Explicit natural gradient updates for Cholesky factor in Gaussian variational approximation

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Abstract

Stochastic gradient methods have enabled variational inference for high-dimensional models and large data. However, the steepest ascent direction in the parameter space of a statistical model is given not by the commonly used Euclidean gradient, but the natural gradient which premultiplies the Euclidean gradient by the inverted Fisher information matrix. Use of natural gradients can improve convergence significantly, but inverting the Fisher information matrix is daunting in high-dimensions. In Gaussian variational approximation, natural gradient updates of the natural parameters (expressed in terms of the mean and precision matrix) of the Gaussian distribution can be derived analytically, but do not ensure the precision matrix remains positive definite. To tackle this issue, we consider Cholesky decomposition of the covariance or precision matrix and derive explicit natural gradient updates of the Cholesky factor, which depend only on the first instead of the second derivative of the log posterior density, by finding the inverse of the Fisher information matrix analytically. Efficient natural gradient updates of the Cholesky factor are also derived under sparsity constraints incorporating different posterior independence structures.

Keywords: Gaussian variational approximation; Natural gradients; Cholesky factor; Covariance matrix; Sparse precision matrix; Positive definite constraint.

1 Introduction

Variational inference is fast and provides an attractive alternative to Markov chain Monte Carlo (MCMC) methods for approximating intractable posterior distributions in the Bayesian framework. Use of stochastic gradient methods (Robbins and Monro, 1951) has further enabled variational inference for high-dimensional models and large data sets (Hoffman et al., 2013; Salimans and Knowles, 2013). While Euclidean gradients are commonly used in the optimization of the variational objective function, the direction of steepest ascent in the parameter space of statistical models, where distance between probability distributions is measured using the Kullback-Leibler (KL) divergence, is actually given by the natural gradient (Amari, 1998). Stochastic optimization based on natural gradients has been found to be more robust with the ability to avoid or escape plateaus, resulting in faster convergence (Rattray et al., 1998). Martens (2020) shows that natural gradient descent can be seen as a second order optimization method, with the Fisher information matrix taking the place of the Hessian and having more favorable properties.
The natural gradient is computed by premultiplying the Euclidean gradient with the inverse of the Fisher information matrix, the computation of which can be highly complex. However, in some cases, natural gradient updates can be simpler than those based on Euclidean gradients, such as for the conjugate exponential family models considered in [Hoffman et al., 2013]. If the variational approximation employs a distribution in the minimal exponential family ([Wainwright and Jordan, 2008]), then the natural gradient of the variational objective function (evidence lower bound) with respect to the natural parameter is just given by the gradient of the evidence lower bound with respect to the mean of the sufficient statistics ([Hensman et al., 2012, Amari, 2016, Khan and Lin, 2017]).

In Gaussian variational approximation ([Opper and Archambeau, 2009]), the true posterior is approximated by a multivariate Gaussian which belongs to the minimal exponential family. Natural gradient updates of the natural parameter can thus be derived analytically as described above. Combined with the theorems of [Bonnet, 1964] and [Price, 1958], these simplify to updates of the mean and precision matrix which depend on the first and second order derivatives of the log posterior density ([Khan et al., 2018]). However, the update for the precision matrix does not ensure that it remains positive definite.

Various approaches have been proposed to deal with the positive definite constraint. [Khan and Lin, 2017] use a back-tracking line search, but that can lead to slow convergence. [Ong et al., 2018b] parametrize the Gaussian in terms of the mean and Cholesky factor of the precision matrix and derive the Fisher information matrix analytically, but compute the natural gradients by solving a linear system numerically. Using chain rule, [Salimbeni et al., 2018] show that the inverse of the Fisher information matrix in alternative parametrizations (which are one-one transformations of the natural parameters) can be computed as a Jacobian-vector product using automatic differentiation. [Ong et al., 2018], [Ong et al., 2018a] and [Tran et al., 2020] consider a factor structure for the covariance matrix, and [Tran et al., 2020] compute the natural gradients using a conjugate gradient linear solver based on a block diagonal approximation of the Fisher information matrix. [Lin et al., 2020] use Riemannian gradient descent with a retraction map (derived using a second-order approximation of the geodesic) to compute a modified update of the precision matrix, that includes an additional term to ensure positive definiteness. [Tran et al., 2020] optimize the covariance matrix on the manifold of symmetric positive definite matrices and derive an update for the covariance based on an approximation of the natural gradient and a popular retraction for the manifold.

In this article, we consider Cholesky decompositions of either the covariance or precision matrix, and derive the inverse of the Fisher information matrix for these parametrizations in closed form. Explicit natural gradient updates for the Cholesky factor are then presented in both cases. In contrast to natural gradient updates of the natural parameter (involving the mean and precision matrix), our updates depend only on the first order derivative of the log posterior density, thus reducing storage and computational costs. Updates of the mean and Cholesky factor based on Euclidean gradients have been presented in [Titsias and Lázaro-Gredilla, 2014], and we demonstrate that corresponding
natural gradient updates only require minor modifications with minimal additional costs.

Gaussian variational approximation has been widely applied in many contexts such as likelihood-free inference using the synthetic likelihood approach (Ong et al., 2018b), Bayesian neural networks in deep learning (Khan et al., 2018), exponential random graph models for network modeling (Tan and Friel, 2020) and factor copula models (Nguyen et al., 2020) which seek to capture the dependence structure of high-dimensional variables using a small number of latent variables via bivariate links. For greater flexibility in accommodating variables which are constrained, skewed or heavy-tailed, a Gaussian variational approximation can be specified for variables which have first undergone independent parametric transformations, resulting in a Gaussian copula variational approximation for the original variables. Han et al. (2016) use a Bernstein polynomial transformation while Smith et al. (2020) employ the transformation of Yeo and Johnson (2000) and the Tukey g-and-h distribution (Yan and Genton, 2019) to improve the normality and symmetry of the original variables. Our natural gradient updates of the mean and Cholesky factor can be applied to improve convergence in stochastic gradient ascent in any context where a Gaussian density is used as an approximating density (such as those discussed above).

In high-dimensional models, sparsity constraints can be imposed on the covariance matrix by assuming a diagonal or block-diagonal structure according to the variational Bayes restriction (see, e.g. Titsias and Lázaro-Gredilla, 2014; Tan, 2021). Alternatively, the precision matrix can be assumed to adopt a structure that reflects the conditional independence structure in the true posterior, as demonstrated in state space models and generalized linear mixed models by Tan and Nott (2018). The ADVI (automatic differentiation variational inference) algorithm (Kucukelbir et al., 2017) in Stan (Stan Development Team, 2019) allows the user to fit Gaussian variational approximations with either a diagonal or full covariance matrix and provides a library of transformations to convert constrained variables onto the real line. However, it does not permit specification of other sparsity structures and uses Euclidean gradients to update the Cholesky factor in stochastic gradient ascent. While sparsity constraints can be imposed in Euclidean gradients simply by setting relevant entries to zero, the same does not necessarily apply to natural gradients due to the need to premultiply the Euclidean gradient by the Fisher information matrix. We further derive efficient natural gradient updates in the case where (i) the covariance matrix has a block-diagonal structure such as in reparametrized variational Bayes (RVB, Tan, 2021) and (ii) the precision matrix reflects the posterior conditional independence structure in a hierarchical model (Tan and Nott, 2018).

This article is organized as follows. Section 2 introduces the notation used in this article and Section 3 describes stochastic variational inference based on Euclidean gradients. In Section 4, we define the natural gradient and discuss its use in stochastic variational inference. Section 5 presents the natural gradient updates of the mean and Cholesky factor of either the covariance or precision matrix in Gaussian variational approximation. Section 6 derives efficient natural gradient updates when different sparsity constraints are imposed. We conclude with a discussion in Section 7.
2 Notation

Let $A$ be a $d \times d$ matrix. We use $\text{vec}(A)$ to denote the $d^2 \times 1$ vector obtained by stacking the columns of $A$ in order from left to right, and $K$ the $d^2 \times d^2$ commutation matrix such that $K\text{vec}(A) = \text{vec}(A^T)$. Let $N = (K + I_{d^2})/2$.

Let $\text{vech}(A)$ denote the $d\frac{(d+1)}{2} \times 1$ vector obtained from $\text{vec}(A)$ by omitting supradiagonal elements. If $A$ is symmetric, then $D\text{vech}(A) = \text{vec}(A)$ where $D$ denotes the duplication matrix, and $D^+\text{vec}(A) = \text{vech}(A)$ where $D^+ = (D^T D)^{-1}D^T$ denotes the Moore-Penrose inverse of $D$. Let $L$ denote the $d\frac{(d+1)}{2} \times d^2$ elimination matrix where $L\text{vec}(A) = \text{vech}(A)$. Note that $L^T\text{vech}(A) = \text{vec}(A)$ if $A$ is lower triangular.

To simplify notation, we use $K$, $D$ and $L$ to denote the commutation, duplication and elimination matrices generally and their dimensions should be inferred from the context. More details and identities on these matrices can be found in Magnus and Neudecker (1980) and Magnus and Neudecker (2019).

Let $\otimes$ denote the Kronecker product such that $\text{vec}(AXB) = (B^T \otimes A)\text{vec}(X)$ and $\odot$ the elementwise Hadamard product. We use $\bar{A}$ to denote the lower triangular matrix derived from $A$ by replacing all supradiagonal elements by zero. Let $\text{diag}(A)$ denote the $d \times 1$ vector containing the diagonal elements of $A$, and $\text{dg}(A)$ denote the diagonal matrix derived from $A$ by replacing all non-diagonal elements by zero. Define $\bar{A} = \bar{A} - \text{dg}(A)/2$.

If $a$ is a vector, then $\text{diag}(a)$ denotes the diagonal matrix having $a$ as the diagonal. Let $\nabla_\lambda L, \nabla^2_\lambda L$ and $\nabla^2_\lambda,\alpha L$ denote $\partial L/\partial \lambda, \partial^2 L/\partial \lambda \partial \lambda^T$ and $\partial^2 L/\partial \lambda \partial \alpha^T$ respectively for vectors $\lambda$ and $\alpha$.

3 Stochastic variational inference

Let $p(y|\theta)$ denote the likelihood of unknown variables $\theta \in \mathbb{R}^d$ given observed data $y$. Suppose a prior distribution $p(\theta)$ is specified and the true posterior distribution $p(\theta|y) = p(y|\theta)p(\theta)/p(y)$ is intractable. In variational inference, $p(\theta|y)$ is approximated by a density $q_\lambda(\theta)$ with parameters $\lambda \in \Omega$, which are chosen to minimize the KL divergence between $q_\lambda(\theta)$ and $p(\theta|y)$. As

$$
\log p(y) = \int q_\lambda(\theta) \log \frac{q_\lambda(\theta)}{p(\theta|y)} d\theta + \int q_\lambda(\theta) \log \frac{p(y,\theta)}{q_\lambda(\theta)} d\theta,
$$

minimizing the KL divergence with respect to $\lambda$ is equivalent to maximizing the evidence lower bound on the log marginal likelihood. If we let $h_\lambda(\theta) = \log[p(y,\theta)/q_\lambda(\theta)]$, then the evidence lower bound,

$$
\mathcal{L}(\lambda) = E_{q_\lambda(\theta)}[\log p(y,\theta) - \log q_\lambda(\theta)] = E_{q_\lambda(\theta)}[h_\lambda(\theta)]
$$
is the variational objective function to be maximized with respect to $\lambda$. When $\mathcal{L}$ is intractable, stochastic gradient ascent can be used for optimization. Starting with some initial estimate $\lambda^{(1)}$, an update

$$\lambda^{(t+1)} = \lambda^{(t)} + \rho_t \hat{\nabla}_\lambda \mathcal{L}(\lambda^{(t)})$$

(1)
is performed at iteration $t$, where $\hat{\nabla}_\lambda \mathcal{L}(\lambda^{(t)})$ is an unbiased estimate of the Euclidean gradient $\nabla_\lambda \mathcal{L}$ evaluated at $\lambda^{(t)}$. Under regularity conditions, $\lambda^{(t)}$ will converge to a local maximum of $\mathcal{L}$ if the stepsize $\rho_t$ satisfies $\sum_{t=1}^{\infty} \rho_t = \infty$ and $\sum_{t=1}^{\infty} \rho_t^2 < \infty$ (Spall 2003). In practice, an adaptive stepsize sequence such as Adam (Kingma and Ba 2015) is often used.

### 3.1 Euclidean gradient of evidence lower bound

The Euclidean gradient of $\mathcal{L}$ with respect to $\lambda$ is given by

$$\nabla_\lambda \mathcal{L} = \int [\nabla_\lambda q_\lambda(\theta)] h_\lambda(\theta) d\theta - \int q_\lambda(\theta) \nabla_\lambda \log q_\lambda(\theta) d\theta$$

$$= \int [\nabla_\lambda q_\lambda(\theta)] h_\lambda(\theta) d\theta$$

$$= \nabla_\lambda E_{q_\lambda(\theta)}[h(\theta)].$$

(2)
The second term in the first line of (2) is the expectation of the score function which is zero. In the last line, we have dropped the subscript $\lambda$ from $h_\lambda(\cdot)$ so that it is clearer that the gradient $\nabla_\lambda$ applies only to $q_\lambda(\theta)$ as can be seen from the second line. Estimates of $\nabla_\lambda \mathcal{L}$ can be computed in different ways and existing techniques can be broadly divided into two approaches.

The first is to apply the log derivative trick or score function method, which is based on the fact that $\nabla_\lambda q_\lambda(\theta) = q_\lambda(\theta) \nabla_\lambda \log q_\lambda(\theta)$. From (2), this enables us to write

$$\nabla_\lambda \mathcal{L} = E_{q_\lambda(\theta)}[\nabla_\lambda \log q_\lambda(\theta) h(\theta)],$$

and an unbiased estimate of $\nabla_\lambda \mathcal{L}$ is $\hat{\nabla}_\lambda \mathcal{L} = \nabla_\lambda \log q_\lambda(\theta) h(\theta)$ where $\theta$ is simulated from $q_\lambda(\theta)$. Despite being widely applicable, such gradient estimates tend to have high variance leading to slow convergence. Various techniques have been proposed to reduce their variance such as the use of control variates (Paisley et al. 2012), Rao-Blackwellization (Ranganath et al. 2014) and importance sampling (Ruiz et al. 2016).

The second approach is to apply the reparametrization trick (Kingma and Welling 2014; Rezende et al. 2014; Titsias and Lázaro-Gredilla 2014), writing $\theta = \mathcal{T}_\lambda(z)$, where $\mathcal{T}_\lambda(\cdot)$ is a differentiable function and $z$ are random variables whose distribution $p(z)$ is independent of $\lambda$. From (2), after applying chain rule, we obtain

$$\nabla_\lambda \mathcal{L} = \nabla_\lambda \int p(z) h(\mathcal{T}_\lambda(z)) dz = E_{p(z)}[\nabla_\lambda \theta \nabla_\theta h(\theta)],$$

(3)
where \( \theta = T_\lambda(z) \). Hence an unbiased estimate is \( \hat{\nabla}_\lambda \mathcal{L} = \nabla_\lambda \theta \nabla_\theta h(\theta) \) where \( z \) is simulated from \( p(z) \). With the reparametrization trick, \( h \) becomes a direct function of \( \lambda \) and gradient information from \( h(\cdot) \) can be harnessed more effectively. Gradients computed in this way typically have lower variance than in the score function approach and very often, only a single sample from \( p(z) \) is required for computing the unbiased estimate \( \hat{\nabla}_\lambda \mathcal{L} \). For instance, if \( q_\lambda(\theta) \) is \( N(\mu, CC^T) \), where \( CC^T \) is the Cholesky decomposition of the covariance matrix, we can use the transformation \( \theta = Cz + \mu \) where \( z \sim N(0, I_d) \). More generally, for distributions outside the location-scale family, let \( F_\lambda(\theta) \) denote the cdf of \( q_\lambda(\theta) \). If \( F_\lambda(\theta) \) is differentiable, then we can use the transformation \( \theta = \lambda^{-1}(z) \), where \( z \sim U[0, 1] \). This approach can be applied easily to distributions with tractable inverse cdf such as the exponential, Cauchy, logistics and Weibull distributions.

4 Natural gradient of evidence lower bound

In stochastic variational inference, we are interested in finding the parameter \( \lambda \) of \( q_\lambda(\theta) \) that maximizes the evidence lower bound \( \mathcal{L}(\lambda) \). The Fisher information matrix of \( q_\lambda(\theta) \) is defined as

\[
F_\lambda = -E_{q_\lambda(\theta)}[\nabla^2 \log q_\lambda(\theta)].
\]

Let the distance between two probability distributions be measured using the KL divergence. Applying a second order Taylor series expansion,

\[
\text{KL}(q_\lambda(\theta)\|q_{\lambda+d\lambda}(\theta)) = \int q_\lambda(\theta) \log \frac{q_\lambda(\theta)}{q_{\lambda+d\lambda}(\theta)} d\theta \\
\approx E_{q_\lambda(\theta)}\{\log q_\lambda(\theta) - [\log q_\lambda(\theta) + d\lambda^T \nabla_\lambda \log q_\lambda(\theta) + \frac{1}{2}d\lambda^T \nabla^2_\lambda \log q_\lambda(\theta) d\lambda]\} \\
= \frac{1}{2}d\lambda^T F_\lambda d\lambda,
\]

since \( E_{q_\lambda(\theta)}[\nabla_\lambda \log q_\lambda(\theta)] = 0 \). From [Amari (2016)](Amari2016), if \( d\lambda \) is sufficiently small, the distance between two points, \( \lambda \) and \( \lambda + d\lambda \), in the parameter space can be defined as

\[
2\text{KL}(q_\lambda(\theta)\|q_{\lambda+d\lambda}(\theta)) = d\lambda^T F_\lambda d\lambda = \|d\lambda\|_{F_\lambda}^2.
\]

Thus, the distance between two nearby parameters \( \lambda \) and \( \lambda+d\lambda \) is not given by \( d\lambda^T d\lambda \) as in a Euclidean space, but by \( d\lambda^T F_\lambda d\lambda \). The set of all distributions \( q_\lambda(\theta), \lambda \in \Omega \) is a manifold where each point \( \lambda \) denotes a probability density function and the KL divergence provides the manifold with a Riemannian structure. We say that the manifold is Riemannian with norm \( \|d\lambda\|_{F_\lambda} = \sqrt{d\lambda^T F_\lambda d\lambda} \) if the Riemannian metric \( F_\lambda \) is positive definite.

Suppose we want to find the steepest ascent direction of \( \mathcal{L}(\lambda) \) at \( \lambda \). [Amari (1998)](Amari1998) defines this direction as the vector \( a \) that maximizes \( \mathcal{L}(\lambda + a) \) where \( \|a\|_{F_\lambda} = \epsilon \) for a small constant \( \epsilon \). Using the method of Lagrange multipliers, let

\[
\mathcal{L} = \mathcal{L}(\lambda + a) - \alpha(\|a\|_{F_\lambda}^2 - \epsilon^2) = \mathcal{L}(\lambda) + a^T \nabla_\lambda \mathcal{L}(\lambda) - \alpha(a^T F_\lambda a - \epsilon^2).
\]
Setting $\nabla_a \mathcal{L} = \nabla_\lambda \mathcal{L}(\lambda) - 2\alpha F_\lambda a$ to zero gives $a \propto F_\lambda^{-1} \nabla_\lambda \mathcal{L}(\lambda)$. Hence the steepest ascent direction for $\mathcal{L}(\lambda)$ in the parameter space of $q_\lambda(\theta)$ is given by the natural gradient,

$$\tilde{\nabla}_\lambda \mathcal{L} = F_\lambda^{-1} \nabla_\lambda \mathcal{L},$$

which premultiplies the Euclidean gradient by the inverse of the Fisher information matrix, provided $F_\lambda$ is positive definite (see also [Amari 1998, 2016; Martens 2020]). Replacing the estimate of the Euclidean gradient in (1) with that of the natural gradient then results in the natural gradient update,

$$\lambda^{(t+1)} = \lambda^{(t)} + \rho_t F_\lambda^{-1} \tilde{\nabla}_\lambda \mathcal{L}(\lambda^{(t)}).$$

If $\xi \equiv \xi(\lambda)$ is a smooth reparametrization of the variational density, then the Fisher information matrix

$$F_\xi = -\mathbb{E}_{q_\xi(\theta)}[\nabla_\xi^2 \log q_\xi(\theta)] = J F_\lambda J^T,$$

where $J = \nabla_\xi \lambda$ is the Jacobian matrix ([Lehmann and Casella 1998]). If $\xi$ is, in addition, an invertible function of $\lambda$, then $J$ is invertible and the natural gradient is given by

$$\tilde{\nabla}_\xi \mathcal{L} = F_{\xi}^{-1} \nabla_\xi \mathcal{L}$$

$$= (J^{-T} F_\lambda^{-1} J^{-1}) J (\nabla_\lambda \mathcal{L})$$

$$= (\nabla_\lambda \xi)^T \tilde{\nabla}_\lambda \mathcal{L}. \quad (4)$$

Thus, it is easy to interchange among different parametrizations which are smooth invertible functions of each other.

### 4.1 Variational approximation in exponential family

Suppose $q_\lambda(\theta)$ belongs to an exponential family and

$$q_\lambda(\theta) = H(\theta) \exp[\phi(\theta)^T \lambda - A(\lambda)], \quad (5)$$

where $\lambda \in \Omega$ is the natural parameter, $\phi(\theta)$ are the sufficient statistics and $A(\lambda)$ is the cumulant or log-partition function. Then

$$m = \mathbb{E}_{q_\lambda(\theta)}[\phi(\theta)] = \nabla_\lambda A(\lambda), \quad \text{Var}_{q_\lambda(\theta)}[\phi(\theta)] = \nabla_\lambda^2 A(\lambda),$$

and the Fisher information matrix,

$$F_\lambda = -\mathbb{E}_{q_\lambda(\theta)}[\nabla_\lambda^2 \log q_\lambda(\theta)] = \nabla_\lambda^2 A(\lambda) = \nabla_\lambda m.$$ 

$F_\lambda$ is positive definite and invertible if the exponential family representation in (5) is minimal, or equivalently, if the mapping $m : \Omega \rightarrow \mathcal{M}$ is one-one, where $\mathcal{M}$ is the set of realizable mean parameters ([Wainwright and Jordan 2008, pp. 40, 62–64].)
Applying chain rule, $\nabla_\lambda L = \nabla_\lambda m \nabla_m L = F_\lambda \nabla_m L$. Hence the natural gradient,

$$\tilde{\nabla}_\lambda L = F_\lambda^{-1} \nabla_\lambda L = \nabla_m L,$$  \hspace{1cm} (6)

can be computed by finding the gradient of $L$ with respect to the mean parameter without computing the Fisher information matrix directly (Khan and Lin 2017).

4.2 Gaussian variational approximation

A popular option for $q_\lambda(\theta)$ is the multivariate Gaussian $N(\mu, \Sigma)$, with mean $\mu$ and covariance matrix $\Sigma$ (Opper and Archambeau 2009). If some variables in $\theta$ are constrained, we can first transform them to be unconstrained using for instance, the library of transformations in Stan (Kucukelbir et al. 2017). Alternatively, we can consider Gaussian copula variational approximation (Han et al. 2016; Smith et al. 2020) if some variables in $\theta$ are skewed or heavy-tailed.

The multivariate Gaussian can be represented as a member of the exponential family in (5) by writing

$$q_\lambda(\theta) = (2\pi)^{-d/2} \exp \left\{ \phi(\theta)^T \lambda - \frac{1}{2} \mu^T \Sigma^{-1} \mu - \frac{1}{2} \log |\Sigma| \right\},$$

where

$$\phi(\theta) = \begin{bmatrix} \theta \\ \text{vech}(\theta \theta^T) \end{bmatrix}, \quad \lambda = \begin{bmatrix} \Sigma^{-1} \mu \\ -\frac{1}{2} \Sigma^{-1} D^T \text{vec}(\Sigma) \end{bmatrix}, \quad m = \begin{bmatrix} \mu \\ \text{vech}(\Sigma + \mu \mu^T) \end{bmatrix}.$$ 

From (6), the natural gradient of $L$ with respect to the natural parameters $\lambda$ can be obtained simply by finding the gradient of $L$ with respect to the mean parameters $m$. Let $m_1 = \mu$ and $m_2 = \text{vech}(\Sigma + \mu \mu^T)$, and introduce $\zeta = (\zeta_1^T, \zeta_2^T)^T$, where

$$\zeta_1 = \mu = m_1, \quad \zeta_2 = \text{vech}(\Sigma) = m_2 - \text{vech}(m_1 m_1^T).$$

Then

$$\nabla_m \zeta = \begin{bmatrix} \nabla m_1 \zeta_1 \\ \nabla m_2 \zeta_1 \\ \nabla m_1 \zeta_2 \\ \nabla m_2 \zeta_2 \end{bmatrix} = \begin{bmatrix} I_d & 0_{d(d+1)/2 \times d} \\ 0_{d(d+1)/2 \times d} & I_{d(d+1)/2} \end{bmatrix}.$$

More details are given in Appendix A. Applying chain rule, the natural gradient is

$$\tilde{\nabla}_\lambda L = \nabla_m L = \nabla_m \zeta \nabla_\zeta L = \begin{bmatrix} \nabla_\mu L & -2(\nabla_\zeta L_\mu) \\ D^T \text{vec}(\nabla_\zeta L) \end{bmatrix},$$  \hspace{1cm} (7)

where $\nabla_{\text{vech}(\Sigma)} L = D^T \nabla_{\text{vech}(\Sigma)} L_\Sigma = D^T \text{vec}(\nabla_\Sigma L)$. From (2) and the Theorems of Bonnet.
\( \nabla_\mu L = \int [\nabla_\mu q_\lambda(\theta)] h(\theta) d\theta = E_{q_\lambda(\theta)}[\nabla_\theta h(\theta)], \)

\( \nabla_\Sigma L = \int [\nabla_\Sigma q_\lambda(\theta)] h(\theta) d\theta = \frac{1}{2} E_{q_\lambda(\theta)}[\nabla_\theta^2 h(\theta)]. \)

Substituting these results in (7),

\[
\tilde{\nabla}_\lambda L = E_{q_\lambda(\theta)} \left[ \nabla_\theta h(\theta) - \nabla_\theta^2 h(\theta) \mu \right].
\]

Let \( \theta^{(t)} \) denote a sample generated from \( q_\lambda(\theta) \) at iteration \( t \). The natural gradient update of \( \lambda \) is

\[
\left[ \Sigma^{(t+1)^{-1}} \mu^{(t+1)} \right] = \left[ \Sigma^{(t)^{-1}} \mu^{(t)} \right] + \rho_t \left[ \nabla_\theta h(\theta^{(t)}) - \nabla_\theta^2 h(\theta^{(t)}) \mu^{(t)} \right],
\]

which simplifies to

\[
\Sigma^{(t+1)^{-1}} = \Sigma^{(t)^{-1}} - \rho_t \nabla_\theta^2 h(\theta^{(t)}),
\]

\[
\mu^{(t+1)} = \mu^{(t)} + \rho_t \Sigma^{(t+1)^{-1}} \nabla_\theta h(\theta^{(t)}).
\]

The natural gradient update of \( \Sigma^{-1} \) derived in this manner does not ensure \( \Sigma^{-1} \) remains positive definite and it also depends on the second derivative of \( h(\theta) \).

5 Natural gradient updates for mean and Cholesky factor of Gaussian variational approximation

To ensure that the covariance or precision matrix remains positive definite in the optimization, we consider different parametrizations of \( q_\lambda(\theta) \) based on Cholesky decompositions. Updating only the Cholesky factor instead of the full covariance or precision matrix may also reduce computation and storage costs. The first parametrization is

\[
\lambda_1 = (\mu^T, \text{vech}(C)^T)^T \text{ where } \Sigma = CC^T
\]

and the second parametrization is

\[
\lambda_2 = (\mu^T, \text{vech}(T)^T)^T \text{ where } \Sigma^{-1} = TT^T,
\]

where \( C \) and \( T \) are lower triangular matrices. For these parametrizations, \( \lambda_1 \) and \( \lambda_2 \) are not the natural parameters of \( q_\lambda(\theta) \). Hence the natural gradient cannot be computed simply by using (6) and it is necessary to find \( F_\lambda^{-1} \). We show that \( F_\lambda^{-1} \) and hence the natural gradient updates can be evaluated analytically for the parametrizations in (8) and (9).
First, we find the Euclidean gradients of $L$ with respect to $\lambda_1$ and $\lambda_2$ using the reparametrization trick. Let $z \sim N(0, I_d)$ and $\phi(z)$ denote the density of $z$. From (3), $\nabla_\lambda L = E_{\phi(z)}[\nabla_\lambda \theta \nabla_\theta h(\theta)]$. For $\lambda_1$, let $\theta = Cz + \mu$. Then

$$\nabla_{\lambda_1} \theta = \begin{bmatrix} \nabla_{\mu \theta} \\ \nabla_{\text{vech}(\theta)} \end{bmatrix} = \begin{bmatrix} I_d \\ L(z \otimes I_d) \end{bmatrix} \quad \text{and} \quad \nabla_{\lambda_1} L = E_{\phi(z)} \left[ \begin{bmatrix} \nabla_\theta h(\theta) \\ \text{vech}(G_1) \end{bmatrix} \right],$$

since $L(z \otimes I_d)\nabla_\theta h(\theta) = L\text{vec}(\nabla_\theta h(\theta)z^T) = \text{vech}(G_1) = \text{vech}(\tilde{G}_1)$, where $G_1 = \nabla_\theta h(\theta)z^T$. Next, we find the Fisher information matrix $F_{\lambda_i}$ and its inverse for each parametrization $\lambda_i$, $i = 1, 2$. The natural gradient is then given by $\nabla_{\lambda_i} \mathcal{L} = F_{\lambda_i}^{-1} \nabla_{\lambda_i} L$. To find the inverse, we require Lemma 1 whose proof is given in Appendix B. The results are then summarized in Theorem 1.

**Lemma 1.** If $\Lambda$ is a $d \times d$ lower triangular matrix, then

$$\mathcal{I}(\Lambda) = L\{(\Lambda^{-1} \otimes \Lambda^{-T}K + I_d \otimes \Lambda^{-T}\Lambda^{-1})L^T = 2L(I_d \otimes \Lambda^{-T})N(I_d \otimes \Lambda^{-1})L^T,$$

and

$$\mathcal{I}(\Lambda)^{-1} = \frac{1}{2}L(I_d \otimes \Lambda)L^T(LNL^T)^{-1}L(I_d \otimes \Lambda^T)L^T.$$

Let $G$ be any $d \times d$ matrix. Then

$$\mathcal{I}(\Lambda)^{-1} \text{vech}(G) = \text{vech}(\Lambda \tilde{H}),$$

where $H = \Lambda^T \tilde{G}$.

**Theorem 1.** For $i = 1, 2$, the Fisher information matrix of $q_{\lambda_i}(\theta)$ and its inverse are given by

$$F_{\lambda_i} = \begin{bmatrix} \Sigma^{-1} & 0 \\ 0 & \mathcal{I}(\Lambda_i) \end{bmatrix} \quad \text{and} \quad F_{\lambda_i}^{-1} = \begin{bmatrix} \Sigma^{-1} & 0 \\ 0 & \mathcal{I}(\Lambda_i)^{-1} \end{bmatrix},$$

where $\Lambda_1 = C$ and $\Lambda_2 = T$. The natural gradient is

$$\nabla_{\lambda_i} \mathcal{L} = E_{\phi(z)} \left[ \begin{bmatrix} \Sigma \nabla_\theta h(\theta) \\ \text{vech}(\Lambda_i \tilde{H}_i) \end{bmatrix} \right],$$

where $H_i = \Lambda_i^T \tilde{G}_i$, $\theta = Cz + \mu$ for $\lambda_1$ and $\theta = T^{-T}z + \mu$ for $\lambda_2$. 

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Proof. The Fisher information matrix is given by $F = -\mathbb{E}_{q_{\lambda}(\theta)}[\nabla_\theta^2 \ell_q]$, where
\[
\ell_q = \log q_{\lambda}(\theta) = -\frac{d}{2} \log(2\pi) - \frac{1}{2} \log |\Sigma| - \frac{1}{2}(\theta - \mu)^T \Sigma^{-1}(\theta - \mu).
\]
If $\lambda = \lambda_1$, $\Sigma = CC^T$ and if $\lambda = \lambda_2$, $\Sigma^{-1} = TT^T$. We have
\[
\begin{align*}
\nabla^2_{\lambda_1} \ell_q &= - \begin{bmatrix} \Sigma^{-1} & (z^T \otimes \Sigma^{-1} + C^{-T} \otimes z^T C^{-1}) L^T \\
L\{(zz^T - I_d)C^{-1} \otimes C^{-T} + C^{-1} \otimes C^{-T} zz^T\} K + zz^T \otimes \Sigma^{-1} & L^T \end{bmatrix}, \\
\nabla^2_{\lambda_2} \ell_q &= - \begin{bmatrix} \Sigma^{-1} & -z^T \otimes I_d + T \otimes z^T T^{-1} \end{bmatrix} L^T \\
& \quad \times \{(T^{-1} \otimes T^{-T}) K + I_d \otimes T^{-T} zz^T T^{-1}\} L^T.
\end{align*}
\]
Since $E_{\phi(z)}(z) = 0$ and $E_{\phi(z)}(zz^T) = I_d$, we obtain $F_{\lambda_1}$ in (10) by applying Lemma 1. Since $F_{\lambda_1}$ is a block-diagonal matrix and each of the blocks is invertible, applying Lemma 1 again gives $F_{\lambda_2}^{-1}$ in (10). Finally, the natural gradient is given by
\[
\nabla_{\lambda_1} \mathcal{L} = F_{\lambda_1}^{-1} \nabla_{\lambda_1} \mathcal{L} = \begin{bmatrix} \Sigma & 0 \\
0 & \mathcal{J}(\lambda_1)^{-1} \end{bmatrix} E_{\phi(z)} \left[ \nabla_{\theta} h(\theta) \right] = E_{\phi(z)} \left[ \Sigma \nabla_{\theta} h(\theta) \right],
\]
where we have applied the last result in Lemma 1. More details are given in Appendix C.

The stochastic variational inference algorithms for updating $\mu$ and $C$ where $\Sigma = CC^T$ are outlined in Figure 1. For comparison, Algorithm 1a on the left is based on Euclidean gradients while Algorithm 1b on the right is based on natural gradients. Similarly, the algorithms for updating $\mu$ and $T$ where $\Sigma^{-1} = TT^T$ are given in Figure 2, where Algorithm 2a is based on Euclidean gradients while Algorithm 2b is based on natural gradients.

**Algorithm 1a** (Update $\mu$ and $C$ using Euclidean gradients)

- Initialize $\mu^{(t)}$ and $C^{(t)}$.
- For $t = 1, 2, \ldots$,
  1. Generate $z \sim N(0, I_d)$ and compute $\theta^{(t)} = C^{(t)} z + \mu^{(t)}$.
  2. Compute $\hat{G}_1$, where $G_1 = \nabla_{\theta} h(\theta^{(t)}) z^T$.
  3. Update $\mu^{(t+1)} = \mu^{(t)} + \rho_t \nabla_{\theta} h(\theta^{(t)})$.
  4. Update $C^{(t+1)} = C^{(t)} + \rho_t \hat{G}_1$.

**Algorithm 1b** (Update $\mu$ and $C$ using natural gradients)

- Initialize $\mu^{(t)}$ and $C^{(t)}$. For $t = 1, 2, \ldots$,
  1. Generate $z \sim N(0, I_d)$ and compute $\theta^{(t)} = C^{(t)} z + \mu^{(t)}$.
  2. Compute $G_1$, where $G_1 = \nabla_{\theta} h(\theta^{(t)}) z^T$.
  3. Compute $\hat{H}_1$ where $H_1 = C^{(t)T} G_1$.
  4. Update $\mu^{(t+1)} = \mu^{(t)} + \rho_t C^{(t)} C^{(t)T} \nabla_{\theta} h(\theta^{(t)})$.
  5. Update $C^{(t+1)} = C^{(t)} + \rho_t C^{(t)} \hat{H}_1$.

Figure 1: Stochastic variational inference algorithms for updating $\mu$ and $C$ where $\Sigma = CC^T$.

To ensure that the Cholesky factor $C$ is unique, we may restrict its diagonal entries to be positive. This can be done (see, e.g. Tan and Nott, 2018) by defining a lower triangular matrix $C'$ such that $C'_{ii} = \log(C_{ii})$ and $C'_{ij} = C_{ij}$ if $i > j$, and applying the stochastic
Algorithm 2a (Update $\mu$ and $T$ using Euclidean gradients)

Initialize $\mu^{(1)}$ and $T^{(1)}$.
For $t = 1, 2, \ldots$,
1. Generate $z \sim N(0, I_d)$ and compute $\theta^{(t)} = T^{(t)-1} z + \mu^{(t)}$.
2. Compute $G_2$, where $G_2 = -T^{(t)-1} z [\nabla_{\theta} h(\theta^{(t)})]^T T^{(t)-1}$.
3. Update $\mu^{(t+1)} = \mu^{(t)} + \rho_t \nabla_{\theta} h(\theta^{(t)})$.
4. Update $T^{(t+1)} = T^{(t)} + \rho_t G_2$.

Algorithm 2b (Update $\mu$ and $T$ using natural gradients)

Initialize $\mu^{(1)}$ and $T^{(1)}$. For $t = 1, 2, \ldots$,
1. Generate $z \sim N(0, I_d)$ and compute $\theta^{(t)} = T^{(t)-1} z + \mu^{(t)}$.
2. Compute $G_2$, where $G_2 = -T^{(t)-1} z [\nabla_{\theta} h(\theta^{(t)})]^T T^{(t)-1}$.
3. Compute $H_2$ where $H_2 = T^{(t)} G_2$.
4. Update $\mu^{(t+1)} = \mu^{(t)} + \rho_t T^{(t)-1} \nabla_{\theta} h(\theta^{(t)})$.
5. Update $T^{(t+1)} = T^{(t)} + \rho_t T^{(t)} H_2$.

Figure 2: Stochastic variational inference algorithms for updating $\mu$ and $T$ where $\Sigma^{-1} = TT^T$.

gradient updates to $C'$ instead. From [4],

$$\tilde{\nabla}_{\text{vech}(C')} L = \{ \nabla_{\text{vech}(C')} \text{vech}(C') \}^T \tilde{\nabla}_{\text{vech}(C')} L = \text{vech}(L_C) \odot \tilde{\nabla}_{\text{vech}(C')} L,$$

where $\nabla_{\text{vech}(C')} \text{vech}(C') = \text{diag}[\text{vech}(L_C)]$ and $L_C$ is a $d \times d$ lower triangular matrix with diagonal equal $1/\text{diag}(C)$ and ones elsewhere. Thus the update 5) in algorithm 1b can be replaced with

$$C'(t+1) = C'(t) + \rho_t L C'(t) \odot C'(t) \tilde{H}_1.$$

A similar modification can be made to ensure the Cholesky factor $T$ is unique in Algorithm 2b.

6 Imposing sparsity

In high-dimensional hierarchical models, it may be useful to impose sparsity constraints on the covariance or precision matrix, and on their corresponding Cholesky factors. For Algorithms 1a and 2a, updates of sparse Cholesky factors can be obtained simply by extracting entries in the Euclidean gradients corresponding to nonzero entries in the Cholesky factors. However, the same does not necessarily apply to natural gradients due to premultiplication of the Euclidean gradient by the Fisher information matrix. In this section, we derive efficient natural gradient updates of the Cholesky factors in the case where (i) the covariance matrix has a block-diagonal structure corresponding to the assumption in variational Bayes, such as in RVB [Tan 2021] and (ii) the precision matrix reflects the posterior conditional independence structure in a hierarchical model.
6.1 Block-diagonal covariance structure

Suppose the covariance matrix has a block-diagonal structure,

\[ \Sigma = \text{blockdiag}(\Sigma_1, \ldots, \Sigma_N). \]

Then \( C = \text{blockdiag}(C_1, \ldots, C_N) \), where \( C_iC_i^T \) is the Cholesky decomposition of each \( \Sigma_i \) and \( C_i \) is a \( d_i \times d_i \) lower triangular matrix with \( \sum_{i=1}^N d_i = d \). This approach of assuming a block-diagonal covariance matrix is used in reparametrized variational Bayes (RVB, Tan, 2021), where the local variables in a hierarchical model are first transformed so that they are independent of each other and of the global variables a posteriori before applying variational Bayes. In this case, \( \lambda = (\mu^T, \text{vech}(C_1)^T, \ldots, \text{vech}(C_N)^T)^T \). Let \( \mu = (\mu_1^T, \ldots, \mu_N^T)^T \), \( \theta = (\theta_1^T, \ldots, \theta_N^T)^T \) and \( z = (z^T, \ldots, z_N^T)^T \) be corresponding partitionings so that

\[ \theta = Cz + \mu = \begin{bmatrix} C_1z_1 \\ \vdots \\ C_Nz_N \end{bmatrix} + \mu. \]

Extending earlier results, we have

\[
\nabla_\lambda \theta = \begin{bmatrix} \nabla_\mu \theta \\ \nabla_{\text{vech}(C_1)} \theta \\ \vdots \\ \nabla_{\text{vech}(C_N)} \theta \end{bmatrix} = \begin{bmatrix} I_d \\ L(z_1 \otimes I_{d_1}) & \cdots & 0 \\ \vdots \\ 0 & \cdots & L(z_N \otimes I_{d_N}) \end{bmatrix}
\]

and

\[
\nabla_\lambda \mathcal{L} = E_{\phi(z)} \left[ \begin{bmatrix} \nabla_{\theta^i} h(\theta) \\ L(z_1 \otimes I_{d_1}) \nabla_{\theta_1} h(\theta) \\ \vdots \\ L(z_N \otimes I_{d_N}) \nabla_{\theta_N} h(\theta) \end{bmatrix} \right] = E_{\phi(z)} \left[ \begin{bmatrix} \nabla_{\theta} h(\theta) \\ \text{vech}(\bar{G}_{11}) \\ \vdots \\ \text{vech}(\bar{G}_{1N}) \end{bmatrix} \right],
\]

where \( G_{1i} = \nabla_{\theta_i} h(\theta)z_i^T \) for \( i = 1, \ldots, N \). In this case,

\[
\ell_q = -\frac{d}{2} \log(2\pi) - \sum_{i=1}^N \left\{ \log |C_i| + \frac{1}{2} (\theta_i - \mu_i)^T C_i^{-T} C_i C_i^T (\theta_i - \mu_i) \right\}.
\]

The Fisher information matrix \( F_\lambda \) can be shown to be a block-diagonal matrix with \( N + 1 \) blocks, where the inverse of each of the last \( N \) blocks can be found using Lemma. Thus the natural gradient is given by

\[
\tilde{\nabla}_\lambda \mathcal{L} = F_\lambda^{-1} \nabla_\lambda \mathcal{L}
\]
where \( H_{1i} = C_i^T \bar{G}_{1i} \) for \( i = 1, \ldots, N \).

The above result is useful as it shows that to find the natural gradient, it is sufficient to compute \( \bar{G}_{1i} \) and \( H_{1i} \) and \( C_i \bar{H}_{1i} \) for \( i = 1, \ldots, n \). Hence, \( C, \bar{G}_1 = \text{blockdiag}(\bar{G}_{11}, \ldots, \bar{G}_{1N}) \) and \( \bar{H}_1 = \text{blockdiag}(\bar{H}_{11}, \ldots, \bar{H}_{1N}) \) can all be stored and computed as sparse block lower triangular matrices in Algorithm 1b. The procedure is outlined in Algorithm 1c. For example, Figure 3 illustrates the nonzero entries in \( C^T, \bar{G}_1 \) and \( H_1 = C^T \bar{G}_1 \) using shaded regions when there are \( N = 4 \) blocks in \( \Sigma \). If we apply Algorithm 1b naively by computing the full \( \bar{G}_1 \) (where \( G_1 = \nabla_{\theta} h(\theta)z^T \)), \( H_1 = C^T \bar{G}_1 \) and \( \bar{C} \bar{H}_1 \), and then updating only the nonzero entries in \( C \), we would get the same answer but a lot of resources are wasted because \( \bar{G}_1 \) and \( \bar{H}_1 \) are actually very sparse when \( \Sigma \) is block-diagonal. With this approach, the additional computation required to use Algorithm 1b (with natural gradients) instead of Algorithm 1a (with Euclidean gradients) will be insignificant even for high-dimensional problems.

![Figure 3: Shaded regions denote the nonzero entries in \( C^T, \bar{G}_1 \) and \( H_1 = C^T \bar{G}_1 \) when \( \Sigma \) is a block-diagonal matrix with 4 blocks.](image)

### 6.2 Sparse precision matrix

Consider a hierarchical model where \( p(y, \theta) = p(\theta_G) \prod_{i=1}^n p(y_i|b_i, \theta_G)p(b_i|\theta_G) \) and \( \theta = (b_1^T, \ldots, b_n^T, \theta_G^T)^T \). Then the local variables \( b_1, \ldots, b_n \) are independent of each other conditional on the global variables \( \theta_G \). Hence we can consider the precision matrix \( \Omega = \Sigma^{-1} \) with Cholesky decomposition \( TT^T \) to be of the form

\[
\Omega = \begin{bmatrix}
    \Omega_1 & \cdots & 0 \\
    \vdots & \ddots & \vdots \\
0 & \cdots & \Omega_n \\
\end{bmatrix}
\quad \text{and} \quad
T = \begin{bmatrix}
    T_1 & \cdots & 0 & 0 \\
    \vdots & \ddots & \vdots & \vdots \\
0 & \cdots & T_n & 0 \\
\end{bmatrix},
\]

where \( T_1, \ldots, T_n \) and \( T_G \) are lower triangular matrices of orders \( d_1, \ldots, d_n \) and \( d_G \). Let

\[
\lambda = (\mu^T, \text{vech}(T_1)^T, \text{vec}(T_{G1})^T, \ldots, \text{vech}(T_n)^T, \text{vec}(T_{Gn})^T, \text{vech}(T_G)^T)^T.
\]
Algorithm 1c (Block-diagonal covariance matrix)

Initialize $\mu^{(1)}$ and $C^{(1)}$ where $C = \text{blockdiag}(C_1, \ldots, C_N)$.
For $t = 1, 2, \ldots$,
1. Generate $z \sim \text{N}(0, I_d)$ and compute $\theta^{(t)} = C^{(t)} z + \mu^{(t)}$.
2. Compute $G_1 = \text{blockdiag}(G_{11}, \ldots, G_{1N})$.
3. Compute $\bar{H}_1$ where $H_1 = C^{(t)T} G_1$.
4. Update $\mu^{(t+1)} = \mu^{(t)} + \rho_t C^{(t)} C^{(t)T} \nabla_{\theta} h(\theta^{(t)})$.
5. Update $C^{(t+1)} = C^{(t)} + \rho_t C^{(t)} \bar{H}_1$.

Algorithm 2c (Sparse precision matrix)

Initialize $\mu^{(1)}$ and $T^{(1)}$ for $T$ in (11).
For $t = 1, 2, \ldots$,
1. Generate $z \sim \text{N}(0, I_d)$ and compute $\theta^{(t)} = T^{(t)-1} z + \mu^{(t)}$.
2. Find $u = T_D^{(t)T} z$ and $v = T^{(t)-1} \nabla_{\theta} h(\theta^{(t)})$.
3. Compute $\bar{G}_2$ in (12).
4. Compute $\bar{H}_2$ where $H_2 = T_D^{(t)T} \bar{G}_2$.
5. Update $\mu^{(t+1)} = \mu^{(t)} + \rho_t T^{(t)-T} T^{(t)-1} \nabla_{\theta} h(\theta^{(t)})$.
6. Update $T^{(t+1)} = T^{(t)} + \rho_t T^{(t)} \bar{H}_2$.

Figure 4: Stochastic variational inference algorithms based on natural gradients.

For this ordering, the Fisher information matrix $F_\lambda$ is a block diagonal matrix. Let $\mu = (\mu_1^T, \ldots, \mu_n^T, \mu_G^T)^T$, $\theta = (\theta_1^T, \ldots, \theta_n^T, \theta_G^T)^T$ and $z = (z_1^T, \ldots, z_n^T, z_G^T)^T$ be corresponding partitionings. In addition, let $T_D = \text{blockdiag}(T_1, \ldots, T_n, T_G)$ and $u = T_D^{T} z = (u_1^T, \ldots, u_n^T, u_G^T)^T$, where $u_i = T_i^{-T} z_i$ for $i = 1, \ldots, n$ and $u_G = T_G^{-T} z_G$. We have

$$T^{-1} = \begin{bmatrix}
T_1^{-1} & \ldots & 0 & 0 \\
\vdots & \ddots & \vdots & \vdots \\
0 & \ldots & T_n^{-1} & 0 \\
-T_G^{-1} T_1 T_1^{-1} & \ldots & -T_G^{-1} T_n T_n^{-1} T_G^{-1} & 0
\end{bmatrix}$$
and $\theta = T^{-T} z + \mu = \begin{bmatrix}
T_1^{-T} w_1 \\
\vdots \\
T_n^{-T} w_n \\
u_G
\end{bmatrix}$.

where $w_i = z_i - T_G^{T} u_G$ for $i = 1, \ldots, n$. Then

$$\nabla_\lambda \theta = [\nabla_{\mu} \theta^T \quad \nabla_{\text{vec}(T_1)} \theta^T \quad \nabla_{\text{vec}(T_G)} \theta^T \ldots \quad \nabla_{\text{vec}(T_n)} \theta^T \quad \nabla_{\text{vec}(T_G)} \theta^T \quad \nabla_{\text{vec}(T_G)} \theta^T]^T$$

$$= \begin{bmatrix}
I_d \\
-L(T_1^{-1} \otimes T_1^{-T} w_1) & \ldots & 0 & 0 \\
-(T_1^{-1} \otimes u_G) & \ldots & 0 & 0 \\
\vdots & \ddots & \vdots & \vdots \\
0 & \ldots & -L(T_n^{-1} \otimes T_n^{-T} w_n) & 0 \\
0 & \ldots & -(T_n^{-1} \otimes u_G) & 0 \\
L(T_G^{-1} T_1 T_1^{-1} \otimes u_G) & \ldots & L(T_G^{-1} T_G T_n^{-1} \otimes u_G) & -L(T_G^{-1} \otimes u_G)
\end{bmatrix}.$$
Let \( v = T^{-1} \nabla_\theta h(\theta) = (v_1, \ldots, v_n, v_G) \), where \( v_i = T_i^{-1} \nabla_\theta h(\theta) \) for \( i = 1, \ldots, n \) and \( v_G = T_G^{-1}[\nabla_\theta h(\theta) - \sum_{i=1}^n T_{Gi}T_i^{-1} \nabla_\theta h(\theta)] \). The Euclidean gradient is given by

\[
\nabla_\lambda \mathcal{L} = E_{\phi(z)} \left[ \begin{array}{c}
\nabla_\theta h(\theta) \\
\text{vech}( - T_i^T u_i v_i^T ) \\
\text{vec}( - u_G v_i^T ) \\
\text{vech}( G_{2G} )
\end{array} \right]_{i=1,\ldots,n},
\]

where \( G_{2G} = -u_G v_G^T \).

Next, we derive the natural gradient by finding the inverse of the Fisher information matrix explicitly. In this case,

\[
\ell_q = -\frac{d}{2} \log(2\pi) + \log |T_G| + \sum_{i=1}^N \log |T_i| - \frac{1}{2} \sum_{i=1}^n (\theta_i - \mu_i)^T T_i T_i^T (\theta_i - \mu_i)
\]

\[
- \frac{1}{2} (\theta_G - \mu_G)^T \left( \sum_{i=1}^n T_{Gi}T_i^T + T_G T_G^T \right) (\theta_G - \mu_G) - (\theta_G - \mu_G)^T \sum_{i=1}^n T_{Gi}T_i^T (\theta_i - \mu_i).
\]

and the Fisher information matrix is \( F_{\lambda} = \text{blockdiag}(\Sigma^{-1}, F_1, \ldots, F_n, \mathcal{I}(T_G)) \), where

\[
F_i^{-1} = \left[ \begin{array}{cc}
\mathcal{I}(T_i)^{-1} & \mathcal{I}(T_i)^{-1} L(I_d \otimes T_i^{-T} T_G^T) \\
I_d \otimes T_G T_G^T & (I_d \otimes T_{Gi}T_i^T)^{-1} L^T \mathcal{I}(T_i)^{-1} L(I_d \otimes T_i^{-T} T_G^T)
\end{array} \right].
\]

The natural gradient,

\[
\tilde{\nabla}_\lambda \mathcal{L} = F_{\lambda}^{-1} \nabla_\lambda \mathcal{L} = E_{\phi(z)} \left[ \begin{array}{c}
\Sigma \nabla_\theta h(\theta) \\
\text{vech}(T_i \tilde{H}_{2i}) \\
\text{vec}(T_{Gi} \tilde{H}_{2i} - T_G z G i v_i^T ) \\
\text{vech}(T_G \tilde{H}_{2G})
\end{array} \right]_{i=1,\ldots,n},
\]

where \( H_{2i} = T_i^T \tilde{G}_{2i} \) and \( G_{2i} = -u_i v_i^T \) for \( i = 1, \ldots, n \), and \( H_{2G} = T_G^T \tilde{G}_{2G} \). Derivation details are given in Appendix \( \text{[D]} \). To compute the natural gradient, we need to first find \( u = T_D^{-T} z \) and \( v = T^{-1} \nabla_\theta h(\theta) \). Then we compute

\[
\tilde{G}_2 = \left[ \begin{array}{cccc}
\tilde{G}_{21} & \ldots & 0 & 0 \\
\vdots & \ddots & \vdots & \vdots \\
0 & \ldots & \tilde{G}_{2n} & 0 \\
-u_G v_1^T & \ldots & -u_G v_n^T & \tilde{G}_{2G}
\end{array} \right], \quad G_2 = \left[ \begin{array}{cccc}
u_1 v_1^T & \ldots & 0 & 0 \\
\vdots & \ddots & \vdots & \vdots \\
0 & \ldots & u_n v_n^T & 0 \\
u_G v_1^T & \ldots & u_G v_n^T & u_G v_G^T
\end{array} \right].
\]
Note that $\bar{G}_2$ has the same sparsity structure as $T$. Define $H_2 = T_D^T \bar{G}_2$ so that

$$H_2 = \begin{bmatrix} T_1^T \bar{G}_{21} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & T_n^T \bar{G}_{2n} & 0 \end{bmatrix}, \quad \bar{H}_2 = \begin{bmatrix} \bar{H}_{21} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \bar{H}_{2n} & 0 \end{bmatrix}.$$  

Finally,

$$T \bar{H} = \begin{bmatrix} T_1 \bar{H}_{21} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & T_n \bar{H}_{2n} & 0 \end{bmatrix}. $$

The procedure is outlined in Algorithm 2c.

## 7 Conclusion

In Gaussian variational approximation, the natural gradient update of the precision matrix does not ensure positive definiteness. To tackle this issue, we consider Cholesky decompositions of the covariance or precision matrix and derive natural gradient updates of the Cholesky factor in each case. As these parametrizations are not given in terms of the natural parameter, we need to find the inverse of the Fisher information matrix. We demonstrate that this inverse can be found analytically and present the natural gradient updates of the Cholesky factors in closed form. These natural gradient updates can potentially improve convergence in stochastic gradient ascent and can be used in any context where the variational approximation is a multivariate Gaussian. Sparsity constraints can also be imposed to incorporate assumptions in variational Bayes or conditional independence structure in the posterior and efficient natural gradient updates are also derived in several of these cases.

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A Natural gradient of $\mathcal{L}$ with respect to natural parameters

Differentiating $\zeta_2 = m_2 - \vech(m_1 m_1^T)$ with respect to $m_1$, we obtain

$$d\zeta_2 = -D^+ \text{vec}(m_1 dm_1^T + dm_1 m_1^T)$$

$$= -D^+ (I_d^2 + K)(I_d \otimes m_1)dm_1$$

$$= -2D^+DD^+(I_d \otimes m_1)dm_1$$

$$= -2D^+(I_d \otimes m_1)dm_1$$

We have used the properties $I_d^2 + K = 2DD^+$ and $D^+D = I_{d(d+1)/2}$.

B Proof of Lemma [1]

To prove Lemma [1] we require several results regarding the elimination matrix $L$ from Magnus and Neudecker [1980], which are stated in Lemma [2] for ease of reference.

**Lemma 2.** If $P$ and $Q$ are lower triangular $d \times d$ matrices, then

(i) $LL^T = I_{d(d+1)/2}$;

(ii) $(LNL^T)^{-1} = 2I_{d(d+1)/2} - LKL^T$;

(iii) $N = DLN$;

(iv) $L^T L(P^T \otimes Q)L^T = (P^T \otimes Q)L^T$ or the transpose, $L(P \otimes Q^T)L^T = L(P \otimes Q^T)$;

(v) $L(P^T \otimes Q)L^T = D^T(P^T \otimes Q)L^T$ or the transpose, $L(P \otimes Q^T)L^T = L(P \otimes Q^T)D$.

**Proof.** The proofs can be found respectively in Lemma 3.2 (ii), Lemma 3.4 (ii), Lemma 3.5 (ii) and Lemma 4.2 (i) and (iii), of [Magnus and Neudecker] [1980].

**Proof of Lemma [1].** From the left-hand side,

$$\mathcal{J}(\Lambda) = L\{K(\Lambda^{-T} \otimes \Lambda^{-1}) + I_d \otimes \Lambda^{-T} \Lambda^{-1}\}L^T$$

$$= L\{K(\Lambda^{-T} \otimes I_d)(I_d \otimes \Lambda^{-1}) + (I_d \otimes \Lambda^{-T})(I_d \otimes \Lambda^{-1})\}L^T$$

$$= L\{(I_d \otimes \Lambda^{-T})K(I_d \otimes \Lambda^{-1})\}L^T$$

$$= L(I_d \otimes \Lambda^{-1})(K + I_d^2)(I_d \otimes \Lambda^{-1})L^T$$

$$= 2L(I_d \otimes \Lambda^{-T})N(I_d \otimes \Lambda^{-1})L^T.$$

Using the results in Lemma [2] we have

$$\{2L(I_d \otimes \Lambda^{-T})N(I_d \otimes \Lambda^{-1})L^T\} \{\frac{1}{2}L(I_d \otimes \Lambda)L^T(LNL^T)^{-1}L(I_d \otimes \Lambda^T)L^T\}$$

$$= L(I_d \otimes \Lambda^{-T})(DLN)(I_d \otimes \Lambda^{-1})(I_d \otimes \Lambda)L^T(LNL^T)^{-1}L(I_d \otimes \Lambda^T)L^T$$

$$= L(I_d \otimes \Lambda^{-T})L^T(LNL^T)^{-1}L(I_d \otimes \Lambda^T)L^T$$

$$= L(I_d \otimes \Lambda^{-T})L^T L(I_d \otimes \Lambda^T)L^T$$

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\[
= L(I_d \otimes \Lambda^{-T})(I_d \otimes \Lambda^T)L^T \\
= LL^T = I_{d(d+1)/2}. [\text{(iv)}]
\]

The roman letters in square brackets on the right indicate which parts of Lemma 2 are used. Finally,

\[
\mathcal{J}(\Lambda)^{-1}\text{vech}(G) = \frac{1}{2}L(I_d \otimes \Lambda)L^T(LNL^T)^{-1}L(I_d \otimes \Lambda^T)L^T\text{vech}(\bar{G}) \\
= \frac{1}{2}L(I_d \otimes \Lambda)L^T(2I_{d(d+1)/2} - LKL^T)L(I_d \otimes \Lambda^T)\text{vec}(\bar{G}) [\text{Lemma 2(ii)}] \\
= \frac{1}{2}L(I_d \otimes \Lambda)(2I_d - L^T LK)L^T L\text{vec}(\Lambda^T G) \\
= \frac{1}{2}L(I_d \otimes \Lambda)(2I_d - L^T LK)L^T\text{vech}(\bar{H}) \\
= \frac{1}{2}L(I_d \otimes \Lambda)(2I_d - L^T LK)\text{vech}(H) \\
= L(I_d \otimes \Lambda)\text{vech}(\bar{H}) - \frac{1}{2}L(I_d \otimes \Lambda)L^T LK \text{vech}(\bar{H}) \\
= L\text{vech}(\Lambda \bar{H}) - \frac{1}{2}L(I_d \otimes \Lambda)L^T\text{vech}(\bar{H}^T) \\
= \text{vech}(\Lambda \bar{H}) - \frac{1}{2}L(I_d \otimes \Lambda)L^T \text{vech}(\text{d}g(\bar{H})) \\
= \text{vech}(\Lambda \bar{H}) - \frac{1}{2}\text{vech}(\text{d}g(\bar{H})) \\
= \text{vech}(\Lambda \bar{H}).
\]

\[\square\]

C Proof of Theorem 1

The following lemma is useful in the proof of Theorem 1

Lemma 3. Let \( x \) be a vector of length \( d \) and \( T \) be a \( d \times d \) matrix. Then

\[
d\left( \frac{1}{2}x^TTT^Tx \right) = \text{vec}(xx^TT^T)d\text{vec}(T).
\]

If \( T \) is invertible, then

\[
d\left( \frac{1}{2}x^TT^{-1}T^{-1}x \right) = -\text{vec}(T^{-T}T^{-1}xx^TT^{-T})d\text{vec}(T).
\]

Proof.

\[
d\left( \frac{1}{2}x^TTT^Tx \right) = \frac{1}{2}[x^T(dT)^TT^Tx + x^TT(dT)^Tx] \\
= x^T(dT)^TT^Tx = \text{tr}(Txx^TT^T(dT)) \\
= \text{vec}(xx^TT^Td\text{vec}(T)).
\]

\[
d\left( \frac{1}{2}x^TT^{-T}T^{-1}x \right) = -\frac{1}{2}[x^T(-T^{-T}T^{-1}T^{-T}x + x^TT^{-T}T^{-1}(dT)^T(-T^{-1}x)] \\
= -x^T(-T^{-T}T^{-1}T^{-1}x = -\text{tr}(T^{-1}xx^TT^{-T}T^{-1}(dT)) \\
= -\text{vec}(T^{-T}T^{-1}xx^TT^{-T})d\text{vec}(T).
\]
In this case, \( \nabla_{\mu} \ell_q = \Sigma^{-1}(\theta - \mu) \) and \( \nabla_{\mu}^2 \ell_q = -\Sigma^{-1} \).

### C.1 Cholesky decomposition of covariance matrix

In this case, \( \theta = Cz + \mu \). Differentiating \( \nabla_{\mu} \ell_q = C^{-T}C^{-1}(\theta - \mu) \) w.r.t. \( C \),

\[
\text{d}(\nabla_{\mu} \ell_q) = -[C^{-T}(dC^T)C^{-T}C^{-1} + C^{-T}C^{-1}(dC)C^{-1}](\theta - \mu)
\]

\[
= -[C^{-T}(dC^T)C^{-T}z + C^{-T}C^{-1}(dC)z]
\]

\[
= -[(z^TC^{-1} \otimes C^{-T})K + (z^T \otimes C^{-T}C^{-1})]L^T \text{dvech}(C).
\]

\[
\therefore \nabla_{\mu, \text{vech}(C)} \ell_q = -[C^{-T} \otimes z^T C^{-1} + z^T \otimes \Sigma^{-1}]L^T.
\]

Differentiating \( \ell_q \) w.r.t. \( C \) and applying Lemma \( 3 \)

\[
d\ell_q = -\text{tr}(C^{-1}dC) + \text{vec}(C^{-T}C^{-1}(\theta - \mu)(\theta - \mu)^T C^{-T})d\text{dvec}(C).
\]

\[
= -\text{vec}(C^{-T})^T d\text{dvec}(C) + \text{vec}(C^{-T}zz^T)L^T d\text{dvech}(C)
\]

\[
= [-\text{vec}(C^{-T}) + \text{vec}(C^{-T}zz^T)]^T L^T d\text{dvech}(C)
\]

\[
\therefore \nabla_{\text{vech}(C)} \ell_q = L\text{vec}[C^{-T}(zz^T - I_d)] = \text{vech}[C^{-T}(zz^T - I_d)].
\]

Since \( z = C^{-1}(\theta - \mu) \), differentiating \( z \) with respect to \( \text{vech}(C) \),

\[
dz = -C^{-1}(dC)C^{-1}(\theta - \mu) = -C^{-1}(dC)z.
\]

Differentiating \( \nabla_{\text{vech}(C)} \ell_q = \text{vech}[C^{-T}(zz^T - I_d)] \) w.r.t. \( C \),

\[
d\nabla_{\text{vech}(C)} \ell_q = L\text{vec}[-C^{-T}dC^TC^{-T}(zz^T - I_d) + C^{-T} \{ z(dz^T) + dz(z^T) \}]
\]

\[
= -L \{ [(zz^T - I_d)C^{-1} \otimes C^{-T}]Kd\text{dvec}(C) + \text{vec}[C^{-T}zz^T(dC^T)C^{-T} + C^{-T}C^{-1}dCzz^T] \}
\]

\[
= -L \{ [(zz^T - I_d)C^{-1} \otimes C^{-T}]K + (C^{-1} \otimes C^{-T}zz^T)K + (zz^T \otimes \Sigma^{-1})L^T d\text{dvech}(C) \}.
\]

\[
\therefore \nabla^2_{\text{vech}(C)} \ell_q = -L \{ [(zz^T - I_d)C^{-1} \otimes C^{-T} + C^{-1} \otimes C^{-T}zz^T]K + zz^T \otimes \Sigma^{-1} \}L^T.
\]

Taking negative expectations with respect to \( g_{\lambda_1}(\theta) \), we have by Lemma \( 4 \)

\[
-\mathbb{E}_{g_{\lambda_1}(\theta)}[\nabla^2_{\text{vech}(C)} \ell_q] = L \{ (C^{-1} \otimes C^{-T})K + (I_d \otimes C^{-T}C^{-1}) \}L^T = \mathcal{J}(C).
\]

### C.2 Cholesky decomposition of precision matrix

In this case, \( z = T^T(\theta - \mu) \) and

\[
\ell_q = -\frac{d}{2} \log(2\pi) + \log |T| - \frac{1}{2} (\theta - \mu)TT^T(\theta - \mu).
\]
Differentiating $\nabla_{\mu} \ell_q = TT^T(\theta - \mu)$ w.r.t. $T$,

$$d(\nabla_{\mu} \ell_q) = [(dT)T^T + T(dT^T)](\theta - \mu) = ((\theta - \mu)^T T \otimes I_d + ((\theta - \mu)^T \otimes T)K)L^T \text{dvech}(T)$$

$$\therefore \nabla_{\mu,\text{vech}(T)}^2 \ell_q = ((\theta - \mu)^T T \otimes I_d + T \otimes (\theta - \mu)^T)L^T$$

Taking negative expectations with respect to $q_{\lambda_2}(\theta)$, we have by Lemma 3

$$-E_{q_{\lambda_2}(\theta)}[\nabla_{\text{vech}(T)}^2 \ell_q] = L\{(T^{-1} \otimes T^{-T})K + I_d \otimes T^{-T}T^{-1}\}L^T = \mathcal{J}(T).$$

**D Sparse precision matrix**

Differentiating $\ell_q$ with respect to $T_i$ and applying Lemma 3

$$d\ell_q = \text{tr}(T_i^{-1}dT_i) - \text{vec}[(\theta_i - \mu_i)(\theta_i - \mu_i)^T dT_i]$$

$$= \text{vec}\{T_i^{-1}(\theta_i - \mu_i)(\theta_i - \mu_i)^T dT_i\} - \text{vec}((\theta_i - \mu_i)(\theta_i - \mu_i)^T dT_i)$$

$$\therefore \nabla_{\text{vech}(T_i)} \ell_q = \text{vech}\{(T_i^{-1} - (\theta_i - \mu_i)(\theta_i - \mu_i)^T T_i - (\theta_i - \mu_i)(\theta_i - \mu_i)^T T_i + (\theta_i - \mu_i)(\theta_i - \mu_i)^T T_i G_i\}.$$
Differentiating $\nabla_{\text{vec}(T_i)} \ell_q$ with respect to $T_{G_i}$,
\[
\text{d} \nabla_{\text{vec}(T_i)} \ell_q = -L \text{vec}[\{(\theta_i - \mu_i)(\theta_G - \mu_G)^T dT_{G_i}\} \daddr{vec}(T_{G_i})
= -L\{I_{d_i} \otimes (\theta_i - \mu_i)(\theta_G - \mu_G)^T\} \daddr{vec}(T_{G_i}),
\]
\[
\nabla_{\text{vec}(T_i), \text{vec}(T_G)} \ell_q = -L\{I_{d_i} \otimes T_i^{-T}(z_i - T_{G_i}^{-T} z_G)z_G^{-T} T_{G_i}^{-1}\}.
\]
\[
-E[\nabla_{\text{vec}(T_i), \text{vec}(T_G)} \ell_q] = -L\{I_{d_i} \otimes T_i^{-T} T_{G_i}^{-T} T_{G_i}^{-1}\}.
\]

Differentiating $\ell_q$ with respect to $T_{G_i}$,
\[
\text{d} \ell_q = \text{vec}[(\theta_G - \mu_G)(\theta_G - \mu_G)^T T_{G_i} + (\theta_G - \mu_G)(\theta_i - \mu_i)^T T_i]^T \daddr{vec}(T_{G_i}).
\]
\[
\nabla_{\text{vec}(T_G_i)} \ell_q = \text{vec}[(\theta_G - \mu_G)(\theta_G - \mu_G)^T T_{G_i} + (\theta_G - \mu_G)(\theta_i - \mu_i)^T T_i].
\]

Differentiating $\ell_q$ with respect to $T_G$,
\[
\text{d} \ell_q = \text{tr}(T_{G_i}^{-1} \text{d} T_{G_i}) - \text{vec}[(\theta_G - \mu_G)(\theta_G - \mu_G)^T T_{G_i}]^T L^T \daddr{vec}(T_{G_i})
= \text{vec}[T_{G_i}^{-T} - (\theta_G - \mu_G)(\theta_G - \mu_G)^T T_{G_i}]^T L^T \daddr{vec}(T_{G_i}).
\]
\[
\nabla_{\text{vec}(T_G)} \ell_q = \text{vec}[T_{G_i}^{-T} - (\theta_G - \mu_G)(\theta_G - \mu_G)^T T_{G_i}].
\]

Differentiating $\nabla_{\text{vec}(T_G)} \ell_q$ with respect to $T_G$,
\[
\text{d} \nabla_{\text{vec}(T_G)} \ell_q = -L \text{vec}[(T_{G_i}^{-T} dT_{G_i})^T T_{G_i}^{-T} + (\theta_G - \mu_G)(\theta_G - \mu_G)^T dT_G]
= -L[(T_{G_i}^{-1} \otimes T_{G_i}^{-T}) K + I_{d_G} \otimes (\theta_G - \mu_G)(\theta_G - \mu_G)^T L^T] \daddr{vec}(T_{G_i}).
\]
\[
\nabla_{\text{vec}(T_G)} \ell_q = -L[(T_{G_i}^{-1} \otimes T_{G_i}^{-T}) K + I_{d_G} \otimes T_{G_i}^{-T} z_G z_G^{-T} T_{G_i}^{-1}] L^T.
\]
\[
-E[\nabla_{\text{vec}(T_G)} \ell_q] = L[(T_{G_i}^{-1} \otimes T_{G_i}^{-T}) K + I_{d_G} \otimes T_{G_i}^{-T} T_{G_i}^{-1}] L^T = \mathcal{J}(T_G).
\]

Thus the Fisher information matrix is a block diagonal, where
\[
F_i = \begin{bmatrix} A_i & B_i \\ B_i^T & D_i \end{bmatrix} \quad \text{and} \quad \begin{aligned}
A_i &= \mathcal{J}(T_i) + L(I_{d_i} \otimes T_i^{-T} T_{G_i}^{-1} T_{G_i}^{-1} T_{G_i}^{-1} T_{G_i}^{-1} T_{G_i}^{-1}) L^T, \\
B_i &= -L(I_{d_i} \otimes T_i^{-T} T_{G_i}^{-1} T_{G_i}^{-1} T_{G_i}^{-1} T_{G_i}^{-1} T_{G_i}^{-1}), \\
D_i &= I_{d_i} \otimes T_{G_i}^{-T} T_{G_i}^{-1}.
\end{aligned}
\]

Since $D_i^{-1} = I_{d_i} \otimes T_{G_i} T_{G_i}^{-T}$, and $B_i D_i^{-1} = -L(I_{d_i} \otimes T_{G_i}^{-T} T_{G_i}^{-1} T_{G_i}^{-1} T_{G_i}^{-1} T_{G_i}^{-1} T_{G_i}^{-1} T_{G_i}^{-1}) L^T$.
and $A_i - B_i D_i^{-1} B_i^T = \mathcal{I}(T_i)$. Hence

$$F_i^{-1} = \begin{bmatrix}
\mathcal{I}(T_i)^{-1} \\
(I_d \otimes T_G T_i^{-1}) L^T \mathcal{I}(T_i)^{-1} \\
I_d \otimes T_G T_i^T + (I_d \otimes T_G T_i^{-1}) L^T \mathcal{I}(T_i)^{-1} L(I_d \otimes T_i^{-1} T_G^T)
\end{bmatrix}. $$

The natural gradient

$$\begin{bmatrix}
\tilde{\nabla}_{\text{vech}(T_i)} \mathcal{L} \\
\tilde{\nabla}_{\text{vec}(T_i)} \mathcal{L}
\end{bmatrix} = F_i^{-1} \begin{bmatrix}
\text{vech}(-T_i^{-T} w_i v_i^T) \\
\text{vec}(-u_i G_i)
\end{bmatrix}. $$

We have

$$\begin{align*}
\tilde{\nabla}_{\text{vech}(T_i)} \mathcal{L} &= \mathcal{I}(T_i)^{-1} \text{vech}(-T_i^{-T} w_i v_i^T) + L(I_d \otimes T_i^{-T} T_G^T) \text{vech}(-u_i G_i)
\end{align*}$$

where $G_{2i} = -T_i^{-T} z_i v_i^T$ and $H_{2i} = T_i^T \bar{G}_{2i}$. In addition,

$$\begin{align*}
\tilde{\nabla}_{\text{vec}(T_i)} \mathcal{L} &= (I_d \otimes T_G T_i^T) \text{vec}(-u_i G_i) + (I_d \otimes T_G T_i^{-1}) L^T \text{vech}[T_i \{H_{2i} - \text{dg}(\bar{H}_{2i})/2]\}
\end{align*}$$

Finally,

$$\begin{align*}
\tilde{\nabla}_{\text{vec}(T_G)} \mathcal{L} &= \mathcal{I}(T_G)^{-1} \text{vech}(G_{2G}) = \text{vech}(T_G \bar{H}_{2G})
\end{align*}$$

where $H_{2G} = T_G^T \bar{G}_{2G}$. 

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