^\top)^\top \) provide a unique parameterization of \( \Omega \). If \( (Y_1, \ldots, Y_m)^\top \sim N(0, \Omega) \), each angle is related to a partial correlation as

\[
 \cos \vartheta_{i,j} = \text{Corr}(Y_i, Y_j | Y_1, \ldots, Y_{j-1}) \equiv \rho_{i,j|1:(j-1)}.
\]

Each angle is transformed to the real line by setting \( \eta_{i,j} = \Phi^{-1}(\vartheta_{i,j}/\pi) \). Each partial correlation \( \rho_{i,j|1:(j-1)} = 0 \) iff \( \eta_{i,j} = 0 \), so that shrinkage of \( \eta_{i,j} \) towards zero is equivalent to shrinking these partial correlations to zero representing conditional independence between \( Y_i \) and \( Y_j \).

The parameters are stacked into the vector \( \eta = (\eta_2^\top, \ldots, \eta_r^\top)^\top \equiv (\eta_1, \eta_2, \ldots, \eta_{(r-1)/2})^\top \), with \( \eta_i = (\eta_{i,1}, \ldots, \eta_{i,i-1})^\top \). The horseshoe prior (Carvalho et al., 2010) is used to provide adaptive shrinkage towards zero (i.e. regularization), where

\[
 \eta_s | \xi, \chi_s \sim N(0, \chi_s), \quad \chi_s | \nu_s \sim \mathcal{G}^{-1} \left( \frac{1}{2}, \frac{1}{2\nu_s} \right), \quad \xi | \kappa \sim \mathcal{G}^{-1} \left( \frac{1}{2}, \frac{1}{\kappa} \right), \quad \nu_1, \ldots, \nu_{(r-1)/2}, \kappa \sim \mathcal{G}^{-1} \left( \frac{1}{2}, 20 \right),
\]

where \( \mathcal{G}^{-1}(a, b) \) is an inverse gamma distribution with parameters \( a \) and \( b \). The posterior densities of parameters that are regularized using the horseshoe prior are funnel-shaped and difficult to approximate (Betancourt and Girolami, 2015, Ghosh et al., 2019). To address this, Ingraham and Marks (2017) suggest adopting the “non-centered” re-parameterization

\[
 \eta_s = \tau_s \sqrt{\xi} \chi_s, \text{ for } s = 1, \ldots, r(r-1)/2,
\]

which simplifies the geometry of the posterior so that it is easier to approximate. Here, \( \chi^\top, \nu^\top, \xi, \kappa \) are all positive, so we further transform them to the real line using logarithmic transformations. With this, the model parameter vector \( \theta = (\tau^\top, \log \chi^\top, \log \xi, \log \nu^\top, \log \kappa)^\top \). The posterior
\( p(\theta|y) \propto p(y|\theta)p(\theta) = g(\theta) \) and its gradient \( \nabla_\theta \log g(\theta) \) are available in closed form and are given in the Online Appendix.

### 4.2 U.S. income inequality

The copula model is used to model the dependence between changes in income inequality in U.S. states from 1916 to 2018. Inequality is measured using the annual Gini coefficient, where higher values indicate higher income inequality. Data for the study were sourced from Mark Frank’s webpage at [www.shsu.edu/eco_mwf/inequality.html](http://www.shsu.edu/eco_mwf/inequality.html), which are constructed from tax filings at the Inland Revenue Service using an approach detailed in Frank (2009). Due to missing early observations the states of Alaska and Hawaii were removed, while the District of Columbia (Washington D.C.) was included. Let \( GINI_{t,j} \) denote the Gini coefficient in year \( t \) for state \( j \), then we set \( y_{t,j} = GINI_{t,j} - GINI_{t-1,j} \) and estimate the marginal distribution in each state using a kernel density estimate (KDE). These are non-Gaussian, so that a copula model is appropriate; see Figure A1 in the Web Appendix. The copula data \( u_{t,j} \) are then computed, and posterior inference evaluated for the two cases below.

**Two U.S. states inequality example**

The first estimation is for the \( r = 2 \) most populous states of California and Texas. Here, \( (\theta_1, \ldots, \theta_5)^\top = (\tau_1, \log \chi_1, \log \xi, \log \nu_1, \log \kappa)^\top \) and we consider this case because in a low-dimensional setting the posterior can be computed using MCMC methods, allowing comparison with our VA. Figure 5 plots the univariate marginals \( p(\theta_i|y) \) and bivariate marginals \( p(\theta_i, \theta_j|y) \) evaluated using MCMC. The posteriors are unimodal, skewed and dependent—precisely the type of distribution that can be captured well using an elliptical copula model. Figure 6 plots the equivalent marginals of the \( t \)-copula VA, with \( t_{\gamma_i} \) being Double-YJ transforms and \( K = 5 \) factors (i.e. \( B = 5 \times 5 \)). These are given by (10) and bivariate slices of (9). The VA captures key features of the posterior distribution well, including the location, skew and dependence. There is some mild under-estimation of the posterior variance, which is a common feature of fixed-form VAs that may be rectified using a
post-estimation adjustment (Yu et al., 2021).

49 U.S. states inequality example

The second case is estimation for all \( r = 49 \) U.S. states, so that \( \Omega \) has \( 49(48/2) = 1176 \) unique elements and, when including the horseshoe regularization hyper-parameters, \( \theta \) has \( m = 3530 \) elements. Table 2 summarizes the results for 20 different VAs with differing numbers of columns \( K \) for matrix \( B \) and transformations \( t_{\gamma_i} \) employed. When the identity transformation \( t_{\gamma_i}(\theta_i) = \theta_i \) is used, the VA is simply a t-distribution with a factor covariance matrix. When \( K = 0 \) the scale matrix \( \Sigma \) is diagonal and the VA is a mean field approximation over each element of \( \theta \).

The number of variational parameters \( |\lambda| \) and the time taken to complete 1,000 steps of the SGA algorithm are reported. We found 15,000 steps is sufficient to calibrate each VA; for example, calibration took two hours for the t-copula with \( K = 15 \) and the YJ transformation for \( t_{\gamma_i} \) using an un-optimized implementation on a low end desktop. Also reported is the median lower bound over the last 500 steps, labeled as \( \text{LB} \), with higher values indicating more accurate calibration. By this measure the copula VAs are all more accurate than a t-distribution, and the t-copula with \( K = 15 \) and the YJ transformation for \( t_{\gamma_i} \) is the most accurate. For \( K = 20 \) the highly parameterized dependence structure can be harder to calibrate well using first order stochastic optimization methods, leading to lower values of \( \text{LB} \).

For the Gaussian copula data model, the level of pairwise dependence between the states can be measured by the matrix of Spearman correlations \( \Omega^s = \frac{6}{\pi} \arcsin(\frac{1}{2} \Omega) \), where the \( \arcsin \) function is applied element-wise to \( \frac{1}{2} \Omega \). Figure A2 plots the point estimate of \( \Omega^s \) from the optimal t-copula VA to the posterior. This estimate was obtained by simulating draws of \( \theta \) from the VA, evaluating the resulting draws of \( \Omega^s \) and computing their mean. To further visualize the results, we select the five contiguous western states of AZ, CA, NV, OR and WA, and then plot the marginal variational posteriors of the pairwise Spearman correlations for these states in Figure 7. This is undertaken for both the mean field t-distribution and the optimal t-copula, and the impact of employing the more accurate copula model VA can be seen; for example, the posterior estimate for the correlation...
Table 2: Summary of 20 VAs to the Posterior of the Gaussian Copula Model for U.S. Inequality

| $t_{\alpha i}$ | Number of Columns in $B$ | \(K = 0\) | \(K = 5\) | \(K = 10\) | \(K = 15\) | \(K = 20\) |
|---------------|--------------------------|-----------|-----------|-----------|-----------|-----------|
| Number of Variational Parameters $|\lambda|$ | | | | | |
| Identity      | 7,061                    | 24,711    | 42,361    | 60,011    | 77,661    |
| iGH           | 14,121                   | 31,771    | 49,421    | 67,071    | 84,721    |
| YJ            | 10,591                   | 28,241    | 45,891    | 63,541    | 81,191    |
| Double YJ     | 14,121                   | 31,771    | 49,421    | 67,701    | 84,721    |
| Time (Mins. per 1000 Steps) | | | | | |
| Identity      | 5.6                      | 5.9       | 6.4       | 8.3       | 13.1      |
| iGH           | 5.6                      | 6.1       | 6.6       | 8.8       | 13.7      |
| YJ            | 5.6                      | 5.9       | 6.4       | 8.3       | 13.2      |
| Double YJ     | 5.5                      | 5.9       | 6.5       | 8.4       | 13.2      |

The computation was implemented in serial using MATLAB on a low end DELL desktop with an Intel i7-10700 CPU @ 2.9Ghz.

between WA and AZ is located at a lower value. The posteriors of other elements in $\Omega^s$ (unreported) are affected similarly.

5 Discussion

This paper aims to refine and extend the high-dimensional copula VI approach outlined in Smith et al. (2020), making five contributions. First, Section 2 clarifies why implicit copula models are an attractive choice of VA in high dimensions, compared to other copula VAs. Second, an adjustment to the learnable transformations that define the implicit copula is proposed that increases the accuracy of the VA. Third, it is shown how to implement the re-parameterization trick for a sub-class of elliptical copulas. This is useful in practice because employing the re-parameterization gradient at (1) can increase the efficiency of SGA algorithms greatly. Fourth, it is shown how spherical co-ordinates can be used to represent the factor decomposition of the constrained scale matrix $\Sigma$ of an elliptical copula. Last, it is demonstrated how the proposed copula VI method can
be used to approximate the complex posterior of a regularized correlation matrix. This is a difficult posterior to evaluate exactly in high dimensions using standard MCMC methods.

Elliptical copula VI is an attractive black box method for posteriors that are unimodal, have positive and negative dependencies between parameters, and exhibit high levels of skew, as in Figures 5 and 6. Gunawan et al. (2021) also employ implicit copula VI, but with a mixture of normals for $\psi \sim F$. This further extends the dependence structure of the VA, although calibration is more computationally demanding because the re-parameterization trick cannot be used directly. Compositions of parametric transformations can be considered at (7), although experiments (unreported) suggest little to no improvement in the accuracy of the VA. However, a promising direction for future work is to consider a Gaussian or other process for $\psi \sim F$. The resulting implicit copula is a “copula process” (Wilson and Ghahramani, 2010) which can admit a more complex dependence structure for the VA, while still exploiting the computational advantages outlined here.
Appendix A  Gradients for implementation of SGA

This appendix provides the gradients to implement SGA with the re-parameterization trick for the proposed VA at (9). They do not vary by choice of target density, and MATLAB code for their evaluation is provided in the Supplementary Material.

Expression for $\nabla_\theta \log q_\lambda(\theta)$

The gradient at (6) is

$$\nabla_\theta \log q_\lambda(\theta) = \frac{g'_{m,\omega}(\psi^T \Sigma^{-1} \psi)}{g_{m,\omega}(\psi^T \Sigma^{-1} \psi)} \cdot 2 \frac{\partial \psi}{\partial \theta} \Sigma^{-1} \psi + \left( \frac{t''_{\gamma_1} \left( \frac{\theta_1 - \mu_1}{\sigma_1} \right)}{t'_{\gamma_1} \left( \frac{\theta_1 - \mu_1}{\sigma_1} \right) \sigma_1}, \ldots, \frac{t''_{\gamma_m} \left( \frac{\theta_m - \mu_m}{\sigma_m} \right)}{t'_{\gamma_m} \left( \frac{\theta_m - \mu_m}{\sigma_m} \right) \sigma_m} \right)^T,$$

with

$$\frac{\partial \psi}{\partial \theta} = \text{diag} \left( t'_{\gamma_1} \left( \frac{\theta_1 - \mu_1}{\sigma_1} \right) \sigma_1, \ldots, t'_{\gamma_m} \left( \frac{\theta_m - \mu_m}{\sigma_m} \right) \sigma_m \right).$$

Expressions for $t'_{\gamma_j}$ and $t''_{\gamma_j}$ are provided in Table 1 of Smith et al. (2020) for both the YJ and iGH transformations, which are very fast to compute. The derivatives of compositions of these two transformations are also easily computed using a trivial application of the chain rule. Expressions for $g_{m,\omega}$ and $g'_{m,\omega}$ are given in Table 1 for the four elliptical copula. For the Gaussian copula the first ratio simplifies to $\frac{g'_{m,\omega}(\psi^T \Sigma^{-1} \psi)}{g_{m,\omega}(\psi^T \Sigma^{-1} \psi)} = -1/2$, while for the t copula it simplifies to $\frac{g'_{m,\omega}(\psi^T \Sigma^{-1} \psi)}{g_{m,\omega}(\psi^T \Sigma^{-1} \psi)} = -\frac{v+m}{2v} \left[ 1 + \left( \frac{\psi^T \Sigma^{-1} \psi}{\nu} \right)^{-1} \right].$

Expression for $\frac{\partial \theta(\varepsilon,\lambda)}{\partial \lambda}$

Denote $A = [d \ B]$ to be the matrix of elements $a_{j,k}, \boldsymbol{x} = (\boldsymbol{x}_1^T, \ldots, \boldsymbol{x}_m^T)^T, P_1 = [0_{K \times 1} \ I_K]^T$ and $P_2 = (1, 0_{1 \times K})^T$. The derivatives of $\theta$ with respect to $\lambda = (\mu^T, \sigma^T, \gamma^T, \tau^T, \omega^T)^T$ are

$$\frac{\partial \theta(\varepsilon,\lambda)}{\partial \mu} = I_m, \quad \frac{\partial \theta(\varepsilon,\lambda)}{\partial \sigma} = \text{diag} \left( t^{-1}_{\gamma_1}(\psi_1), \ldots, t^{-1}_{\gamma_m}(\psi_m) \right),$$

$$\frac{\partial \theta(\varepsilon,\lambda)}{\partial \gamma} = \text{diag} \left( \sigma_1 t^{-1}_{\gamma_1}(\psi_1), \ldots, \sigma_m t^{-1}_{\gamma_m}(\psi_m) \right),$$

$$\frac{\partial \theta(\varepsilon,\lambda)}{\partial \tau} = \frac{\partial \theta}{\partial \psi} \frac{\partial \psi}{\partial \tau}, \quad \frac{\partial \theta(\varepsilon,\lambda)}{\partial \omega} = \frac{\partial \theta}{\partial \psi} \frac{\partial \psi}{\partial \omega},$$

$$\frac{\partial \theta(\varepsilon,\lambda)}{\partial \varepsilon} = \frac{\partial \theta(\varepsilon,\lambda)}{\partial \psi} \frac{\partial \psi}{\partial \varepsilon}.$$
where
\[
\frac{\partial \theta}{\partial \psi} = \text{diag} \left( \sigma_1 \frac{\partial t_{z_1}^{-1}(\psi_1)}{\partial \psi_1}, \ldots, \sigma_m \frac{\partial t_{n_m}^{-1}(\psi_m)}{\partial \psi_m} \right),
\]
\[
\frac{\partial \kappa}{\partial \tau} = \text{blockdiag} \left( \frac{\partial \kappa_1}{\partial \tau_1}, \ldots, \frac{\partial \kappa_m}{\partial \tau_m} \right)
\]
with \(\frac{\partial \kappa_j}{\partial \tau_j} = \text{diag} (\phi(\tau_{j,1}) \pi, \ldots, \phi(\tau_{j,K-1}) \pi, \phi(\tau_{j,K}) \pi),\) and
\[
\frac{\partial \psi}{\partial \kappa} = \sqrt{w} \left[ (z^T P_1^T) \otimes I_m + \text{diag} (\epsilon) \left( P_2^T \otimes I_m \right) \right] K_{K+1,m} \frac{\partial A^T}{\partial \kappa},
\]
with \(\frac{\partial A^T}{\partial \kappa} = \text{blockdiag} \left( \frac{\partial a_1}{\partial \kappa_1}, \ldots, \frac{\partial a_m}{\partial \kappa_m} \right)\) and
\[
\left\{ \frac{\partial a_i}{\partial \kappa_i} \right\}_{j,l} = \begin{cases} 
\cos (\kappa_{i,j}) \cos (\kappa_{i,l}) \prod_{s \in \{1, \ldots, j-1\} \setminus \{l\}} \sin (\kappa_{i,s}) & \text{If } l < j \land j < K + 1 \\
- \prod_{s=1}^{j} \sin (\kappa_{i,s}) & \text{If } l = j \land j < K + 1 \\
\cos (\kappa_{i,l}) \prod_{s \in \{1, \ldots, j-1\} \setminus \{l\}} \sin (\kappa_{i,s}) & \text{If } l < j \land j = K + 1 \\
0 & \text{Otherwise}
\end{cases}
\]

Here, \(K_{K+1,m}\) denotes the relevant commutation matrix. For details on the derivation of these expressions see the Online Appendix. The terms \(\frac{\partial t_{z_1}^{-1}(\cdot)}{\partial \tau_j}\) and \(\frac{\partial t_{\psi_1}^{-1}(\cdot)}{\partial \psi_j}\) are provided in Table 1 of Smith et al. (2020) for both the YJ and iGH transformations.

For the Gaussian and Laplace distributions it is unnecessary to evaluate the derivative \(\frac{\partial \psi}{\partial \omega}\) because \(\omega = \emptyset\). However, in general \(\psi = \sqrt{w} (Bz + D\epsilon)\) with \(w = F_W^{-1}(u; \omega)\), so that
\[
\frac{\partial \psi}{\partial \omega} = (Bz + D\epsilon) \times \left\{ \frac{1}{2 \left( F_W^{-1}(u; \omega) \right)^{1/2}} \left( \frac{\partial}{\partial \omega} F_W^{-1}(u; \omega) \right) \right\}
\]
For the \(t\) distribution \(\omega = \nu, F_W^{-1}(u; \omega) = \nu / F_X^{-1}(1 - u; \nu)\) with \(F_X\) the distribution function of \(X \sim \chi^2(\nu)\), and \(\frac{\partial}{\partial \omega} F_W^{-1}(u; \omega)\) is computed numerically.
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Marginal densities $q_i^{\text{SLN2020}}$ (yellow line) and $q_{\lambda_i}$ at (red line) of optimal VAs to two skew normal (SN) target densities (blue line). Both target distributions have the same Pearson skew of 0.8553 and standard deviation $\sigma_{SN} = 1$. Panel (a) plots VA densities when the target mean is $\mu_{SN} = 15$, and panel (b) plots VA densities when the target mean is $\mu_{SN} = 0$. Also reported are the KL divergences for the optimal approximations.
Figure 2: Kullback-Leibler Divergence of Gaussian Copula VA Marginals

KL divergence of optimal marginal approximations to SN target densities. The SN distributions have a Pearson skew of 0.8553, but different means $\mu_{SN}$ and standard deviations $\sigma_{SN}$. Gaussian approximations have KL divergence of 0.172 for all target densities (black dashed line), and the approximation $q_\lambda$ at (10) has KL divergence of 0.009 for all target densities (solid black line). The KL divergence of $q_i^{SLN2020}$ is plotted as curves for four values of $\sigma_{SN}$ and $0 < \mu_{SN} < 60$. The two cases corresponding to Figure 2(a,b) are indicated with circles.
Panels (a)–(c) are for the $t$-copula VA proposed here, and panels (d)–(f) are for the Gaussian copula VA in Smith et al. (2020). In each panel the exact posterior moment (computed using MCMC) is plotted on the horizontal axis, and moment of the VA on the vertical axis. The posterior means, standard deviations and Pearson’s skew are plotted in the first, second and third columns, respectively. In each panel there is a scatter of $m = 509$ points for each of three variational estimators that correspond to the YJ (blue circles), iGH (red cross) and YJ-Double (yellow square) transformations for $t_{\gamma_i}$. For panels (a)–(e), the results are very similar so most points are close to each other and hard to distinguish.
Marginal posterior densities for three random effects. Each panel plots the exact posterior computed by MCMC (black line), the t-copula VA at $q_\lambda$ (red line) and that in Smith et al. (2020) (yellow line) for the iGH transformation.
Figure 5: Exact Posterior for the Two U.S. States Inequality Example

Exact posterior of $(\theta_1, \ldots, \theta_5) = (\tau_1, \log \chi_1, \log \nu_1, \log \xi, \log \kappa)$ computed using MCMC. The univariate marginals $p(\theta_i|y)$ are on the leading diagonals, and the bivariate marginals $p(\theta_i, \theta_j|y)$ are on the off-diagonals.
Figure 6: Variational Posterior for the Two U.S. States Inequality Example

Posterior estimates of \((\theta_1, \ldots, \theta_5)^\top = (\tau_1, \log \chi_1, \log \nu_1, \log \xi, \log \kappa)^\top\) using the copula VA with (adjusted) YJ transformations. The marginals \(q_{\lambda_i}(\theta_i)\) are on the leading diagonals, and the bivariate marginals—which are bivariate slices of \([9]\)—are on the off-diagonals.
Variational posterior densities of the 10 Spearman correlations between the contiguous western U.S. states of WA, OR, CA, NV and AZ. The posterior for the more accurate optimal t-copula is in blue, while that from the mean field t-distribution is in black.
Online Appendix for “Implicit copula variational inference”

This Online Appendix has two parts:

**Part A**: Additional Details and Results for Section 3.

**Part B**: Additional Results for the U.S. Inequality Example.
Part A: Additional Details and Results for Section 3
This appendix provides further details on the priors and the required gradients and derivatives for the SGA algorithm.

A.1 Priors and gradients

Priors
The priors for all the parameters in the model are
\[ \tau_s \sim N(0, 1), \quad \chi_s|\nu_s \sim G^{-1} \left( \frac{1}{2}, \frac{1}{\nu_s} \right), \quad \xi|\kappa \sim G^{-1} \left( \frac{1}{2}, \frac{1}{\kappa} \right), \quad \nu_1, \ldots, \nu_{r(r-1)/2}, \kappa \sim G^{-1} \left( \frac{1}{2}, 20 \right). \]

To conduct variational inference we transform all parameters to the real line as follows:
(i) \( \chi_s \) is transformed to \( \tilde{\chi}_s = \log \chi_s \);
(ii) \( \xi \) is transformed to \( \tilde{\xi} = \log \xi \);
(iii) \( \nu_s \) is transformed to \( \tilde{\nu}_s = \log \nu_s \);
(iv) \( \kappa \) is transformed to \( \tilde{\kappa} = \log \kappa \).

After the transformations we obtain the following prior density functions (using the Jacobians of the change of variables)
(i) \( p(\tau_s) = \phi_1 (\tau_s; 0, 1) ; \)
(ii) \( p(\tilde{\chi}_s|\nu_s) \propto \left( \frac{1}{\nu_s} \right)^{0.5} \exp \left( -\frac{1}{2} \tilde{\chi}_s - \frac{1}{\nu_s \exp(\tilde{\chi}_s)} \right) ; \)
(iii) \( p(\tilde{\xi}|\kappa) \propto \left( \frac{1}{\kappa} \right)^{0.5} \exp \left( -\frac{1}{2} \tilde{\xi} - \frac{1}{\kappa \exp(\tilde{\xi})} \right) ; \)
(iv) \( p(\tilde{\nu}_s) \propto \exp \left( -\frac{1}{2} \tilde{\nu}_s - \frac{20}{\exp(\tilde{\nu}_s)} \right) ; \)
(v) \( p(\tilde{\kappa}) \propto \exp \left( -\frac{1}{2} \tilde{\kappa} - \frac{20}{\exp(\tilde{\kappa})} \right) . \)

Log-posterior
\[ \log g(\theta) = \log p(y|\theta) + \log p(\theta) \]
\[ = - \frac{N}{2} \log |\Omega| - \frac{1}{2} \sum_{i=1}^{N} x_i^\top (\Omega^{-1} - I_r) x_i + \log p(\theta) \] (15)

Gradient
The model-specific gradient vector for the parameters of the copula model is:
\[ \nabla_\theta \log g(\theta) = \left( \nabla_\tau \log g(\theta)^\top, \nabla_{\tilde{\chi}} \log g(\theta)^\top, \nabla_{\tilde{\xi}} \log g(\theta)^\top, \nabla_{\tilde{\nu}} \log g(\theta)^\top, \nabla_{\tilde{\kappa}} \log g(\theta)^\top \right)^\top. \]
The different terms in this gradient can be computed as

\[
\nabla_r \log g(\theta) = \left(\sqrt{\xi} \sqrt{\chi} \right) \circ \frac{\partial \log g(\theta)}{\partial \eta}^\top - \tau
\]

\[
\nabla_\chi \log g(\theta) = \frac{1}{2} \tau \circ \left(\sqrt{\xi} \sqrt{\chi} \right) \circ \frac{\partial \log g(\theta)}{\partial \eta}^\top + \nabla_\chi \log p(\bar{\chi} | \bar{\nu})
\]

\[
\nabla_\nu \log g(\theta) = \nabla_\nu \log p(\bar{\chi} | \bar{\nu}) + \nabla_\nu \log p(\bar{\nu})
\]

\[
\nabla_\xi \log g(\theta) = \frac{1}{2} \frac{\partial \log g(\theta)}{\partial \eta} \left(\tau \circ \sqrt{\xi} \sqrt{\chi} \right) - \frac{1}{2} + \frac{1}{\kappa \xi}
\]

\[
\nabla_\kappa \log g(\theta) = -\frac{1}{2} + \frac{1}{\kappa \xi} - \frac{1}{2} + \frac{1}{\kappa}
\]

where \(\nabla_\chi \log p(\bar{\chi} | \bar{\nu}) = \left(-\frac{1}{2} + \frac{1}{\nu_1 x_1}, \ldots, -\frac{1}{2} + \frac{1}{\nu_r (r-1)/2 x_r (r-1)/2}\right)^\top\),

\[\nabla_\nu \log p(\bar{\chi} | \bar{\nu}) = \left(-\frac{1}{2} + \frac{1}{\nu_1 x_1}, \ldots, -\frac{1}{2} + \frac{1}{\nu_r (r-1)/2 x_r (r-1)/2}\right)^\top,\]

\[
\frac{\partial \log g(\theta)}{\partial \eta} = \left[-\frac{N}{2} \text{vec}(\Omega^{-1})^\top \frac{\partial \Omega}{\partial L} - \frac{1}{2} \left(\sum_{i=1}^N x_i x_i^\top \right) \frac{\partial \Omega^{-1}}{\partial \Omega} \frac{\partial \Omega}{\partial L}\right] \frac{\partial L}{\partial \theta} \frac{\partial \theta}{\partial \eta}
\]

\[
\frac{\partial \Omega}{\partial L} = (I_r + K_r) (L \otimes L)
\]

\[
\frac{\partial \Omega^{-1}}{\partial L} = -\Omega^{-1} \otimes \Omega^{-1}
\]

\[
\frac{\partial \theta}{\partial \eta} = \text{blockdiag} \left(\frac{\partial \theta_1}{\partial \eta_1}, \ldots, \frac{\partial \theta_r}{\partial \eta_r}\right)
\]

\[
\frac{\partial \theta_i}{\partial \eta_i} = \text{diag} \left[\phi(\eta_{i,1}) \pi, \ldots, \phi \left(\eta_{i,i} + \Phi^{-1} \left(\frac{1}{4}\right) \right) \frac{2\pi}{\kappa}\right]
\]

Finally, \(\partial L / \partial \theta\) is a matrix with elements \(\left(\partial L / \partial \theta\right)_{(j-1)r+i,(i-1)r+k} = \frac{\partial l_{i,j}}{\partial \theta_{i,k}}\), where

\[
\frac{\partial l_{i,j}}{\partial \theta_{i,k}} = \begin{cases} 
\cos (\theta_{i,i-1}) \prod_{s=1}^{i-2} \sin (\theta_{i,s}) & \text{If } i > 1 \land j = i \land k = i - 1 \\
\sin (\theta_{i,i-1}) \frac{\cos (\theta_{i,k})}{\sin (\theta_{i,k})} \prod_{s=1}^{i-2} \sin (\theta_{i,s}) & \text{If } i > 1 \land j = i \land k < i - 1 \\
-\prod_{s=1}^{i-1} \sin (\theta_{i,s}) & \text{If } i > 1 \land j < i \land k = j \\
\cos (\theta_{i,j}) \frac{\cos (\theta_{i,k})}{\sin (\theta_{i,k})} \prod_{s=1}^{j-1} \sin (\theta_{i,s}) & \text{If } i > 1 \land j < i \land k < j \\
0 & \text{Otherwise.}
\end{cases}
\]

If not specified, all remaining elements of \(\partial L / \partial \theta\) are zero.
Part B: Gradients for \( q \)

In this section we will denote \( A = [d \ B] \) to be the matrix with elements \( a_{j,k} \) and \( \mathbf{x} = (\mathbf{x}_1^\top, \ldots, \mathbf{x}_m^\top)^\top \).

We need to compute the derivatives of \( \theta \) with respect to all the elements in \( \lambda = (\mu^\top, \sigma^\top, \gamma^\top, \tau^\top)^\top \):

\[
\begin{align*}
\frac{\partial \theta(\varepsilon, \lambda)}{\partial \mu} &= I_m \\
\frac{\partial \theta(\varepsilon, \lambda)}{\partial \sigma} &= \text{diag} \left( t_{\gamma_1^{-1}}(\psi_1), \ldots, t_{\gamma_m^{-1}}(\psi_m) \right) \\
\frac{\partial \theta(\varepsilon, \lambda)}{\partial \gamma} &= \text{diag} \left( \sigma_1 \frac{\partial t_{\gamma_1^{-1}}(\psi_1)}{\partial \gamma_1}, \ldots, \sigma_m \frac{\partial t_{\gamma_m^{-1}}(\psi_m)}{\partial \gamma_m} \right) \\
\frac{\partial \theta(\varepsilon, \lambda)}{\partial \gamma_j} &= \frac{\partial \theta}{\partial \phi} \frac{\partial \phi}{\partial \mathbf{x}} \\
\frac{\partial \theta(\varepsilon, \lambda)}{\partial \gamma_m} &= \frac{\partial \theta}{\partial \phi} \frac{\partial \phi}{\partial \mathbf{x}} \\
\frac{\partial \theta(\varepsilon, \lambda)}{\partial \tau} &= \frac{\partial \theta}{\partial \psi} \frac{\partial \psi}{\partial \mathbf{x}} \\
\frac{\partial \theta(\varepsilon, \lambda)}{\partial \omega} &= \frac{\partial \theta}{\partial \psi} \frac{\partial \psi}{\partial \mathbf{x}}
\end{align*}
\]

For the last derivative we need to compute the three terms \( \frac{\partial \theta}{\partial \psi} \), \( \frac{\partial \psi}{\partial \mathbf{x}} \), and \( \frac{\partial \mathbf{x}}{\partial \tau} \). The first term can be computed as

\[
\frac{\partial \theta}{\partial \psi} = \text{diag} \left( \sigma_1 \frac{\partial t_{\gamma_1^{-1}}(\psi_1)}{\partial \psi_1}, \ldots, \sigma_m \frac{\partial t_{\gamma_m^{-1}}(\psi_m)}{\partial \psi_m} \right).
\]

The third term is given as \( \frac{\partial \mathbf{x}}{\partial \tau} = \text{blockdiag} \left( \frac{\partial \mathbf{x}}{\partial \tau_1}, \ldots, \frac{\partial \mathbf{x}}{\partial \tau_m} \right) \), with

\[
\frac{\partial \mathbf{x}_j}{\partial \tau_j} = \text{diag} \left( \phi(\tau_j, 1) \pi, \ldots, \phi(\tau_j, K-1) \pi, \phi(\tau_j, K) \pi, 2 \pi \right).
\]

For the second term we know that:

\[
\begin{align*}
\frac{\partial \psi}{\partial \mathbf{x}} &= \sqrt{w} \left[ (z^\top \otimes I_m) \frac{\partial B}{\partial \mathbf{x}} + \text{diag} (\varepsilon) \frac{\partial d}{\partial \mathbf{x}} \right] \\
\text{with} \quad \frac{\partial B}{\partial \mathbf{x}} &= \frac{\partial B}{\partial A^\top} \frac{\partial A^\top}{\partial \mathbf{x}} \\
\frac{\partial d}{\partial \mathbf{x}} &= \frac{\partial d}{\partial A^\top} \frac{\partial A^\top}{\partial \mathbf{x}}
\end{align*}
\]

We can write \( B = AP_1 \) and \( d = AP_2 \) where \( P_1 = [0_{K \times 1} \ I_K]^\top \) and \( P_2 = (1, 0_{1 \times K})^\top \). Then \( \frac{\partial B}{\partial A^\top} \) can be easily computed after noting that

\[
\text{vec} (B) = \left( P_1^\top \otimes I_m \right) \text{vec} (A) = \left( P_1^\top \otimes I_m \right) K_{K+1,m} \text{vec} (A^\top)
\]

where \( K_{K+1,m} \) denotes a commutation matrix. Then

\[
\frac{\partial B}{\partial A^\top} = \left( P_1^\top \otimes I_m \right) K_{K+1,m}.
\]
The term $\frac{\partial d}{\partial A}$ can be computed by noting that

$$\text{vec}(d) = \left(P_2^\top \otimes I_m\right)\text{vec}(A) = \left(P_2^T \otimes I_m\right)K_{K+1,m}\text{vec}(A^\top)$$

so that

$$\frac{\partial d}{\partial A^\top} = \left(P_2^T \otimes I_m\right)K_{k+1,m}.$$

The elements of the derivative $\frac{\partial A^\top}{\partial \kappa}$ can be computed as

$$\left\{\frac{\partial a_i}{\partial \kappa_i}\right\}_{j,l} = \begin{cases} 
\cos(\kappa_{i,j})\cos(\kappa_{i,l})\prod_{s \in \{1,\ldots,j-1\}}\sin(\kappa_{i,s}) & \text{If } l < j \wedge j < K + 1 \\
-\prod_{s=1}^{l} \sin(\kappa_{i,s}) & \text{If } l = j \wedge j < K + 1 \\
\cos(\kappa_{i,l})\prod_{s \in \{1,\ldots,j-1\}}\sin(\kappa_{i,s}) & \text{If } l < j \wedge j = K + 1 \\
0 & \text{Otherwise}
\end{cases}$$

Replacing all the terms above into (16) we can show that

$$\frac{\partial \psi}{\partial \kappa} = \sqrt{w}\left[(\varepsilon^T P_1^\top) \otimes I_m + \text{diag} (\varepsilon) \left(P_2^T \otimes I_m\right)\right] K_{K+1,m} \frac{\partial A^\top}{\partial \kappa}.$$
Part B: Additional Results for the U.S. Inequality Example

Figure A1: Marginal Data Density Estimates for Nine Most Populous U.S. States

Marginal density estimates of $g_i(y) = \frac{4}{dy}G_j(y)$ for the nine most populous U.S. states. In each panel the KDE (black line) is used to compute the copula data $u_{t,j} = G_j(y_{t,j})$, while the fitted Gaussian (green line) is plotted for comparison.
Posterior mean estimates of Spearman correlation matrix $\Omega^*$ for all 49 U.S. states in our data. The means are obtained by simulating Monte Carlo iterates $\theta \sim q_{\lambda^*}$ from the calibrated optimal t-copula VA.