
Variational Inference in Location-Scale Families: Exact Recovery of the Mean and Correlation Matrix

Charles C. Margossian

Center for Computational Mathematics
Flatiron Institute

Lawrence K. Saul

Center for Computational Mathematics
Flatiron Institute

Abstract

Given an intractable target density p , variational inference (VI) attempts to find the best approximation q from a tractable family \mathcal{Q} . This is typically done by minimizing the exclusive Kullback-Leibler divergence, $\text{KL}(q||p)$. In practice, \mathcal{Q} is not rich enough to contain p , and the approximation is misspecified even when it is a unique global minimizer of $\text{KL}(q||p)$. In this paper, we analyze the robustness of VI to these misspecifications when p exhibits certain symmetries and \mathcal{Q} is a location-scale family that shares these symmetries. We prove strong guarantees for VI not only under mild regularity conditions but also in the face of severe misspecifications. Namely, we show that (i) VI recovers the mean of p when p exhibits an *even* symmetry, and (ii) it recovers the correlation matrix of p when in addition p exhibits an *elliptical* symmetry. These guarantees hold for the mean even when q is factorized and p is not, and for the correlation matrix even when q and p behave differently in their tails. We analyze various regimes of Bayesian inference where these symmetries are useful idealizations, and we also investigate experimentally how VI behaves in their absence.

1 INTRODUCTION

In many problems, it is necessary to approximate an intractable distribution p . Variational inference (VI) posits a parameterized family \mathcal{Q} of tractable distributions, and within this family it attempts to find the

best approximation to p [Jordan et al., 1999, Wainwright and Jordan, 2008, Blei et al., 2017]. This is typically done by minimizing the exclusive Kullback-Leibler (KL) divergence with respect to the parameters of \mathcal{Q} . An important application of VI lies in Bayesian inference, where the primary computational task is to approximate the posterior distribution.

In practice, $p \notin \mathcal{Q}$. For example, we may set \mathcal{Q} to be a family of factorized distributions—the so-called *mean-field* approximation [Peterson, 1987, Hinton and Camp, 1993, Parisi, 1998]—even when p does not factorize, or to be the family of multivariate Gaussian distributions even when p is non-Gaussian. Still, while the best approximation in \mathcal{Q} may not exactly match p , we may hope that it captures certain key features such as its mean and correlation matrix.

Several empirical studies report that VI accurately estimates the mean of p ; this is true even when the approximation is misspecified to a degree that other quantities, such as the variance and entropy, are poorly estimated [e.g MacKay, 2003, Turner and Sahani, 2011, Blei et al., 2017, Giordano et al., 2018, Margossian et al., 2024]. These results are nuanced by other examples in which VI poorly estimates expectation values [Huggins et al., 2020, Zhang et al., 2022]. There is therefore a need for a theory that explains the empirical successes of VI, but also cautions against its potential failures.

In this paper, we analyze the robustness of VI when \mathcal{Q} is a location-scale family. Our first main result is a guarantee for VI’s estimate of the mean. In particular, we show that if the target density p and each approximation $q \in \mathcal{Q}$ are endowed with a point of symmetry, then a stationary point of $\text{KL}(q||p)$ is found by matching these points of symmetry. Under further conditions, we show that this stationary point is unique and also a global minimizer. Thus, VI is guaranteed to locate this point, which corresponds to the mean of p , provided we have a well-performing optimizer. These conditions allow for several misspecifications in \mathcal{Q} : for example, q may be factorized while p is not, or the tails

of q may be lighter (or heavier) than those of p . At the same time, the assumption of symmetry is satisfied by many location-scale families (e.g., Gaussian, Laplace, student-t).

Our second main result is a guarantee for VI’s estimate of the correlation matrix. We consider the setting where p exhibits an elliptical symmetry and \mathcal{Q} is a location-scale family whose base density is spherically symmetric. Here, under similar assumptions, we show that $\text{KL}(q||p)$ has a unique minimizer that correctly estimates the correlation matrix of p . We note that VI finds this solution even when no $q \in \mathcal{Q}$ matches the tail behavior of p nor correctly estimates its covariances.

We complement our theoretical results with an empirical study of VI in location-scale families. We experiment with both synthetic targets, in which we control the amount of symmetry in p , and with real-world posteriors from problems in Bayesian inference. When VI is used for Bayesian inference—to estimate a posterior p over model parameters from data—we observe that this posterior tends to be symmetric in the limits of *both* small and large amounts of data. Our experiments also probe VI in intermediate regimes where p is less amenable to symmetric approximations. Code to reproduce all experimental results and figures in this paper can be found at https://github.com/charlesm93/VI_location_robust.

Related work. There is a rich literature on the robustness of VI to misspecifications of \mathcal{Q} . While we focus on VI’s estimates of the mean and correlation matrix, others have examined estimates of the marginal likelihood [Jordan et al., 1999, Li and Turner, 2016], the corresponding maximum likelihood estimator [Wang and Blei, 2018], importance weights when q is used as a proposal distribution [Yao et al., 2018, Vehtari et al., 2024], and estimators for various measures of uncertainty [e.g. MacKay, 2003, Turner and Sahani, 2011, Margossian and Saul, 2023, Katsevich and Rigollet, 2024, Margossian et al., 2024]. Researchers have also investigated the frequentist properties of variational Bayes estimators: that is, how well does the first moment of q recover a true value z^* which underlies a data generating process [e.g Alquier and Ridgway, 2020, Yang et al., 2020, Zhang and Gao, 2020].

Extending this literature, we identify weak conditions under which VI *exactly* recovers the mean, including in non-asymptotic regimes, thereby formalizing past empirical observations [e.g MacKay, 2003, Blei et al., 2017, Giordano et al., 2018]. Previous works have used the Wasserstein distance to bound the error of VI’s estimates [Huggins et al., 2020, Biswas and Mackey, 2023]. While these works provide a post-hoc diagnostic, ours provides a complementary theoretical guar-

antee. Katsevich and Rigollet [2024] also provide theoretical guarantees for the recovery of the mean, in the case where \mathcal{Q} is the family of Gaussians. Their results are non-asymptotic, although exact recovery of the mean is only achieved asymptotically. To our knowledge, our work is the first to provide guarantees for VI with elliptically symmetric distributions and to investigate its ability to recover the correlation matrix.

Many analyses rely on settings where the posterior p asymptotically approaches a Gaussian, per the Bernstein-von Mises theorem [van der Vaart, 1998]. Our analysis does not explicitly consider asymptotic limits, nor does it require p to be Gaussian. Rather, our work leverages the presence in p of even and elliptical symmetries; these symmetries are observed in Gaussian distributions (and in many other distributions besides). Hence, the techniques in this paper can also be applied to asymptotic analyses of VI that invoke the Bernstein-von Mises theorem.

2 PRELIMINARIES

In this section we review the main ideas and assumptions behind VI, as well as how it is used in practice. We then consider particular symmetries that a target density may exhibit and discuss why they are useful idealizations for certain regimes of Bayesian inference.

2.1 Variational inference in practice

The primary computational task in VI is to minimize the exclusive KL divergence

$$\text{KL}(q||p) = \int [\log q(z) - \log p(z)] q(z) dz, \quad (1)$$

over $q \in \mathcal{Q}$, where \mathcal{Q} is a continuously parameterized family of tractable distributions. Typically, it is only possible to evaluate an unnormalized target density \tilde{p} , and the best approximation in \mathcal{Q} is computed by maximizing the evidence lower bound (ELBO),

$$\text{ELBO} = \int [\log \tilde{p}(z) - \log q(z)] q(z) dz. \quad (2)$$

When this integral cannot be evaluated exactly, it can be approximated via Monte Carlo using draws from q . A similar approach also produces estimates of the gradient of the ELBO with respect to the variational parameters of \mathcal{Q} . Often, it is assumed that the target density p and each $q \in \mathcal{Q}$ have support over all of \mathbb{R}^d . This condition for p can be met by transforming constrained latent variables, as in automatic differentiation VI [ADVI; Kucukelbir et al., 2017]; for example, we may apply a logarithmic transformation to a positive variable.

2.2 Assumptions for theoretical analysis

Our goal in this paper is to provide conditions under which VI is guaranteed to correctly estimate certain properties of the target density p . By this, we mean first that the KL divergence in eq. (1) has a unique minimizer in the family \mathcal{Q} , and second that this minimizer shares the desired properties of p even when $p \notin \mathcal{Q}$. To provide these guarantees, we must make additional assumptions on \mathcal{Q} and p .

2.2.1 Location-scale families

Our analysis begins by supposing that \mathcal{Q} is a location-scale family or a subfamily thereof. In the following definition and throughout the paper, we use $S^{\frac{1}{2}}$ to denote the principal square-root of a positive-definite matrix S .

Definition 1. Let q_0 be a density over \mathbb{R}^d . A location-scale family \mathcal{Q} is a two-parameter family $\{q_{\nu,S}\}$ of densities over \mathbb{R}^d satisfying

$$q_{\nu,S}(z) = q_0(S^{-\frac{1}{2}}(z-\nu))|S|^{\frac{1}{2}} \quad (3)$$

for all $z, \nu \in \mathbb{R}^d$ and $d \times d$ positive-definite matrices S . We say that q_0 is the base density of the family \mathcal{Q} and that ν and S are its location and scale parameters.

Remark 2. The square-root of a matrix is not uniquely defined and other choices may be considered. Our analysis only requires the determinant of the square-root to be positive. This condition is verified by the principle square-root but also the Cholesky factor of S .

Definition 3. A location family \mathcal{Q} is a one-parameter subfamily $\{q_\nu\}$ of location-scale densities that share the same scale parameter.

Location-scale families are used widely in statistics: examples include the Gaussian, Laplace, student-t, and Cauchy families. They are also particularly relevant to black box VI [e.g Ranganath et al., 2014, Kucukelbir et al., 2017, Cai et al., 2024], where the variational approximation is often taken to be Gaussian. Location-scale distributions are simple to manipulate, and they can be sampled using the *reparameterization trick* [Kingma and Welling, 2014, Rezende et al., 2014, Titsias and Lázaro-Gredilla, 2014], which produces low variance Monte Carlo estimators of the ELBO and its gradient.

2.2.2 Even and elliptical symmetries

Our analysis focuses on the setting where the target density p and the base density $q_0 \in \mathcal{Q}$ exhibit certain symmetries. We define these symmetries next.

Definition 4. (Even and odd symmetry.) We say a function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is even-symmetric about a location point $\nu \in \mathbb{R}^d$ if for all $\zeta \in \mathbb{R}^d$ it satisfies

$$f(\nu + \zeta) = f(\nu - \zeta). \quad (4)$$

Similarly, we say a function f is odd-symmetric about a location point ν if for all $\zeta \in \mathbb{R}^d$ it satisfies

$$f(\nu + \zeta) = -f(\nu - \zeta). \quad (5)$$

Definition 5. (Spherical symmetry.) We say a density $p(\zeta)$ is spherically symmetric if the density can be written as a function $\|\zeta\|$; that is, if $\|\zeta_1\| = \|\zeta_2\|$, then $p(\zeta_1) = p(\zeta_2)$.

Definition 6. (Elliptical symmetry.) We say a density $p(z)$ is elliptically symmetric about $\nu \in \mathbb{R}^d$ if there exists a positive-definite matrix $M \in \mathbb{R}^{d \times d}$ such that the density of $\zeta = M^{-\frac{1}{2}}(z-\nu)$ is spherically symmetric. In this case we call M the scale matrix of p .

Remark 7. If $p(z)$ is elliptically symmetric with scale matrix M , then $\text{Corr}_p[z_i, z_j] = M_{ij}/\sqrt{M_{ii}M_{jj}}$.

We emphasize, per the previous remark, that the correlation matrix of an elliptically symmetric distribution is determined by its scale matrix, even though its covariance matrix is not.

Assumptions of symmetry form the cornerstone of our analysis. Specifically, we analyze VI in cases where (i) p is even-symmetric and \mathcal{Q} is a location family whose base density q_0 is also even-symmetric, and (ii) p is elliptically symmetric and \mathcal{Q} is a location-scale family whose base density q_0 is spherically symmetric.

2.2.3 Regularity conditions on p

VI recasts the problem of inference as one of optimization. It is generally difficult to prove guarantees for non-convex problems in optimization, and this difficulty is also present in our setting. To prove the strongest guarantees for VI, our analysis places further assumptions on the target density: specifically, we assume that $\log p$ is concave on all of \mathbb{R}^d and strictly concave on some open set of \mathbb{R}^d . We also assume that p is differentiable, and that $\log p$ and each $q \in \mathcal{Q}$ satisfy the assumptions of the dominated convergence theorem to permit differentiating under the integral sign. (More concretely, the reader may assume that each $q \in \mathcal{Q}$ has finite moments of all orders, and that $\|\nabla \log p(z)\|$ can be bounded by some polynomial in $\|z\|$.)

2.3 Symmetries and Bayesian inference

We now briefly examine how exact or approximate symmetries of the target density, p , arise in various regimes of Bayesian inference. In a Bayesian analysis,

we seek to compute the posterior distribution $\pi(z|x)$ of a latent random variable z conditioned on some observation (or collection of observations) x . This posterior distribution is given by

$$\pi(z|x) \propto \pi(z)\pi(x|z), \quad (6)$$

where $\pi(z)$ is the prior distribution, and $\pi(x|z)$, the likelihood function. When VI is used for Bayesian analysis, the target density we approximate is $p(z) = \pi(z|x)$, and eq. (6) reveals how p may come to exhibit exact or approximate symmetries.

Common symmetry. The posterior $\pi(z|x)$ will inherit any common symmetry of the prior $\pi(z)$ and the likelihood $\pi(x|z)$ — for example, if the latter are both even or elliptically symmetric *about the same point*. This scenario is unlikely, although it can arise in empirical Bayes [Carlin and Louis, 2000]. If $\pi(x|z)$ and $\pi(z)$ are symmetric about different points, then the posterior $\pi(z|x)$ will not in general exhibit any symmetry. An exception occurs when both $\pi(x|z)$ and $\pi(z)$ are Gaussian, in which case $\pi(z|x)$ is also Gaussian.

Dominating prior. If the prior $\pi(z)$ is symmetric and “dominates” the likelihood, i.e. $\pi(z|x) \approx \pi(z)$, then the posterior inherits its symmetry to some degree. This occurs if the data is sparse and the likelihood uninformative.

Dominating likelihood. Conversely, suppose the likelihood dominates. This can occur if the prior $\pi(z)$ is flat (i.e. independent of z) or we have a large collection of observations x such that $\pi(z|x)$ is very strongly peaked. In particular, we know per the Bernstein-von-Mises theorem that asymptotically, and under certain regularity conditions, the posterior becomes provably Gaussian (and hence even-symmetric) in the limit of a large number of independent observations. We note, however, that the likelihood $\pi(x|z)$ for a *finite* number of observations does not generally exhibit a point of symmetry even when those observations are individually generated by even-symmetric distributions (e.g., Cauchy, Laplace); this breakdown occurs because the product of non-Gaussian distributions with *different* points of even-symmetry does not itself, in general, exhibit a point of even symmetry. Empirically, though, we find that such likelihoods tend to be approximately symmetric provided that the data is non-adversarial; see Appendix A for more discussion.

Fig. 1 illustrates how the symmetry of a posterior depends on the regime (sparse versus rich data) of Bayesian inference, and specifically on the number of observations, N , in a Bayesian logistic regression. We consider the model

$$\begin{aligned} \beta_0, \beta_1, \beta_2 &\stackrel{\text{iid}}{\sim} \text{Laplace}(0, 0.5), \\ y_i &\sim \text{Bernoulli}(\text{logit}^{-1}(\boldsymbol{\beta}^T \mathbf{x}_i)), \end{aligned} \quad (7)$$

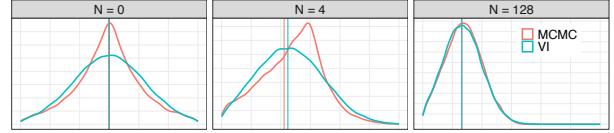


Figure 1: *Posterior distribution of β_1 for a Bayesian logistic regression with N examples. Vertical lines indicate the means estimated by MCMC and VI. These estimates match when the posterior is symmetric ($N=0, 128$) and differ when it is not ($N=4$).*

where $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2)$ and $\mathbf{x}_i = (1, x_{i1}, x_{i2})$ is the i^{th} component of a design matrix with two covariates. We compare the posteriors estimated by ADVI and, as a benchmark, long runs of Markov chain Monte Carlo (MCMC) for different numbers of examples. Both algorithms are implemented in the statistical software Stan [Carpenter et al., 2017]; see Appendix C.1 for details of these algorithms and Appendix C.2 for additional experimental results. Figure 1 plots these estimated posterior distributions for β_1 and $N=0, 4, 128$ examples. We see that the true posterior, as reported by MCMC, is even-symmetric for $N=0$ (where the posterior reduces to the prior) and very nearly symmetric for $N=128$, but clearly asymmetric for $N=4$, a regime where neither the prior nor the likelihood dominates.

Fig. 1 illustrates another result: the posterior mean is accurately estimated by VI when the posterior is symmetric ($N=0$ and $N=128$), but less accurately estimated when it is not ($N=4$). We now formalize this result, providing guarantees for VI when the target density is even-symmetric.

3 EXACT RECOVERY OF MEAN

In this section we prove that there are fairly broad conditions under which VI exactly recovers the mean of the target density. We also use simple examples to illustrate the scope of this result and various caveats. In all that follows, we assume that p and the base density $q_0 \in \mathcal{Q}$ have support on all of \mathbb{R}^d ; we also assume the regularity conditions on p in section 2.2.3.

3.1 Theoretical Statement

Our first theorem shows how VI is able to capitalize on an even symmetry of the target density.

Theorem 8 (Exact Recovery of Mean). *Let \mathcal{Q} be a location family whose base distribution q_0 is even-symmetric about the origin. If p is even-symmetric about μ , then $KL(q_\nu || p)$ has a stationary point at $\nu = \mu$; furthermore, if $\log p$ is concave on \mathbb{R}^d and strictly con-*

cave on some open set of \mathbb{R}^d , then this stationary point is a unique minimizer of $KL(q_\nu || p)$.

Proof. We start by exploiting the parameterized form of the location family \mathcal{Q} . For $q_\nu \in \mathcal{Q}$, we can compute

$$KL(q_\nu || p) = \int [\log q_\nu(z) - \log p(z)] q_\nu(z) dz, \quad (8)$$

$$= \int [\log q_0(\zeta) - \log p(\nu + \zeta)] q_0(\zeta) d\zeta, \quad (9)$$

$$= -\mathcal{H}(q_0) - \int \log p(\nu + \zeta) q_0(\zeta) d\zeta \quad (10)$$

where in eq. (9) we have shifted the variable of integration (to $\zeta = z - \nu$), and in eq. (10), we have used $\mathcal{H}(q_0)$ to denote the entropy of q_0 . Note that $\mathcal{H}(q_0)$ does not depend on the location parameter ν . The gradient of eq. (10) with respect to ν is therefore given by

$$\nabla_\nu KL(q_\nu || p) = - \int \nabla_\nu [\log p(\nu + \zeta)] q_0(\zeta) d\zeta, \quad (11)$$

$$= - \int \nabla_\zeta [\log p(\nu + \zeta)] q_0(\zeta) d\zeta, \quad (12)$$

where in eq. (11) we have differentiated under the integral sign, and in eq. (12) we have exploited the symmetric appearance of ζ and ν inside the gradient. Now suppose $\nu = \mu$. In this case the gradient is given by

$$\nabla_\nu KL(q_\nu || p) \Big|_{\nu=\mu} = - \int \nabla_\zeta [\log p(\mu + \zeta)] q_0(\zeta) d\zeta. \quad (13)$$

By assumption p is even-symmetric about μ , satisfying $p(\mu + \zeta) = p(\mu - \zeta)$. It follows that the gradient in the integrand of eq. (13) is odd-symmetric, with

$$\nabla_\zeta [\log p(\mu + \zeta)] = -\nabla_\zeta [\log p(\mu - \zeta)]. \quad (14)$$

Also recall, by assumption, that q_0 is even-symmetric about the origin, satisfying $q_0(\zeta) = q_0(-\zeta)$. Thus the integrand in eq. (13) is the product of an odd-symmetric and even-symmetric function, and hence an odd-symmetric function in its own right; accordingly, the integral must vanish when it is performed over all of \mathbb{R}^d . This proves the first claim of the theorem that $\nabla_\nu KL(q_\nu || p) = 0$ when $\nu = \mu$.

Now suppose that $\log p$ is concave on \mathbb{R}^d and strictly concave on some open set of \mathbb{R}^d . Under these assumptions, we show in Lemma 13 of appendix B that $KL(q_\nu || p)$ is strictly convex in ν , and hence the stationary point at $\nu = \mu$ corresponds to a unique minimizer. This proves the theorem. \square

Remark 9. VI also recovers the mean of p when \mathcal{Q} is a location-scale family or a subfamily thereof (e.g., one where the scale matrix is restricted to be diagonal). In this setting, the same steps yield a unique minimizer at $\nu = \mu$ for any value of the scale parameter.

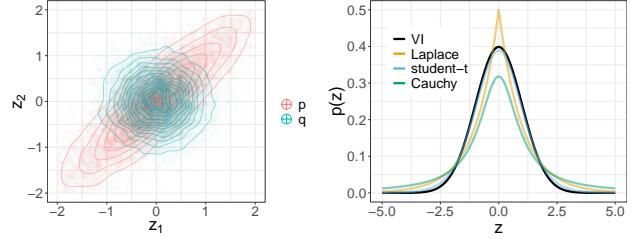


Figure 2: *Robustness of VI to misspecifications.* Left: VI with a factorized Gaussian, q , exactly recovers the mean of a multivariate student-t, p . Right: VI with a univariate Gaussian recovers the point of symmetry in target densities with different tails. This point equals the mean when the target is Laplace or student-t, but not when it is Cauchy (whose mean does not exist).

3.2 Illustrative examples

The content of the theorem is best illustrated by example. We emphasize that the conditions of the theorem allow for severe misspecifications in which the target density p cannot be well approximated over its whole domain by any $q \in \mathcal{Q}$. Our first examples illustrate how VI behaves when \mathcal{Q} is misspecified but still satisfies the conditions of the theorem—in particular, when q is factorized, but p is not, and when p is heavy-tailed, but q is not.

Non-factorized target with heavy tails. Figure 2 (left) illustrates how VI behaves when \mathcal{Q} is the family of Gaussians with diagonal covariance matrices and p is a heavy-tailed two-dimensional student-t with $k = 10$ degrees of freedom and correlation 0.9 between z_1 and z_2 . Despite these misspecifications, p and \mathcal{Q} satisfy all the conditions of the theorem, and VI exactly recovers the mean of p .

Other heavy-tailed targets. Figure 2 (right) illustrates how VI behaves when \mathcal{Q} is the family of one-dimensional Gaussians and p is (i) a Laplace distribution, (ii) a student-t distribution with $k = 10$ degrees of freedom, and (iii) a Cauchy distribution. In all of these cases, VI recovers the point of symmetry of p ; this point is equal to the mean of p for the Laplace and student-t distributions, and to the median of p for the Cauchy distribution (whose mean does not exist).

Our next examples illustrate how VI behaves when the conditions of the theorem are *not* satisfied.

Bimodal target. Figure 3 illustrates how VI behaves when fitting a normal approximation to a balanced mixture of two univariate Gaussians:

$$p(z) = 0.5 \mathcal{N}(z; -m, 1) + 0.5 \mathcal{N}(z; m, 1), \quad (15)$$

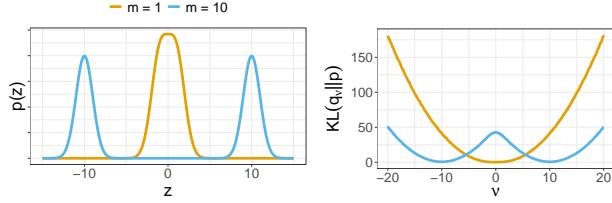


Figure 3: Approximating the mixture p of two normals in eq. (15) when the modes are close ($m=1$) or well separated ($m=10$). Left: probability densities. Right: KL divergence between p and a single normal q_ν with mean ν . Per Theorem 8, $\text{KL}(q_\nu||p)$ has a stationary point at $\nu=0$. This stationary point is a minimizer when $m=1$ but a local maximizer when $m=10$.

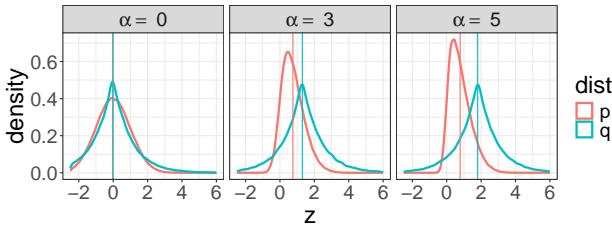


Figure 4: VI approximation of a skewed normal distribution, p , by a Laplace distribution, q . The vertical lines indicate the mean of each distribution. Per Theorem 8, VI correctly estimates the mean of p when $\alpha=0$ and p is symmetric. However, VI's estimate worsens as α increases and p becomes less symmetric.

In this example, p is symmetric about the origin, but it is not log-concave, thus violating one of the theorem's conditions. The figure illustrates two cases—one where the modes of p are close, with $m=1$ in eq. (15), and another, where they are well separated, with $m=10$. Per the theorem, $\text{KL}(q_\nu||p)$ has a stationary point at the origin. However, when p has well-separated modes, this stationary point is not a local minimizer of $\text{KL}(q||p)$; instead it is a local *maximizer*. In this case, VI would not center its approximation at the origin, but instead at one of the two modes.

Asymmetric target. Figure 4 illustrates how VI misestimates the mean when p is not symmetric. In this example, we consider

$$\begin{aligned} p(z) &= \text{skewed-Normal}(z; 0, 1, \alpha) \\ q(z) &= \text{Laplace}(z; \nu, 1), \end{aligned} \quad (16)$$

where $\alpha \in \mathbb{R}$ controls the skewness of p , and the location ν of q is obtained by minimizing $\text{KL}(q||p)$. Note that in this example, because q is Laplace, the variational approximation is misspecified even when p is not skewed. The greater the skewness of p , the less

accurate is VI's estimate of the mean.

4 EXACT RECOVERY OF CORRELATION MATRIX

Next we prove that under fairly broad conditions VI can exactly recover the correlation matrix of the target density. Here again we assume that p and the base density $q_0 \in \mathcal{Q}$ have support on all of \mathbb{R}^d ; we also assume the regularity conditions on p in section 2.2.3.

4.1 Theoretical statement

Our second theorem shows how VI is able to capitalize on an elliptical symmetry of the target density.

Theorem 10 (Exact Recovery of Correlation Matrix). *Let \mathcal{Q} be a location-scale family whose base distribution q_0 is spherically symmetric. If p is elliptically symmetric about μ with scale matrix M , and if $\log p$ is concave on \mathbb{R}^d and strictly concave on some open set of \mathbb{R}^d , then $\text{KL}(q||p)$ has a unique minimizer with respect to the location-scale parameters (ν, S) of \mathcal{Q} at $\nu=\mu$ and $S=\gamma^2 M$ for some $\gamma \in \mathbb{R}$. Per Remark 7, the correlation matrix is recovered at this minimizer.*

Proof. Let $q \in \mathcal{Q}$ with location-scale parameters (ν, S) . Write $q(z) = q_0(\zeta) |S|^{-\frac{1}{2}}$ where $\zeta = S^{-\frac{1}{2}}(z - \nu)$. Then, analogous to eqs. (8–10), we can compute

$$\begin{aligned} \text{KL}(q||p) &= -\mathcal{H}(q_0) - \frac{1}{2} \log |S| \\ &\quad - \int \log p(S^{\frac{1}{2}}\zeta + \nu) q_0(\zeta) d\zeta. \end{aligned} \quad (17)$$

By the assumption of elliptical symmetry, there exists a spherically symmetric density p_0 such that

$$p(z) = p_0(M^{-\frac{1}{2}}(z - \mu)) |M|^{-\frac{1}{2}}. \quad (18)$$

Substituting the above into eq. (17), we obtain a generalization of eq. (10) to location-scale families:

$$\begin{aligned} \text{KL}(q||p) &= -\mathcal{H}(q_0) - \frac{1}{2} \log |S| + \frac{1}{2} \log |M| \\ &\quad - \int \log p_0(M^{-\frac{1}{2}}[S^{\frac{1}{2}}\zeta + \nu - \mu]) q_0(\zeta) d\zeta. \end{aligned}$$

Since p_0 and q_0 are spherically symmetric, they are also even-symmetric about the origin; per Theorem 8, the above is minimized with respect to the location parameter when $\nu=\mu$. Eliminating ν , we find

$$\begin{aligned} \text{KL}(q||p) &= -\mathcal{H}(q_0) - \frac{1}{2} \log |S| + \frac{1}{2} \log |M| \\ &\quad - \int \log p_0(M^{-\frac{1}{2}}S^{\frac{1}{2}}\zeta) q_0(\zeta) d\zeta. \end{aligned} \quad (19)$$

To prove the theorem we must minimize the right side of eq. (19) with respect to the scale parameter S , or

equivalently, with respect to the matrix $J = M^{-\frac{1}{2}}S^{\frac{1}{2}}$. In terms of this matrix, eq. (19) simplifies to

$$\text{KL}(q||p) = -\mathcal{H}(q_0) - \log|J| - \int \log p_0(J\zeta) q_0(\zeta) d\zeta. \quad (20)$$

Eq. (20) shows that after eliminating the location parameter, the remaining objective for VI is strictly convex in J ; this property follows the strict concavity of $\log|J|$ and the assumption that p (and hence also p_0) is log-concave. Hence, any stationary point of eq. (20) corresponds to a unique global minimizer. We will show that such a stationary point occurs when

$$J = \gamma I \quad (21)$$

for some $\gamma > 0$. The rest of the proof uses the symmetry of p_0 and q_0 to verify this ansatz, which in turn implies that $S = \gamma^2 M$.

Since p_0 and q_0 are spherically symmetric, we can define functions $f, g : \mathbb{R} \rightarrow \mathbb{R}$ by the relations

$$f(\|J\zeta\|) = \log p_0(J\zeta), \quad (22)$$

$$g(\|\zeta\|) = q_0(\zeta). \quad (23)$$

We can also compute the gradient of eq. (20) with respect to J in terms of these functions; it is given by

$$\nabla_J \text{KL}(q||p) = -J^{-1} - \int f'(\|J\zeta\|) \frac{J\zeta\zeta^\top}{\|J\zeta\|} g(\|\zeta\|) d\zeta. \quad (24)$$

If a minimizer exists at $J = \gamma I$, then this gradient must vanish there; equivalently, it must be the case that

$$\gamma^{-1} I = - \int f'(\gamma\|\zeta\|) \frac{\zeta\zeta^\top}{\|\zeta\|} g(\|\zeta\|) d\zeta. \quad (25)$$

We complete the proof by showing that eq. (25) determines a unique solution for some $\gamma > 0$.

First we verify that the right side of eq. (25) is a scalar multiple of the identity matrix. To do so, we consider how to perform the i^{th} component of the integration,

$$\int d\zeta_{\setminus\{i\}} \int d\zeta_i \left[f'(\gamma\|\zeta\|) g(\|\zeta\|) \|\zeta\|^{-1} \right] \zeta_j \zeta_i \quad (26)$$

and note that the bracketed term in the integrand is spherically symmetric (and hence also invariant under the change of variables $\zeta_i \rightarrow -\zeta_i$). Now if $i \neq j$, then the integrand as a whole is an odd-symmetric function of ζ_i , and hence the integral over all positive and negative values of ζ_i vanishes. On the other hand, if $i = j$, then from the spherical symmetry of the bracketed term it follows that the integral has the same value for all i . This implies, in turn, that all the diagonal elements on the right side of eq. (25) are equal.

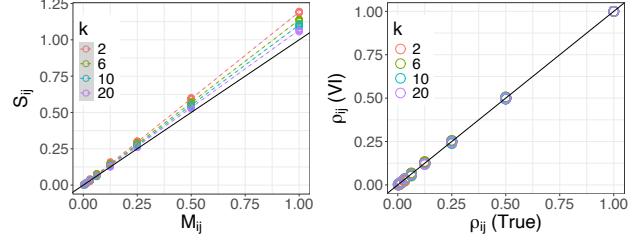


Figure 5: Gaussian approximation of VI to a multivariate student-t with varying degrees of freedom, k . Left: VI's scale matrix S equals the target's scale matrix M , up to a multiplicative constant, which varies with k . Right: for all k , VI exactly recovers the elements ρ_{ij} of the correlation matrix.

It remains to prove that a solution exists for γ . Since each side of eq. (25) is a scalar multiple of the identity matrix, we can solve for γ by equating their traces:

$$\begin{aligned} d\gamma^{-1} &= - \int f'(\gamma\|\zeta\|) g(\|\zeta\|) \|\zeta\|^{-1} \sum_i \zeta_i^2 d\zeta \\ &= - \int f'(\gamma\|\zeta\|) g(\|\zeta\|) \|\zeta\| d\zeta. \end{aligned} \quad (27)$$

We proceed by evaluating the integral in spherical coordinates with $r = \|\zeta\|$. After integrating out the angular coordinates, eq. (27) reduces to

$$d\gamma^{-1} = - \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \int f'(\gamma r) g(r) r^d dr, \quad (28)$$

where we leveraged the fact the surface area of a d -dimensional hypersphere of radius r is $2\pi^{\frac{d}{2}} r^{d-1} / \Gamma(d/2)$. Note that the left side of eq. (28) decreases monotonically with γ from infinity to zero; thus the right side will determine a unique solution if it is a positive non-decreasing function of γ . Now, the log concavity of p implies that the derivative of $\log p$ is monotone. Then, it follows from eqs. (18) and (22) that $-f'(\gamma r)$ is a non-decreasing function of γ . It must also be true that $-f'(0) \geq 0$, since otherwise $\log p$ would have a non-concave kink at the origin. Thus the right side of eq. (28) is indeed a positive non-decreasing function of γ , and a unique solution for γ is determined. \square

4.2 Illustrative examples

Figure 5 illustrates how VI with a Gaussian scale-location family recovers the correlation matrix of multivariate Student-t target densities in \mathbb{R}^{10} . We set

$$p(z) = \text{multi-student-t}(z; k, 0, M), \quad (29)$$

$$q(z) = \mathcal{N}(z; \nu, S), \quad (30)$$

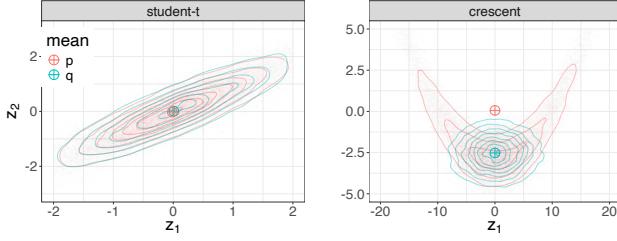


Figure 6: VI with a Gaussian approximation and dense covariance matrix. Left: VI recovers the mean, correlation, and iso-probability contours when the target (student-t) has elliptical symmetry. Right: VI recovers neither the mean nor correlation when the target (crescent) has neither even nor elliptical symmetry.

where k denotes the number of degrees of freedom in the Student-t target, M its scale matrix, and S the covariance matrix of the Gaussian approximation. In this example, the elements of M were one along the diagonal and constant off the diagonal ($S_{ij} = 0.9$ for $i \neq j$). The results in the figure were obtained by ADVI for target densities with heavier tails ($2 \leq k \leq 20$) than q , particularly for small values of k . The results verify Theorem 10: S matches M up to a multiplicative constant and thus yields the exact correlation matrix of p .

Figure 6 (right) shows how VI behaves on the two-dimensional Rosenbrock or *crescent* distribution,

$$\begin{aligned} p(z_1) &= \mathcal{N}(0, 10^2), \\ p(z_2|z_1) &= \mathcal{N}(0.03(z_1 - 100)^2, 1), \end{aligned} \quad (31)$$

which does *not* have elliptical symmetry. In this case, the approximation in eq. (30) recovers neither the mean nor the correlation; see also Table 1. Note, however, that the Rosenbrock distribution is symmetric about the line $z_1 = 0$, and that VI does correctly recover the first component of its mean.

5 NUMERICAL EXPERIMENTS

We now investigate VI on the collection of target distributions in Table 1. Three of these distributions are synthetic: `student` is a student-t distribution with elliptical symmetry and heavy tails, while `mixture` and `crescent` are not even-symmetric. The others in Table 1 arise as posteriors of Bayesian models; these include a centered hierarchical model (`8schools`) with a highly asymmetric posterior [Gelman et al., 2013], a non-centered parameterization of the same model (`8schools_nc`) with better geometry, a binomial regression (`GLM`), a Gaussian process (`disease_map`) [Vanhatalo et al., 2010], and a sparse kernel interaction model (`SKIM`) [Agrawal et al., 2019], applied to a

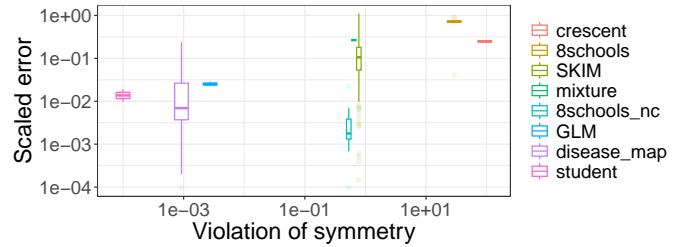


Figure 7: Scaled error in VI’s estimates of the mean, using a Gaussian approximation, versus the asymmetry of its targets. The box plot summarizes the errors for all latent variables. As a trend, VI’s estimates are better when its targets are more symmetric (even if they are not Gaussian). See text for details.

genomic data set [Margossian et al., 2020]. It is unclear how much symmetry is present in the posteriors of the last three models. Further details of each model can be found in Appendix C.3. We fit these targets in Stan with both ADVI and long runs of MCMC, and we use the latter as a stand-in for ground truth.

For each distribution in Table 1, we use a stochastic procedure to assess whether it is approximately even-symmetric. Given a draw z from $p(z)$ —obtained by MCMC for the more complex distributions—we compute the *reflected* sample $z' = 2\mu - z$, where μ is the (estimated) mean of z with respect to the density p . For each (z, z') pair, we then compute the violation

$$\varepsilon(z) = \left| \frac{\log \pi(z|x) - \log \pi(z'|x)}{\log \pi(z|x)} \right|. \quad (32)$$

If $\pi(z|x)$ is even-symmetric about μ , then $\varepsilon(z)$ vanishes for all z . We evaluate $\varepsilon(z)$ at many (MCMC) samples and report the 90th quantile ε_{90} in Table 1.

For each target, we also report how well ADVI estimates its mean, correlation, and covariance. We use

$$\Delta_{\text{mean}} = \frac{|\mathbb{E}_p(z) - \mathbb{E}_q(z)|}{\max(\sqrt{\text{Var}_p(z)}, |\mathbb{E}_p(z)|)} \quad (33)$$

to measure the error of the estimated means. Eq. (33) is both scale-free and numerically stable; see Appendix C.1 for further justification of this choice. We also measure the absolute relative error of the covariances and the absolute error of the correlations (which are already scale-free); in Table 1 we denote these, respectively, by Δ_{cov} and Δ_{corr} .

The plot reveals a trend: VI yields worse estimates as p becomes less symmetric, with the worst estimates obtained for the Rosenbrock distribution (`crescent`) and the centered hierarchical model (`8schools`). Table 1 also reports the error in estimates of the correlations and covariances. Estimates of the former are

Call name	d	Description	ε_{90}	Δ_{mean}	Δ_{corr}	Δ_{cov}
student	2	Elliptical target with heavy tails.	0	0.014	2.42e-3	0.093
disease_map	102	Gaussian process model for epidemiology data.	9.22e-4	0.026	0.017	5.29
GLM	3	Binomial regression for ecological data.	2.73e-3	0.025	0.10	6.71
8schools_nc	10	Non-centered hierarchical model for education data.	0.50	0.004	0.010	1.01
mixture	2	Mixture of two Gaussians with different scales.	0.54	0.26	0.27	23.40
SKIM	305	Sparse kernel interaction model for genetic data.	0.82	0.12	0.014	8.30
8schools	10	Centered hierarchical model for education data.	29.31	0.68	0.11	0.90
Crescent	2	Rosenbrock distribution.	93.48	0.25	0.26	1.395

Table 1: *Scaled errors ($\Delta_{\text{mean}}, \Delta_{\text{corr}}, \Delta_{\text{cov}}$) from VI when estimating the mean, correlation, and covariance of the target density, p . Errors are averaged across all elements of mean vectors and correlation/covariance matrices, and data sets are ordered by the degree to which p violates the assumption of even symmetry, as measured by ε_{90} in eq. (32). As a trend, less symmetric targets yield worse estimates of the mean and correlation; also, the correlation can be well-estimated even when the covariance is not.*

consistently better than the latter. However, the correlation matrix is estimated poorly for the three models that most clearly violate elliptical symmetry (`mixture`, `8schools`, `crescent`).

In summary, blatantly asymmetric distributions produce VI estimators with a large error. Conversely, targets with a near-perfect symmetry yield accurate estimators. Still, it is unclear from our experiments how varying degrees of asymmetry affect the quality of VI estimators. Two intriguing cases are the `8schools_nc` and `mixture` models, which have a comparable violation of symmetry, however the error in `mixture` is noticeably larger.

6 DISCUSSION

In this paper, we have derived broad conditions under which VI with location-scale families exactly recovers the mean and the correlation matrix. Our proofs use basic principles of symmetry to illustrate settings in which $\text{KL}(q||p)$ has a unique global minimizer. The conditions of our theorems allow for several misspecifications: notably, the approximation q need not match the tail behavior of the target p and, when estimating the mean, q can be factorized even though p is not.

In a Bayesian setting, the mean is most commonly used to summarize the posterior, and the correlation, though less often reported, is also of interest. Conceivably, one could employ the scale matrix S returned by VI as a pre-conditioner for other inference algorithms, such as MCMC, which are known to converge more quickly for (approximately) spherically symmetric distributions. This is a direction for future work.

Our results assume that VI algorithms find a minimizer of $\text{KL}(q||p)$, which in practice may not be true. It can be challenging to optimize the ELBO [Dhaka et al., 2020, 2021, Agrawal et al., 2021]; however, re-

cent papers provide convergence guarantees for the optimizations in VI [Lambert et al., 2022, Diao et al., 2023, Domke et al., 2023, Kim et al., 2023, Jiang et al., 2024]. These articles, combined with our paper, ensure that VI converges to useful estimates of its targets. Some of these articles also provide directions for future research, as they consider families of approximations beyond the location-scale families in this paper. For example, Lambert et al. [2022] examine Gaussian mixtures, and Jiang et al. [2024] study the family of all factorized distributions. A natural avenue for future work is to analyze the role of symmetries in the variational approximations for these families.

It would also be interesting to study cases where the target distribution p is nearly symmetric or (at the opposite extreme) highly asymmetric. Another direction for future work is to bound the error of VI’s estimates in terms of measurable violations of symmetry. Such an approach would align with statistical analyses of VI in asymptotic regimes [e.g. Zhang and Gao, 2020, Katsevich and Rigollet, 2024]; these analyses have yielded pre-asymptotic error bounds and shown that exact estimates are recovered asymptotically. A related goal is to construct post-hoc diagnostics which leverage empirical measures of asymmetry (as in Section 5). Our experiments with asymmetric distributions revealed many cases where the error of VI is unacceptably large, and these cases provides further motivation for skewed variational approximations [Tan and Chen, 2024].

Finally, an intriguing conjecture, also deserving of study, is that for each symmetry of p , there is a corresponding statistic that VI under mild conditions can exactly recover.

Acknowledgments

We thank four anonymous referees for their constructive feedback.

References

- Abhinav Agrawal, Daniel R. Sheldon, and Justin Domke. Advances in black-box VI: Normalizing flows, importance weighting, and optimization. *Advances in Neural Information Processing Systems* 33, 2021.
- Raj Agrawal, Jonathan H Huggins, Brians Trippe, and Tamara Broderick. The Kernel interaction trick: Fast Bayesian discovery of pairwise interactions in high dimensions. *International Conference on Machine Learning*, 2019.
- Pierre Alquier and James Ridgway. Concentration of tempered posteriors and of their variational approximations. *The Annals of Statistics*, 48(3):1475–1497, 2020. doi: 10.1214/19-AOS1855.
- Michael Betancourt. A conceptual introduction to Hamiltonian Monte Carlo. *arXiv:1701.02434v1*, 2018.
- Niloy Biswas and Lester Mackey. Bounding Wasserstein distance with couplings. *Journal of the American Statistical Association*, Ahead-of-print:1–12, 2023. doi: 10.1080/01621459.2023.2287773.
- David M. Blei, Alp Kucukelbir, and Jon D. McAuliffe. Variational inference: A review for statisticians. *Journal of the American Statistical Association*, 112:859–877, 2017. doi: 10.1080/01621459.2017.1285773.
- Diana Cai, Chirag Modi, Loucas Pillaud-Vivien, Charles C. Margossian, Robert M. Gower, David M. Blei, and Lawrence K. Saul. Batch and match: black-box variational inference with a score-based divergence. *Proceedings of the 41st International Conference on Machine Learning*, page 5258–5297, 2024.
- Bradley P. Carlin and Thomas A. Louis. *Bayes and Empirical Bayes Methods for Data Analysis*. Chapman & Hall/CRC, 2 edition, 2000.
- Bob Carpenter, Andrew Gelman, Matt Hoffman, Daniel Lee, Ben Goodrich, Michael Betancourt, Marcus A. Brubaker, Jiqiang Guo, Peter Li, and Allen Riddell. Stan: A probabilistic programming language. *Journal of Statistical Software*, 76:1–32, 2017.
- Akash K. Dhaka, Alejandro Catalina, Michael R. Andersen, Måns Magnusson, Jonathan Huggins, and Aki Vehtari. Robust, accurate stochastic optimization for variational inference. *Advances in Neural Information Processing Systems* 33, 2020.
- Akash K. Dhaka, Alejandro Catalina, Manushi Welandawe, Michael R. Andersen, Jonathan Huggins, and Aki Vehtari. Challenges and opportunities in high dimensional variational inference. *Advances in Neural Information Processing Systems* 34, 2021.
- Michael Ziyang Diao, Krishna Balasubramanian, Sinho Chewi, and Adil Salim. Forward-backward gaussian variational inference via jko in the bures-wasserstein space. In *International Conference on Machine Learning*, pages 7960–7991. PMLR, 2023.
- Justin Domke, Robert M. Gower, and Guillaume Garigo. Provable convergence guarantees for black-box variational inference. *Advances in Neural Information Processing Systems* 36, 2023.
- Andrew Gelman, John B. Carlin, Hal S. Stern, David B. Dunson, Ark Vehtari, and Donald B. Rubin. *Bayesian Data Analysis*. Chapman & Hall/CRC Texts in Statistical Science, 2013.
- Rian Giordano, Tamara Broderick, and Michael I. Jordan. Covariances, robustness, and variational Bayes. *Journal of Machine Learning Research*, 19:1–49, 2018.
- Geoffrey E. Hinton and Drew Van Camp. Keeping the neural networks simple by minimizing the description length of the weights. In *Proceedings of the Sixth Annual Conference on Computational Learning Theory*, pages 5–13. ACM, August 1993. doi: 10.1145/168304.168306.
- Matthew D. Hoffman and Andrew Gelman. The no-U-turn sampler: Adaptively setting path lengths in Hamiltonian Monte Carlo. *Journal of Machine Learning Research*, 15:1593–1623, 2014.
- Jonathan H. Huggins, Mikołaj Kasprzak, Trevor Campbell, and Tamara Broderick. Validated variational inference via practical posterior error bounds. In *Proceedings of the 23rd International Conference on Artificial Intelligence and Statistics*, pages 1792–1802, 2020.
- Yiheng Jiang, Sinho Chewi, and Aram-Alexandre Pooladian. Algorithms for mean-field variational inference via polyhedral optimization in the wasserstein space. *Conference on Learning Theory*, 2024.
- Michael I. Jordan, Zoubin Ghahramani, Tommi S. Jaakkola, and Lawrence K. Saul. An introduction to variational methods for graphical models. *Machine Learning*, 37:183–233, 1999.
- Alexander Katsevich and Philippe Rigollet. On the approximation accuracy of gaussian variational inference. *The Annals of Statistics*, 52(4):1384–1409, 2024. doi: 10.1214/24-AOS2321.
- Kyurae Kim, Jisu Oh, Kaiwen Wu, Yi-An Ma, and Jacob R. Gardner. On the convergence and scale parameterizations of black-box variational inference. *Advances in Neural Information Processing Systems* 36, 2023.

-
- Diederik P. Kingma and Max Welling. Auto-encoding variational Bayes. *International Conference on Learning Representations*, 2014.
- Alp Kucukelbir, Dustin Tran, Rajesh Ranganath, Andrew Gelman, and David Blei. Automatic differentiation variational inference. *Journal of Machine Learning Research*, 18:1–45, 2017.
- Marc Lambert, Sinho Chewi, Francis Bach, Silv‘ere Bonnabel, and Philippe Rigollet. Variational inference via wasserstein gradient flows. *Advances in Neural Information Processing Systems*, 35:14434–14447, 2022.
- Yingzhen Li and Richard E. Turner. Rényi divergence variational inference. In *Advances in Neural Information Processing Systems 29*, pages 1073–1081, 2016.
- David J.C. MacKay. *Information theory, inference, and learning algorithms*. Cambridge University Press, 2003.
- Måns Magnusson, Jakob Torgander, Paul-Christian Bürkner, Lu Zhang, Bob Carpenter, and Aki Vehtari. PosteriorDB: Testing, benchmarking and developing bayesian inference algorithms. *arXiv:2407.04967*, 2024.
- Charles C. Margossian and Lawrence K. Saul. The shrinkage-delinkage trade-off: An analysis of factorized Gaussian approximations for variational inference. In *Proceedings of the 39th Conference on Uncertainty in Artificial Intelligence*, pages 1358–1367, 2023.
- Charles C. Margossian, Aki Vehtari, Daniel Simpson, and Raj Agrawal. Hamiltonian Monte Carlo using an adjoint-differentiated Laplace approximation: Bayesian inference for latent gaussian models and beyond. *Advances in Neural Information Processing Systems* 33, 2020.
- Charles C. Margossian, Lucas Pillaud-Vivien, and Lawrence K. Saul. Variational inference for uncertainty quantification: an analysis of trade-offs. *arXiv:2403.13748*, 2024.
- Radford M Neal. Annealed importance sampling. *Statistics and Computing*, 11:125–139, 2001.
- Georgio Parisi. *Statistical Field Theory*. CRC Press, 1998.
- Caroline Peterson. A mean field theory learning algorithm for neural network. *Complex Systems*, 1: 995–1019, 1987.
- Juho Piironen and Aki Vehtari. Sparsity information and regularization in the horseshoe and other shrinkage priors. *Electronic Journal of Statistics*, 11: 5018–5051, 2017.
- Rajesh Ranganath, Sean Gerrish, and David Blei. Black box variational inference. In *Proceedings of the Seventeenth International Conference on Artificial Intelligence and Statistics*, pages 814–822, 2014.
- Danielo Jimenez Rezende, Shakir Mohamed, and Wierstra Daan. Stochastic backpropagation and approximate inference in deep generative models. In *Proceedings of the 31st International Conference on Machine Learning*, pages 1278–1286, 2014.
- Edward A. Roualdes, Brian Ward, Bob Carpenter, Adrian Syboldt, and Seth D. Axen. Bridgestan: Efficient in-memory access to the methods of a Stan model. *Journal of Open Source Software*, 8, 2023.
- Donald B Rubin. Estimation in parallelized randomized experiments. *Journal of Educational Statistics*, 6:377–400, 1981.
- Linda S. L. Tan and Aoxiang Chen. Variational inference based on a subclass of closed skew normals. *Journal of Computational and Graphical Statistics*, pages 1–15, 2024. doi: 10.1080/10618600.2024.2402278.
- Michalis Titsias and Marcos Lázaro-Gredilla. Doubly stochastic variational bayes for non-conjugate inference. In *International Conference on Machine Learning*, pages 1971–1979. PMLR, June 2014.
- Richard E. Turner and Maneesh Sahani. Two problems with variational expectation maximisation for time-series models. In David Barber, A. Taylan Cemgil, and Silvia Chiappa, editors, *Bayesian Time series models*, chapter 5, pages 109–130. Cambridge University Press, 2011.
- Aad van der Vaart. *Asymptotic Statistics*. Cambridge University Press, 1998.
- Jarno Vanhatalo, Ville Pietiläinen, and Aki Vehtari. Approximate inference for disease mapping with sparse Gaussian processes. *Statistics in Medicine*, 29:1580–1607, 2010.
- Aki Vehtari, Daniel Simpson, Andrew Gelman, Yuling Yao, and Jonah Gabry. Pareto smoothed importance sampling. *Journal of Machine Learning Research*, 2024. To appear.
- Martin J. Wainwright and Michael I. Jordan. Graphical models, exponential families, and variational inference. *Foundations and Trends in Machine Learning*, 1(1–2):1–305, 2008.
- Yixin Wang and David M. Blei. Frequentist consistency of variational Bayes. *Journal of the American Statistical Association*, 114:1147–1161, 2018.
- Eunjee Yang, Debdeep Pati, Michael I. Jordan, and Martin J. Wainwright. α -variational inference with statistical guarantees. *The Annals of Statistics*, 48 (2):886–905, 2020. doi: 10.1214/19-AOS1827.

Yuling Yao, Aki Vehtari, Daniel Simpson, and Andrew Gelman. Yes, but did it work?: Evaluating variational inference. In *Proceedings of the 35th International Conference on Machine Learning*, pages 5577–5586, 2018.

Fangzheng Zhang and Chao Gao. Convergence rates of variational posterior distributions. *The Annals of Statistics*, 48(4):2180–2207, 2020.

Lu Zhang, Bob Carpenter, Andrew Gelman, and Aki Vehtari. Pathfinder: Parallel quasi-Newton variational inference. *Journal of Machine Learning Research*, 23(306):1–49, 2022.

Checklist

1. For all models and algorithms presented, check if you include:
 - (a) A clear description of the mathematical setting, assumptions, algorithm, and/or model. **[Yes]**
 - (b) An analysis of the properties and complexity (time, space, sample size) of any algorithm. **[Not Applicable]**
 - (c) (Optional) Anonymized source code, with specification of all dependencies, including external libraries. **[Yes.]**
2. For any theoretical claim, check if you include:
 - (a) Statements of the full set of assumptions of all theoretical results. **[Yes]**
 - (b) Complete proofs of all theoretical results. **[Yes]**
 - (c) Clear explanations of any assumptions. **[Yes]**
3. For all figures and tables that present empirical results, check if you include:
 - (a) The code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL). **[Yes]**
 - (b) All the training details (e.g., data splits, hyperparameters, how they were chosen). **[Yes]**
 - (c) A clear definition of the specific measure or statistics and error bars (e.g., with respect to the random seed after running experiments multiple times). **[Yes]**
 - (d) A description of the computing infrastructure used. (e.g., type of GPUs, internal cluster, or cloud provider). **[Yes]**
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets, check if you include:
 - (a) Citations of the creator If your work uses existing assets. **[Yes]**
 - (b) The license information of the assets, if applicable. **[Not Applicable]**
 - (c) New assets either in the supplemental material or as a URL, if applicable. **[Not Applicable]**
 - (d) Information about consent from data providers/curators. **[Not Applicable]**
 - (e) Discussion of sensible content if applicable, e.g., personally identifiable information or offensive content. **[Not Applicable]**

5. If you used crowdsourcing or conducted research with human subjects, check if you include:
 - (a) The full text of instructions given to participants and screenshots. **[Not Applicable]**
 - (b) Descriptions of potential participant risks, with links to Institutional Review Board (IRB) approvals if applicable. **[Not Applicable]**
 - (c) The estimated hourly wage paid to participants and the total amount spent on participant compensation. **[Not Applicable]**

A SYMMETRY OF LIKELIHOOD

In this appendix, we empirically investigate the symmetry properties of the likelihood. We examine independent and identically distributed observations, meaning the likelihood factorizes as

$$\pi(x | z) = \prod_i \pi(x_i | z). \quad (34)$$

Recall that the likelihood is a function of z , with x kept fixed. We consider the Gaussian, Cauchy, Laplace, and logistic distributions, and take z to be their location parameter. In all these cases, the single-component likelihood $\pi(x_i | z)$ admits a point of symmetry at x_i . However, the product of these single-component likelihoods does not in general have a point of symmetry. The exception is the Gaussian case, where the likelihood is always symmetric about the mean of x .

A natural condition for the likelihood to be symmetric is for the data itself to be symmetric. To illustrate this, we generate N observations. First we create $N = 3$ adversarial samples $x = (-1, 0, 20)$. These observations are deliberately asymmetric, and produce asymmetric likelihoods (Figure 8). Next we generate $N = 3$ ideal samples, $x = (-1, 0, 1)$, which are symmetric and produce symmetric likelihoods. Finally, we randomly draw $N = 10$ and $N = 100$ observations from a symmetric distribution p (somewhat arbitrarily, we chose

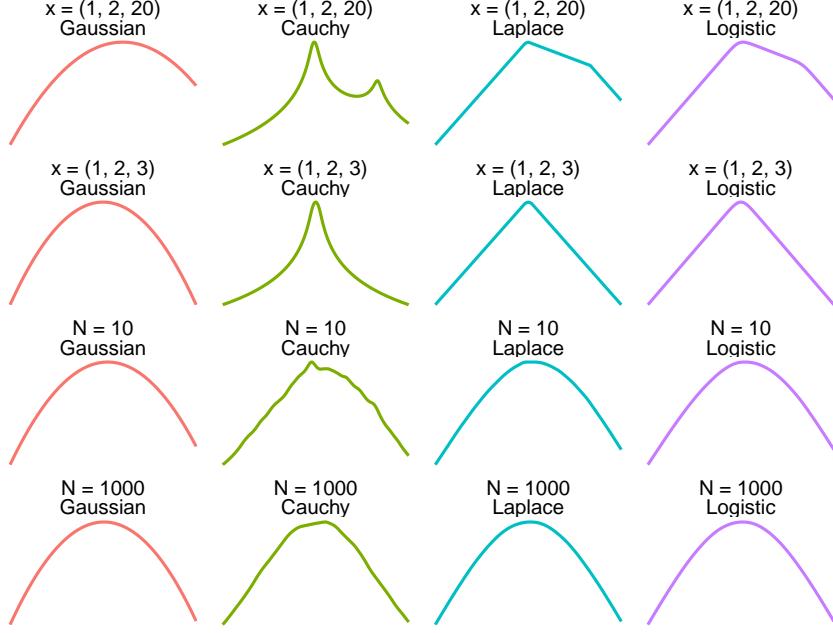


Figure 8: *Symmetry of the log likelihood $f_x(z) = \log \pi(x | z)$.* In the Gaussian case, the likelihood function is always symmetric about the mean of x . Other likelihoods do not in general admit a point of symmetry, as illustrated in the first row. However, if the data is symmetric, the likelihood is also symmetric (second row). Drawing data from a symmetric distribution generates samples which are approximately symmetric, and correspondingly approximately symmetric likelihoods.

p to be Gaussian though any well-behaved symmetric distribution would do). While no particular realization of the data is exactly symmetric, the data is “on average” symmetric. Already for $N = 10$, we find that all non-Gaussian likelihoods are approximately symmetric, with the symmetry becoming stronger for $N = 1000$.

B SUPPORTING PROOFS

In this appendix we prove that the KL divergence in eqs. (8–10) is *strictly* convex in the location parameter ν . This result for $\text{KL}(q_\nu || p)$ is needed in Theorem 8 to prove that VI recovers the exact mean, and it is also needed in Theorem 10 to prove that VI recovers the exact correlation matrix.

We begin by proving two simpler propositions: these propositions show that certain basic properties of strictly convex functions extend to functions that are everywhere convex but only strictly convex on some open set. We begin, in the simplest case, by establishing a property of such functions on the real line.

Proposition 11. *Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be differentiable on \mathbb{R} . Also, let $x_0, x_1 \in \mathbb{R}$ with $x_0 < x_1$, and let*

$$x_\lambda = (1 - \lambda)x_0 + \lambda x_1 \quad (35)$$

for some $\lambda \in (0, 1)$. If f is convex on \mathbb{R} and strictly

convex in a neighborhood of x_λ , then

$$f(x_\lambda) < (1 - \lambda)f(x_0) + \lambda f(x_1) \quad (36)$$

where the above inequality is strict.

Proof. Since f is differentiable, and since $x_0 < x_\lambda < x_1$, we can write

$$f(x_0) = f(x_\lambda) - \int_{x_0}^{x_\lambda} f'(\xi) d\xi, \quad (37)$$

$$f(x_1) = f(x_\lambda) + \int_{x_\lambda}^{x_1} f'(\xi) d\xi. \quad (38)$$

Since f is convex on \mathbb{R} , its derivative is everywhere non-decreasing; also, since f is strictly convex in some interval containing x_λ , its derivative is strictly increasing on this interval. From these observations and the form of eqs. (37–38), we deduce that

$$f(x_0) > f(x_\lambda) - (x_\lambda - x_0)f'(x_\lambda), \quad (39)$$

$$f(x_1) > f(x_\lambda) + (x_1 - x_\lambda)f'(x_\lambda). \quad (40)$$

Next we use eq. (35) to eliminate x_λ from the differences in the above expressions. In this way we find

$$f(x_0) > f(x_\lambda) - \lambda(x_1 - x_0)f'(x_\lambda), \quad (41)$$

$$f(x_1) > f(x_\lambda) + (1 - \lambda)(x_1 - x_0)f'(x_\lambda). \quad (42)$$

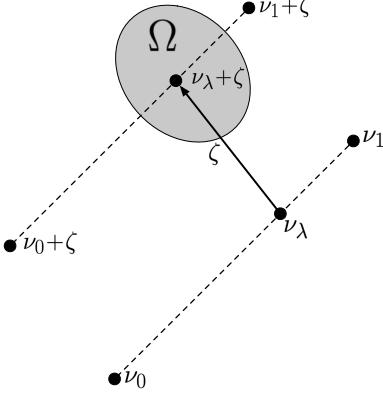


Figure 9: Illustration of the points ν_0 , ν_1 , ν_λ , the translation ζ , and the open set Ω in the proof of Proposition 12.

We obtain the desired result by taking the particular convex combination of these inequalities that cancels out their rightmost terms:

$$(1-\lambda)f(x_0) + \lambda f(x_1) > f(x_\lambda). \quad (43)$$

This proves the result. \square

The next proposition builds on the previous one to establish strict convexity for certain functions over \mathbb{R}^d .

Proposition 12. Let q be a density with positive support on all of \mathbb{R}^d . Let g, h be functions on \mathbb{R}^d related by

$$h(\nu) = \int g(\nu + \zeta) q(\zeta) d\zeta. \quad (44)$$

If g is differentiable, convex on \mathbb{R}^d , and strictly convex on some open set of \mathbb{R}^d , then h is strictly convex on \mathbb{R}^d .

Proof. Let $\nu_0, \nu_1 \in \mathbb{R}^d$, and let $\lambda \in (0, 1)$. Since g is convex, it follows directly from eq. (44) that h is also convex, satisfying

$$h((1-\lambda)\nu_0 + \lambda\nu_1) \leq (1-\lambda)h(\nu_0) + \lambda h(\nu_1). \quad (45)$$

To prove the theorem, we must show additionally that this inequality is *strict*.

Let Ω denote the open set of \mathbb{R}^d in which h is strictly convex, and as shorthand, denote the convex combination of ν_0 and ν_1 in eq. (45) by

$$\nu_\lambda = (1-\lambda)\nu_0 + \lambda\nu_1. \quad (46)$$

We can define another open set Ω_λ in \mathbb{R}^d by translating the points of Ω by an amount $-\nu_\lambda$; namely,

$$\Omega_\lambda = \{\zeta \in \mathbb{R}^d \mid \nu_\lambda + \zeta \in \Omega\}. \quad (47)$$

Then from eq. (44), we can express $h(\nu)$ as the sum of two integrals, one over the set Ω_λ , and one over its complement:

$$h(\nu) = \int_{\Omega_\lambda} g(\nu + \zeta) q(\zeta) d\zeta + \int_{\bar{\Omega}_\lambda} g(\nu + \zeta) q(\zeta) d\zeta \quad (48)$$

In what follows we will be especially focused on the first of these integrals.

Let $\zeta \in \Omega_\lambda$, and consider the illustration of $\nu_0, \nu_1, \nu_\lambda, \zeta$ and Ω in Fig. 9. Define the function $f : \mathbb{R} \rightarrow \mathbb{R}$ by

$$f(x) = g((1-x)\nu_0 + \nu_1 + \zeta). \quad (49)$$

Note that f is convex (since g is convex), and also that by construction, f is strictly convex in some neighborhood of $x = \lambda$, since in this neighborhood the argument of $g((1-x)\nu_0 + \nu_1 + \zeta)$ in eq. (49) belongs to the set Ω_λ . It therefore follows from Proposition 11 that

$$f(\lambda) < (1-\lambda)f(0) + \lambda f(1), \quad (50)$$

or equivalently that

$$g(\nu_\lambda + \zeta) < (1-\lambda)g(\nu_0) + \lambda g(\nu_1), \quad (51)$$

where the above inequality is strict for all $\zeta \in \Omega_\lambda$.

Now we use this inequality to compute a strict lower bound on $h(\nu_\lambda)$. For the first integral in eq. (48), over the set Ω_λ , we have the strict lower bound

$$\int_{\Omega_\lambda} g(\nu_\lambda + \zeta) q(\zeta) d\zeta < \int_{\Omega_\lambda} [(1-\lambda)g(\nu_0) + \lambda g(\nu_1)] q(\zeta) d\zeta, \quad (52)$$

and for the second integral, over the complement of this set, we have the lower bound

$$\int_{\bar{\Omega}_\lambda} g(\nu_\lambda + \zeta) q(\zeta) d\zeta \leq \int_{\bar{\Omega}_\lambda} [(1-\lambda)g(\nu_0) + \lambda g(\nu_1)] q(\zeta) d\zeta. \quad (53)$$

Finally, summing the previous two equations, we obtain the result that

$$h(\nu_\lambda) < (1-\lambda)h(\nu_0) + \lambda h(\nu_1), \quad (54)$$

which is the desired strengthening of eq. (45). The above holds for any $\lambda \in (0, 1)$, $\nu_0, \nu_1 \in \mathbb{R}^d$, and ν_λ given by eq. (46); thus h is strictly convex. \square

We can now prove the main lemma needed for the proofs of Theorems 8 and 10.

Lemma 13. Let \mathcal{Q} be a location family, and for $q_\nu \in \mathcal{Q}$ and some density p , consider the divergence $KL(q_\nu || p)$ as a function of the location parameter $\nu \in \mathbb{R}^d$. If $\log p$ is concave on all of \mathbb{R}^d and strictly concave on some open set of \mathbb{R}^d , then $KL(q_\nu || p)$ is a strictly convex function of the location parameter, ν .

Proof. From eq. (10), the KL divergence is given by

$$\text{KL}(q_\nu || p) = -\mathcal{H}(q_0) - \int \log p(\nu + \zeta) q_0(\zeta) d\zeta. \quad (55)$$

Note that the entropy in this expression, $\mathcal{H}(q_0)$, has no dependence on the location parameter. Thus the lemma follows directly from the previous proposition and the concavity assumptions on $\log p$. \square

C EXPERIMENTAL DETAILS

In this appendix, we provide additional details for all experiments in the paper.

C.1 Algorithms and evaluation metric

For 1-dimensional examples, we minimize $\text{KL}(q||p)$ using a grid-search.

For all other examples, we use the statistical software **Stan** [Carpenter et al., 2017], which supports gradient-based algorithms, and the add-on **bridgeStan** [Roualdes et al., 2023], which enables convenient manipulations of **Stan**'s output. **Stan** transforms all constrained latent variables to the unconstrained scale and so all algorithms, including VI and MCMC, operate over \mathbb{R}^d . We report the quality of the approximation over the unconstrained space. By working in this unconstrained space, we ensure that the experiments align with our theoretical analysis, which assumes that p and q are defined over \mathbb{R}^d .

All experiments are conducted with a 2.8 GHz Quad-Core Intel Core i7 CPU processor. We use the command line interface of **Stan**, specifically **cmdStan** v2.34.1. As a scripting language (i.e. for data manipulation and figures), we use **R** v4.2.3.

C.1.1 Variational inference

In our experiments we use automatic differentiation VI [ADVI; Kucukelbir et al., 2017] where \mathcal{Q} is chosen to be a family of Gaussian distributions. In Section 3.2 we use the “mean-field” mode, meaning the covariance matrix of q is diagonal; for all other experiments, we use the “fullrank” mode and estimate the full covariance matrix. ADVI optimizes the ELBO using stochastic gradient descent, as described in Section 2.1. In order to stabilize the algorithm, we set the default number of Monte Carlo draws to 1,000 per optimization step. For certain problems, we depart from this default, either to stabilize the solution or, for larger problems, to reduce compute time. In particular, for **disease_map** and **SKIM** we reduce the number of Monte Carlo samples per optimization step to 50.

C.1.2 Markov chain Monte Carlo benchmark

As a benchmark, we run long chains of MCMC. Specifically, we use **Stan**'s default sampler, which is a dynamic Hamiltonian Monte Carlo algorithm [Betancourt, 2018, Hoffman and Gelman, 2014]. We use 1,000 warmup iterations and 20,000 sampling iterations.

C.1.3 Evaluation metrics

To assess the quality of VI's approximation, we examine the posterior mean, the posterior correlation matrix, and the posterior covariance matrix. For the mean, we compute

$$\Delta_{\text{mean}} = \frac{|\mathbb{E}_p(z) - \mathbb{E}_q(z)|}{\max(\sqrt{\text{Var}_p(z)}, |\mathbb{E}_p(z)|)}, \quad (56)$$

where the scaling factor is chosen to make the error scale-free and numerically stable. Note that we do not simply compute the relative absolute error, with $\mathbb{E}_p(z)$ in the denominator: though a natural choice, it is unstable when $\mathbb{E}_p(z) \approx 0$. We also do not simply divide by the posterior standard deviation, as this quantity decays to 0 in cases where the data is rich (e.g., **glm**), and this in turn causes any errors in the numerator to be severely penalized. As a result, the performance of VI—when measured relative to the posterior standard deviation—decreases with the number of observations and this effect must be counterbalanced by fine-tuning the optimizer. The metric in eq. (56) was used to safeguard our analysis against these sources of numerical instability.

We report the errors in the correlation and covariance in slightly different ways. For the correlation, we simply report the absolute error

$$\Delta_{\text{corr}} = |\text{Corr}_p(z_i, z_j) - \text{Corr}_q(z_i, z_j)|, \quad (57)$$

noting that the correlation is scale-free. On the other hand, for the covariance, we report the absolute relative error

$$\Delta_{\text{cov}} = \frac{|\text{Cov}_{p(z)} - \text{Cov}_{q(z)}|}{|\text{Cov}_{p(z)}|}. \quad (58)$$

This metric suffers from the usual problem that for covariances close to 0, the error is numerically unstable. We considered adjusting the denominator, as was done for Δ_{mean} , however we do not have good estimates of the variance's variance (i.e. the fourth moment), even with long runs of MCMC. We also did not find that the reported covariance errors were unstable.

C.2 Additional results for Bayesian logistic regression

Figure 10 plots the marginal posterior densities for the Bayesian logistic regression introduced in section 2.3

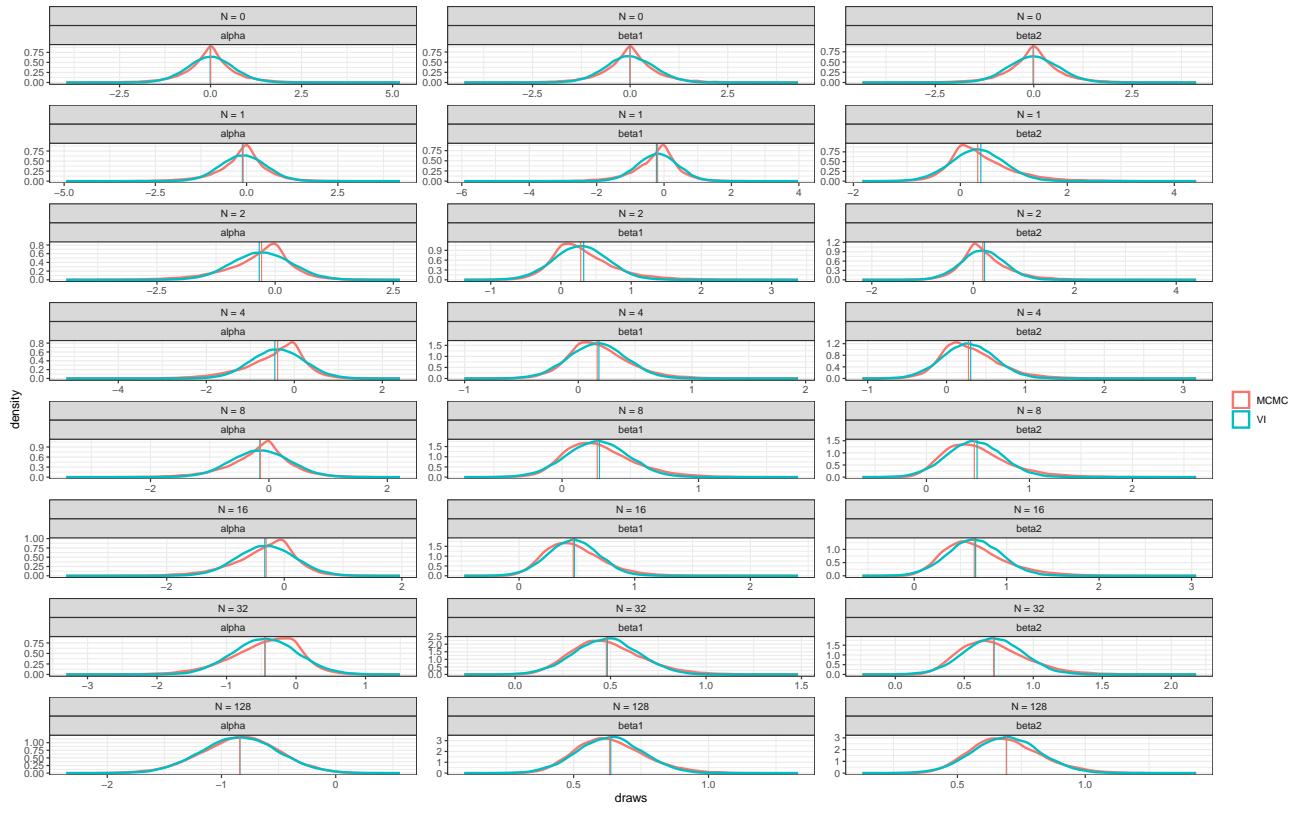


Figure 10: Posterior distributions for α , β_1 , and β_2 for a Bayesian logistic regression with N observations. Vertical lines indicate the means estimated by MCMC and VI. Overall, we find that these estimates match when the posterior is symmetric ($N = 0, N = 128$). In the presence of assymmetry, VI can still correctly estimate the marginal mean for some components, though not all of them.

with $N = 0, 1, 2, 4, 8, 16, 32, 128$ observations. (For clarity, the main body only shows the marginal posteriors for β_1 with $N = 0, 4, 128$. From the figure, we see how the asymmetry manifests for all regression parameters as the number of examples is increased from $N = 0$ (where the prior dominates) to $N = 128$) (where the likelihood dominates). When the posterior is asymmetric, the posterior mean can still be accurately estimated (e.g., $N = 32$), and in many cases we see that one component (but not all three) of the posterior mean is recovered.

C.3 Targets in numerical experiments

In this appendix, we provide details on the targets used in section 5.

student-t ($d = 2$). A multivariate student-t distribution with correlation 0.5 between z_1 and z_2 .

disease_map ($d = 102$). A disease map of Finland to model mortality counts across counties [Vanhatalo et al., 2010]. The model uses a Gaussian process model with an exponentiated squared kernel,

$$k(x_i, x_j) = \alpha^2 \exp\left(-\frac{(x_i - x_j)^T(x_i - x_j)}{\rho^2}\right), \quad (59)$$

where x_i is the two-dimensional coordinate of the i^{th} county. The covariance matrix K of the Gaussian process is then given by $K_{ij} = k(x_i, x_j)$. The full model is

$$\begin{aligned} \rho &\sim \text{invGamma}(2.42, 14.81), \\ \alpha &\sim \text{invGamma}(10, 10), \\ \epsilon &\sim \mathcal{N}(0, I_{n \times n}), \\ L &= \text{Cholesky decompose}(K), \\ \theta &= L\epsilon, \\ y_i &\sim \text{Poisson}(y_e^i e^{\theta_i}). \end{aligned} \quad (60)$$

GLM ($d = 3$). Binomial general linear model for modeling the success rate of Peregrine broods in the French Jura. This model is part of the model data base PosteriorDB [Magnusson et al., 2024] The observations are:

- N , the number of surveyed Peregrine falcons,
- C , the number of Peregrine falcons brooding,
- ye , year covariate,

and the full model is

$$\begin{aligned} \alpha &\sim \mathcal{N}(0, 100^2) \\ \beta_1 &\sim \mathcal{N}(0, 100^2) \\ \beta_2 &\sim \mathcal{N}(0, 100^2) \\ C &\sim \mathcal{B}(N, \text{logit}^{-1}(\alpha + \beta_1 ye + \beta_2 ye^2)) \end{aligned} \quad (61)$$

where $\mathcal{B}(N, p)$ denotes the binomial distribution with total number of trials N and probability of success p .

8schools and **8schools_nc** ($d = 10$). A Bayesian hierarchical model of the effects of a test preparation program across $N = 8$ schools [Rubin, 1981, Gelman et al., 2013]. For each school we observe y_i , the average change in test scores, and σ_i , the sample standard deviation across students. The natural (centered) parameterization (**8schools**) is

$$\begin{aligned} \mu &\sim \mathcal{N}(5, 3^2) \\ \tau &\sim \mathcal{N}^+(0, 5^2) \\ \theta_i &\sim \mathcal{N}(\mu, \tau^2) \\ y_i &\sim \mathcal{N}(\theta_i, \sigma_i^2), \end{aligned} \quad (62)$$

where \mathcal{N}^+ denotes a Gaussian distribution truncated at 0. The latent variables are $z = (\mu, \log \tau, \theta_{1:N})$. This model is known to exhibit an unbounded posterior density with a funnel shape [Neal, 2001]. The non-centered parameterization (**8schools_nc**) alleviates this geometric pathology:

$$\begin{aligned} \mu &\sim \mathcal{N}(5, 3^2) \\ \tau &\sim \mathcal{N}^+(0, 5^2) \\ \epsilon_i &\sim \mathcal{N}(0, 1) \\ \theta_i &= \mu + \tau \epsilon_i \\ y_i &\sim \mathcal{N}(\theta_i, \sigma_i^2). \end{aligned} \quad (63)$$

This data generative process is the same as above, however in this parameterization, the latent variables are $z = (\mu, \log \tau, \epsilon_{1:N})$.

mixture ($d = 2$). A balanced mixture of two two-dimensional Gaussians with different scales and no correlation between components.

$$z_1, z_2 \stackrel{\text{iid}}{\sim} \frac{1}{2} \mathcal{N}(-1, 2) + \frac{1}{2} \mathcal{N}(3, 1). \quad (64)$$

This distribution is neither elliptically nor even-symmetric.

SKIM ($d = 305$). The sparse kernel interaction model (SKIM), developed by Agrawal et al. [2019], is a regularized regression model which accounts for interaction effects between covariates. The model makes a soft selection of regression coefficients using a regularized horseshoe prior [Piironen and Vehtari, 2017]. Following Margossian et al. [2020], we apply the model to a genetic microarray classification data set on prostate cancer. The data set is made up of $N = 102$ patients and $p = 200$ pre-selected genetic covariates. We denote $y \in \{0, 1\}^N$ the binary observations (1: the patient has cancer, 0: the patient has no cancer), and $X \in \mathbb{R}^{N \times p}$ the design matrix.

To specify the full data generating process, we first set the following hyperparameters:

$$\begin{aligned}
p_0 &= 5 \\
s_{\text{global}} &= \frac{p_0}{\sqrt{N}(p - p_0)} \\
\nu_{\text{local}} &= 1 \\
\nu_{\text{global}} &= 1 \\
s_{\text{slab}} &= 2 \\
s_{\text{df}} &= 100 \\
c_0 &= 5.
\end{aligned} \tag{65}$$

Then,

$$\begin{aligned}
\lambda_i &\sim \text{Student}_t(\nu_{\text{local}}, 0, 1) \\
\tau &\sim \text{Student}_t(\nu_{\text{global}}, 0, s_{\text{global}}) \\
c_{\text{aux}} &\sim \text{inv}\Gamma(s_{\text{df}}/2, s_{\text{df}}/2) \\
\chi &\sim \text{InverseGamma}(s_{\text{df}}/2, s_{\text{df}}/2) \\
c &= \sqrt{c_{\text{aux}}} s_{\text{slab}} \\
\tilde{\lambda}_i^2 &= \frac{c^2 \lambda_i^2}{c^2 + \tau^2 \lambda_i^2} \\
\eta_2 &= \tau^2 \chi / c^2 \\
\beta_0 &\sim \mathcal{N}(0, c_0^2) \\
\beta_i &\sim \mathcal{N}(0, \tau^2 \tilde{\lambda}_i^2) \\
\beta_{ij} &\sim \mathcal{N}(0, \eta_2^2 \tilde{\lambda}_i^2 \tilde{\lambda}_j^2) \\
y &\sim \text{Bernoulli}(\text{logit}^{-1}(\beta_0 + X\beta)).
\end{aligned} \tag{66}$$

Following [Agrawal et al. \[2019\]](#), we marginalize out β_i and β_{ij} , using a kernel trick and a Gaussian process reparameterization. To define the Gaussian process covariance matrix K , we first introduce the auxiliary matrices:

$$\begin{aligned}
K_1 &= X \text{ diag}(\tilde{\lambda}^2) X^T \\
K_2 &= [X \circ X] \text{ diag}(\tilde{\lambda}^2) [X \circ X]^T,
\end{aligned} \tag{67}$$

where “ \circ ” denotes the element-wise Hadamard product. Finally,

$$\begin{aligned}
K &= \frac{1}{2} \eta_2^2 (K_1 + 1) \circ (K_1 + 1) - \frac{1}{2} \eta_2^2 K_2 - (\tau^2 - \eta_2^2) K_1 \\
&\quad + c_0^2 - \frac{1}{2} \eta_2^2.
\end{aligned} \tag{68}$$

and

$$\begin{aligned}
\epsilon &\sim \mathcal{N}(0, 1) \\
L &= \text{Cholesky_decompose}(K) \\
f &= L\epsilon \\
y &\sim \text{Bernoulli}(\text{logit}^{-1}(f)).
\end{aligned} \tag{69}$$

Crescent ($d = 2$). See Eq. (31).