Fast and Simple Natural-Gradient Variational Inference with Mixture of Exponential-family Approximations

Wu Lin 1 Mohammad Emtiyaz Khan 2 Mark Schmidt 1

Abstract

Natural-gradient methods enable fast and simple algorithms for variational inference, but due to computational difficulties, their use is mostly limited to minimal exponential-family (EF) approximations. In this paper, we extend their application to estimate structured approximations such as mixtures of EF distributions. Such approximations can fit complex, multimodal posterior distributions and are generally more accurate than unimodal EF approximations. By using a minimal conditional-EF representation of such approximations, we derive simple natural-gradient updates. Our empirical results demonstrate a faster convergence of our natural-gradient method compared to black-box gradient-based methods. Our work expands the scope of natural gradients for Bayesian inference and makes them more widely applicable than before.

1. Introduction

Variational Inference (VI) provides a cheap and quick approximation to the posterior distribution, and is now widely used in many areas of machine learning (Kingma & Welling, 2013; Furmston & Barber, 2010; Wainwright & Jordan, 2008; Hensman et al., 2013; Nguyen et al., 2017). In recent years, many natural-gradient methods have been proposed for VI (Sato, 2001; Honkela et al., 2007; 2011; Hensman et al., 2012; Hoffman et al., 2013; Khan & Lin, 2017). These works have shown that, for specific types of models and approximations, natural-gradient methods can result in simple updates which converge faster than gradient-based methods. For example, stochastic variational inference (SVI) (Hoffman et al., 2013) is a popular natural-gradient method for conjugate exponential-family models. Unfortunately, the simplicity of natural-gradient updates is currently limited to VI with minimal exponential-family (EF) approximations. Such approximations include all minimal (normalized) EF distributions, but not curved or mixture of EF distributions. Such structured approximations are more appropriate for complex and multi-modal posterior distributions, giving a more accurate fit than minimal EF distributions. However, computation of natural-gradients is challenging for them.

In this paper, we propose a simple new natural-gradient method for VI with structured approximations. We define a class of distributions which take a minimal conditional-EF (MCEF) form. This includes many members of mixture and curved EF distributions (see Fig. 1). Using the MCEF representation and an expectation parameterization associated with it, we derive simple natural-gradient updates. Our empirical results show faster convergence of our method compared to gradient descent for VI. Our work extends the simplicity of natural-gradient methods making them more widely applicable than before, while maintaining their fast convergence.

1.1. Related Works

Existing work on natural-gradient VI to obtain EF approximations all assume a minimal representation to ensure invertibility of the FIM. Such methods show fast convergence,
result in simple updates, and lead to a straightforward implementation for many types of models. They have been used for conditionally-conjugate EF models (Sato, 2001; Hoffman et al., 2013) and non-conjugate models (Khan & Lin, 2017), including deep neural networks (Khan et al., 2018; Zhang et al., 2018; Mishkin et al., 2018) and Gaussian processes (Khan et al., 2016; Salimbeni et al., 2018). Our work presents fast and simple updates for approximations that are beyond the reach of these works.

For structured approximations, existing works employ stochastic-gradient methods (Salimans & Knowles, 2013; Hoffman & Blei, 2015; Ranganath et al., 2016; Titsias & Ruiz, 2018; Yin & Zhou, 2018). Such methods are widely applicable, but not as widely used as their mean-field counterparts. This is because they are computationally expensive and slow to converge. Our work attempts to improve these aspects for a flexible class of approximations.

2. Natural-Gradient Variational Inference

We begin with a description of natural-gradient descent for variational inference in probabilistic models. Given a probabilistic model \( p(D, z) \) to model data \( D \) using latent vector \( z \), the goal of Bayesian inference is to compute the posterior distribution: \( p(z|D) = p(D, z)/p(D) \). This requires computation of the marginal likelihood \( p(D) = \int p(D, z)dz \), which is a high dimensional integral and difficult to compute. VI simplifies this problem by approximating the posterior distribution:

\[
q(z|\lambda_z) = h(z) \exp \left[ \langle \phi_z(z), \lambda_z \rangle - A_z(\lambda_z) \right],
\]

where \( q \) denotes the approximating distribution, \( \phi_z(z) \) are the sufficient statistics, \( h(z) \) is the base measure, and \( \lambda_z \in \Omega \) is the natural parameter with \( \Omega \) being the set of valid natural-parameters (the set of \( \lambda_z \) where the log-partition function \( A_z(\lambda_z) \) is finite) and \( \langle \cdot, \cdot \rangle \) denotes an inner product.\(^1\) Such parametrized approximations can be estimated by maximizing the variational lower bound:

\[
\mathcal{L}(\lambda_z) := \mathbb{E}_q[\log p(D, z) - \log q(z|\lambda_z)],
\]

which can be solved by gradient descent, as shown below:

\[
\text{GD} : \quad \lambda_z \leftarrow \lambda_z + \alpha \nabla_{\lambda_z} \mathcal{L}(\lambda_z),
\]

where \( \nabla \) denotes the gradient and \( \alpha > 0 \) is a scalar learning rate. The GD algorithm is simple and convenient to implement by using modern automatic-differentiation methods and the reparameterization trick (Ranganath et al., 2014; Titsias & Lázaro-Gredilla, 2014). Unfortunately, such first-order methods can show suboptimal rates of convergence and be slow in practice.

An alternative approach is to use natural-gradient descent which exploits the information geometry of \( q \) to speed-up convergence. Assuming that the Fisher information matrix (FIM) of \( q(z|\lambda_z) \), denoted by \( \mathbf{F}_z(\lambda_z) \), is positive-definite for all \( \lambda_z \in \Omega \), the natural-gradient descent (NGD) for VI in the natural-parameter space is given as follows:

\[
\text{NGD} : \quad \lambda_z \leftarrow \lambda_z + \beta [\mathbf{F}_z(\lambda_z)]^{-1} \nabla_{\lambda_z} \mathcal{L}(\lambda_z),
\]

The preconditioning of the gradients by the FIM leads to a proper scaling of the gradient in each dimension, and takes into account dependencies between variables. This often leads to faster convergence, particularly when the FIM is well-conditioned.

A naive implementation of (4) would require computation and inversion of the FIM. However, for specific types of models and approximations, NGVI could be simpler to compute than GD. This is true for mean-field VI in conjugate-exponential family models (Hoffman et al., 2013) as well as Bayesian neural networks (Khan et al., 2018; Zhang et al., 2018). This computational efficiency is a result of a simple NGD update to estimate EF approximations, as shown by Khan & Nielsen (2018). For EFs, we can use the expectation-parameter, defined as the function \( \mathbf{m}_z(\lambda_z) := \mathbb{E}_q[\phi_z(z)] \) from \( \Omega \rightarrow \mathcal{M} \), to compute natural-gradients. This is possible because of the following relation,

\[
\nabla_{\lambda_z} \mathcal{L} = \left[ \nabla_{\lambda_z} \mathbf{m}_z^T \right] \nabla_{\mathbf{m}_z} \mathcal{L} = \left[ \mathbf{F}_z(\lambda_z) \right] \nabla_{\mathbf{m}_z} \mathcal{L}
\]

where the first equality is obtained by applying the chain rule and second equality is obtained by noting that \( \nabla_{\lambda_z} \mathbf{m}_z^T = \nabla_{\lambda_z} A(\lambda_z) = \mathbf{F}_z(\lambda_z) \). When the FIM is invertible, we get a simple update for NGD,

\[
\lambda_z \leftarrow \lambda_z + \beta \nabla_{\mathbf{m}_z} \mathcal{L}(\lambda_z),
\]

where the gradient is computed with respect to \( \mathbf{m}_z \). When the above gradient is easier to compute than the gradient with respect to \( \lambda_z \), NGD admits a simpler form than GD. This is the case for many existing works on NGD for VI.

To rewrite NGD as in (6), we need the FIM to be invertible. For EFs, a sufficient condition for invertibility is to use a minimal representation which is defined\(^3\) below using the definition given in Wainwright & Jordan (2008).

**Definition 1** (Minimal EF) A regular EF representation is said to be minimal when there does not exist a nonzero vectors \( \lambda \) such that \( \langle \phi_z(z), \lambda \rangle \) is equal to a constant.

\(^1\)An EF is called regular when \( \Omega \) is an open set.

\(^2\)We assume \( A_z(\lambda_z) \) can be efficiently computed.

\(^3\)A more complete definition is given in Definition 1.3 of Johansen (1979).
This essentially means that they are no linear dependencies in the parameterization of the distribution. When such a nonzero vector exists, we can add/subtract it from \(\Lambda\) without changing the distribution. Minimality ensures that this never happens and the parametrization \(\lambda_z\) is unique and identifiable up to multiplication with a nonsingular affine transformation.

Under a minimal representation, the log-partition function \(A_z(\lambda_z)\) is strictly convex, implying that the FIM is positive-definite.\(^4\) For other types of representation, like curved EFs, the FIM may not be positive-definite. Minimality ensures that the FIM is positive-definite and that NGD is well defined.\(^5\) The NGD update can then be carried out using the expectation parameter which are a one-to-one function, as stated below (Wainwright & Jordan, 2008).

**Theorem 1** The representation (1) is minimal if and only if the mapping \(m_z(\cdot) : \Omega \to \mathcal{M}\) is one-to-one.

Unfortunately, minimal EF approximations are not always appropriate. Such approximations, especially unimodal ones, usually yield poor approximations of multimodal posterior distributions. Structured approximations, such as mixtures of EF distributions, are more suitable for approximating multimodal posteriors. Unfortunately, for such approximations, there is no straightforward way to define a minimal EF representation which can be exploited to derive a simple NGD update. For example, a mixture of EF distributions expressed as

\[
q(z) := \int q(z|w)q(w)dw,
\]

with \(q(z|w)\) as the component and \(q(w)\) as the mixing distribution, may not even have an EF form even when both the terms above are in the EF. A famous example is the finite mixture of Gaussians. The conditions under which the FIM of (7) is invertible are also difficult to characterize in general. Due to these reasons, it is difficult to simplify the NGD update for such structured distributions.

In this paper, we propose a new way to derive simple natural-gradients for structured approximations (7) using a minimal conditional representation which we define next.

### 3. Minimal Conditional-EF Representation

In this section we define a minimal conditional-EF (MCEF) representation of the joint distribution \(q(z, w)\) for structured approximations that take the form (7). Using this, we derive conditions under which the FIM of the joint is invertible, and show that it leads to a simple NGD similar to (6).

We begin with a definition of the conditional EF distribution.

**Definition 2 (Conditional EF)** We call the joint distribution \(q(z, w)\) defined in (7) a conditional EF when its components take the following form:\(^6\)

\[
q(z|w) := h_z(z, w)\exp\left[\langle \phi_z(z, w), \lambda_z \rangle - A_z(\lambda_z, w)\right],
\]

\[
q(w) := h_w(w)\exp\left[\langle \phi_w(w), \lambda_w \rangle - A_w(\lambda_w)\right],
\]

with \(\lambda_w, \phi_w(w)\) and \(A_w(\lambda_w)\) being the natural parameters, sufficient statistics, and log-partition function of \(q(w)\), and \(\lambda_z, \phi_z(z, w)\) and \(A_z(\lambda_z, w)\) are the same for \(q(z|w)\). We denote the set of natural parameters for \(q(z|w)\) and \(q(w)\) by \(\Omega_z\) and \(\Omega_w\) respectively, and assume them to be open.\(^7\)

Note that the sufficient statistics \(\phi_z(z, w)\) and log-partition \(A_z(\lambda_z, w)\) both depend on \(w\), but, conditioned on \(w\), the distribution is parametrized by the natural parameter \(\lambda_z\). For a well-defined conditional EF distribution, \(q(w)\) is a regular EF distribution and conditioned on \(w\), \(q(z|w)\) is also a regular EF distribution. This is a type of conditional exponential-family distribution (Xing et al., 2002; Liang et al., 2009; Lindsey, 1996; Feigin, 1981) with a special conditional structure.

We are interested in an NGD update that can exploit the FIM of the joint distribution. We denote the set of natural parameters by \(\lambda := \{\lambda_z, \lambda_w\}\) and the set of valid \(\lambda_z\) and \(\lambda_w\) by \(\Omega_z\) and \(\Omega_w\) respectively. We define the following FIM in the natural-parameter space \(\Omega_z \times \Omega_w\) as follows:

\[
F_{z,w}(\lambda) := -E_{q(z,w)}[\nabla^2_{\lambda} \log q(z, w)].
\]

This is the FIM of the joint distribution \(q(z, w)\) which is different from the one for the marginal distribution \(q(z)\). Similar to the minimal EF case, our goal now is to find representations where the above FIM is invertible and can be exploited to compute NGD using expectations of the sufficient statistics. The expectation parameters of a CEF can be defined as shown below:

\[
m_z(\lambda_z, \lambda_w) := E_{q(z|w)q(w)}[\phi_z(z, w)],
\]

\[
m_w(\lambda_w) := E_{q(w)}[\phi_w(w)].
\]

We denote the ranges of \(m_z\) and \(m_w\) by \(\mathcal{M}_z\) and \(\mathcal{M}_w\) respectively, and the whole set of expectation parameters

\(^4\)A formal proof can be found in Johansen (1979).

\(^5\)In some cases, when FIM is not invertible, it is still possible to perform NGD by, for example, ignoring the zero eigenvalues or using damping, but the simplification shown in (6) may not be possible.

\(^6\)We assume that \(A_z(\lambda_z, w)\) and \(A_w(\lambda_w)\) can be efficiently computed.

\(^7\)It is possible for \(\Omega_z\) to be non-open since it is an intersection of all of the valid natural-parameter of \(q(z|w)\) for each \(w \sim q(w)\). The set is open when the set of valid natural-parameters for \(q(z|w)\) conditioned on \(w\) does not depend on \(w\), or when the cardinality of the support of \(w\) is finite. For all the examples given in this paper, the set is an open set.
by \( m(\lambda) := \{ m_z, m_w \} \). Since \( \phi_z(z, w) \) and \( A_z(\lambda_z, w) \) both depend on \( w \), we may or may not be able to perform NGD using these expectation parameters. However, we next show NGD is always possible by restricting to a minimal representation of CEFs.

Below we define a minimal representation for CEF which ensures that the \( F_{wz}(\lambda) \) is positive definite, and NGD can be performed using \( m \).

**Definition 3 (Minimal Conditional-EOF (MCEF))** A conditional EF defined in Definition 2 is said to have a minimal representation when \( m_w(\cdot): \Omega_w \to \mathcal{M}_w \) and \( m_z(\cdot, \lambda_w): \Omega_z \to \mathcal{M}_z \) are both one-to-one, \( \forall \lambda_w \in \Omega_w \).

In the next section, we will show that all the examples shown in Figure 1 (See “Examples of MCEFs”) have an MCEF representation. Similar to minimal EFs, an MCEF representation implies that \( F_{wz}(\lambda) \) is positive-definite and invertible, as stated in the following theorem (see a proof in Appendix A).

**Theorem 2** For an MCEF representation given in Definition 3, the FIM \( F_{wz}(\lambda) \) given in (9) is positive-definite and invertible for all \( \lambda \in \Omega \).

Since the FIM is well-defined, it is reasonable to perform natural-gradient steps in the Riemannian manifold defined by \( F_{wz}(\lambda) \). The steps can be taken using an update that takes a simple form, similar to the one shown in (6). As shown in Lemma 5 in Appendix A, similar to (5) for minimal EF, we have the following relationship for MCEFs:

\[
\nabla_{\lambda} L = \left[ \nabla_{\lambda} m^T \right] \nabla_{m} L = [F_{wz}(\lambda)] \nabla_{m} L \quad (12)
\]

Since the FIM is invertible, we can compute the natural-gradient by using gradients with respect to \( m \). The following theorem shows the simplicity of NGD.

**Theorem 3** For minimal conditional-EOF approximations, the following updates are equivalent:

\[
\begin{align*}
\lambda &\leftarrow \lambda + \beta \left[ F_{wz}(\lambda) \right]^{-1} \nabla_{\lambda} L(\lambda) \quad (13) \\
\lambda &\leftarrow \lambda + \beta \nabla_{m} L(\lambda). \quad (14)
\end{align*}
\]

The above theorem generalizes the previous result for minimal EF approximations to minimal conditional-EOF approximations. It also implies that using the expectation parameterization \( m \) enables us to exploit the geometry of the joint \( q(z, w) \) to improve convergence.

4. Examples

In this section, we give examples of approximations with a minimal conditional-EOF form. We discuss finite mixtures of EFs, scale mixtures of Gaussians, and multivariate Skew-Gaussians. We give updates that can be implemented efficiently by using existing NGD implementations, e.g., the variational online Newton (VON) method of Khan et al. (2018). We also propose many new versions. To derive these updates, we use the extended Bonnet’s and Price’s theorems (Lin et al., 2019) for Gaussian mixtures. For exponential-family mixtures, we use the implicit reparameterization trick (Salimans & Knowles, 2013; Figurnov et al., 2018). Lin et al. (2019) discuss a weaker version of the reparameterization trick for exponential-family mixtures.

4.1. Finite Mixture of Exponential Family Distribution

Finite mixtures of EFs are a powerful approximation where components in EF form are mixed using a discrete distributions such as a multinomial distribution, as shown below:

\[
q(z) = \sum_{c=1}^{K} \pi_c q(z|\lambda_c), \quad \text{such that } \sum_{c=1}^{K} \pi_c = 1, \quad (15)
\]

where \( q(z|\lambda_c) \) are EF distributions with natural parameters \( \lambda_c \). The support of \( z \) of all the components is assumed to be the same, and \( \pi_K \) is fixed to \( 1 - \sum_{c=1}^{K-1} \pi_c \).

This distribution cannot be written in an exponential form in general, and therefore none of the existing NGD methods can be used to derive a simple expression for NGVI. Directly applying NGD using the FIM of \( q(z) \) would be too expensive since the number of parameters are in \( O(D^2 K) \), and the FIM could be extremely large when computed naively. Fortunately, the joint distribution does take an MCEF form when all \( q(z|\lambda_c) \) are minimal EFs. A formal statement is given in Appendix B. Using this conditional EF form, we can derive a much simpler NGD update which reduces to simple parallel updates on mixture components.

We will now demonstrate the simplicity of our update for a finite mixture of Gaussians (MOG) where components \( q(z|\lambda_c) := \mathcal{N}(z|\mu_c, \Sigma_c) \) are Gaussian. The sufficient statistics, natural parameters, and expectation parameters of the corresponding EF are given in Table 1.

We consider the following model where the likelihood \( p(D_n|z) \) is defined using neural-network weights \( z \) with a prior \( p(z) \): \( p(D, z) = \prod_{n=1}^{N} p(D_n|z)p(z) \). We approximate the posterior with a MOG by optimizing the following variational lower bound: \( \mathcal{L}(\lambda) := \mathbb{E}_{q(z)}[-h(z)] \) where \( h(z) := \log \frac{q(z)}{p(z)} - \sum_n \log p(D_n|z) \).

We now summarize the NGD update derived in Appendix B. We first generate samples \( (z, w) \) from \( q(z, w) \). The mean \( \mu_c \) and covariance \( \Sigma_c \) are similarly updated by the variational online Newton (VON) algorithm (Khan et al., 2018):

\[
\begin{align*}
\Sigma_c^{-1} &\leftarrow \Sigma_c^{-1} + \beta \delta_c \left[ \nabla^2_{z} h(z) \right]_c, \\
\mu_c &\leftarrow \mu_c - \beta \delta_c \Sigma_c \left[ \nabla_{z} h(z) \right]_c, \quad (16)
\end{align*}
\]

\[
\log \left( \frac{\pi_c}{\pi_K} \right) \leftarrow \log \left( \frac{\pi_c}{\pi_K} \right) - \beta (\delta_c - \delta_K) h(z)
\]
Table 1. We give expressions for various components of \( q(z, w) \) as specified in (8) for a minimal conditional-EF representation. We give three examples. More examples can be found at the Appendix. The first two rows give expressions for the sufficient statistics, and the subsequent rows show natural and expectation parameters. For the first column, \( \mathbb{I}_c(w) \) denotes the indicator function which is 1 when \( w = c \) and 0 otherwise. For the second column, \( \psi \) is the digamma function. For the third column, \( c := \sqrt{2/\pi} \). Note that both the natural and expectation parameters may lie in a constrained set. Due to space limitations, we have not explicitly given the description of these sets.

| \( \phi_w(w) \) | Mixture of Gaussians | T-Distribution | Skew-Gaussian |
|-----------------|----------------------|----------------|--------------|
| \( \mathbb{I}_c(w) \) | \( \{ \mathbb{I}_c(w) \}_{c=1}^K \) | \( -1/w - \log w \) | \( w, w^2 \) |
| \( \phi_z(z, w) \) | \( \{ \mathbb{I}_c(w) z, \mathbb{I}_c(w) z z^T \}_{c=1}^K \) | \( \{ z/w, zz^T/w \} \) | \( \{ z, |w| z, zz^T \} \) |
| \( \lambda_w \) | \( \{ \pi_c \}_{c=1}^{K-1} \) | \( a \) | constants \( \{ 0, \frac{1}{2} \} \) |
| \( m_w(\lambda_w) \) | \( \{ \pi_c \}_{c=1}^{K-1} \) | \( -1 - \log a + \psi(a) \) | constants \( \{ 0, 1 \} \) |
| \( \lambda_z \) | \( \{ \Sigma_c^{-1} \mu_c, -\frac{1}{2} \Sigma_c^{-1} \}_{c=1}^K \) | \( \{ \Sigma^{-1} \mu, -\frac{1}{2} \Sigma^{-1} \} \) | \( \{ \Sigma^{-1} \mu, \Sigma^{-1} \alpha, -\frac{1}{2} \Sigma^{-1} \} \) |
| \( m_z(\lambda) \) | \( \{ \pi_c \mu_c, \pi_c (\mu_c \mu_c^T + \Sigma_c) \}_{c=1}^K \) | \( \{ \mu, \mu \mu^T + \Sigma \} \) | \( \{ \mu + \alpha \mu, \alpha + \epsilon \mu, \\
\mu \mu^T + \alpha \mu^T + \Sigma + \epsilon (\mu \alpha^T + \alpha \mu^T) \} \) |

We now demonstrate the simplicity of our update to obtain a Student’s t-approximation on a Bayesian neural network. We assume the following model with a likelihood \( p(D_n|z) \) specified using a neural network with weights \( z \) and a Student’s t-prior: \( p(D, z) = \prod_{n=1}^N p(D_n|z) T(z|0, I, a_0) \). The Student’s t-prior is better than a Gaussian one if we expect the weights to follow a heavy-tailed distribution. We approximate the posterior by the approximation (17) using parameters \( \Sigma, \mu \), and \( a \). We use the variational lower bound defined in the joint distribution \( p(D, z, w) \) space:

\[
\mathcal{L}(\lambda) = \mathbb{E}_{q(z, w)} \left[ \sum_{n=1}^N \log p(D_n|z) + \log \frac{p(z, w)}{q(z, w)} \right] \tag{18}
\]

Below, we summarize the NGD updates derived in Appendix D. We first sample \( (z, w) \) from \( q \) and randomly sampled an example \( n \). The update is then a small modification of the VON update (Khan et al., 2018):

\[
\Sigma^{-1} - (1 - \beta)\Sigma^{-1} + [u \nabla_z^2 f_n(z) + I/N], \tag{19}
\]

\[
\mu \leftarrow \mu - \beta \Sigma \nabla_z f_n(z) + \mu / N, \tag{20}
\]

\[
a \leftarrow (1 - \beta) a + \beta [a_0 - \delta \Tr (\Sigma^{-1} \nabla_z f_n(z) \Sigma)], \tag{21}
\]

where \( \beta > 0, \delta \leftarrow N u^2 / (2(1 - w)), \) and \( u \) is a pre-multiplier defined below (\( d \) is length of \( z \)): \( u = (a - 1 + d/2)^{-1} \left[ a + (z - \mu)^T \Sigma^{-1} (z - \mu) / 2 \right] \). Similarly, to the previous section, this update can be implemented efficiently using the method of Khan et al. (2018).
Another example is given at Appendix H. Extensions using an Adam-like optimizer for this kind of mixtures are given in Appendix J.

4.3. Gaussian Mean Mixture

We consider the following Gaussian mixture.

\[ q(z|\mu, \alpha, \Sigma) = \int \mathcal{N}(z|u_i, \alpha_i, \Sigma) k \prod_{i=1}^k q(w_i)dw, \]

where \( \alpha \) is a d-by-k matrix and \( z \in \mathbb{R}^d \). An example is the rank-1 covariance Gaussian with \( k = 1, u(w) = w, \) and \( D \) as a diagonal covariance matrix: \( q(z|\mu, \alpha, D) = \int \mathcal{N}(z|u, w\alpha, D)N(w|0, 1)dw = \mathcal{N}(z|\mu, \alpha\alpha^T + D). \)

The multivariate skew Gaussian (Azzalini & Valle, 1996; Genton, 2004), defined below, is another example and allows for non-zero skewness (asymmetric approximations):

\[ q(z|\mu, \alpha, \Sigma) = \int \mathcal{N}(z|u, \alpha, \Sigma)N(w|0, 1)dw. \]

This distribution is not a minimal EF and the FIM of the marginal \( q(z) \) can be singular (Azzalini, 2013). However, the joint distribution is a minimal conditional-EF distribution as we show in Lemma 12 and 13 in Appendix E. The sufficient statistics, natural parameters, expectation parameters of the conditional EF form are given in Table 1.

Similar to other examples, we get a simple and efficient NGD update. We summarize the updates for a model with a neural-network likelihood \( p(D_n|z) \) using weights \( z \) and a Gaussian prior \( \mathcal{N}(z|0, 1) \). Denoting \( f_n(z) = -\log p(D_n|z) \), the lower bound is \( \mathcal{L}(\lambda) := \mathbb{E}_{\lambda(z)}[\sum_n f_n(z) + \log p(z) - \log q(z)] \). The updates derived in Appendix E is a variant of the VON update:

\[
\Sigma^{-1} \leftarrow (1 - \beta)\Sigma^{-1} + \beta (I + N\tilde{g}_0^n) \tag{22}
\]

\[
\mu \leftarrow \mu - \beta \Sigma \left[ \tilde{c}(g_{\mu}^n - c_{\mu}^n) + \mu \right] \tag{23}
\]

\[
\alpha \leftarrow \alpha - \beta \Sigma \left[ \tilde{c}(g_{\alpha}^n - c_{\alpha}^n) + \alpha \right] \tag{24}
\]

where \( \tilde{c} := N/(1 - 2/\pi) \) and \( g_{\mu}^n, g_{\alpha}^n, g_{\alpha}^n \) are gradients obtained by gradient and Hessian of \( f_n(z) \) at a sample of \( q(z) \). The gradients are defined in (53)-(55) in Appendix E.

Another example of the mixture is the exponentially modified Gaussian distribution (Grushka, 1972; Carr & Madan, 2009) given in Appendix F. Extensions using an Adam optimizer for the class of mixtures are given in Appendix J.

5. Generalization to Multilinear EF

We now extend the approach to an approximation with multilinear EFs which contain blocks of natural parameters. We start by specifying a distribution over \( z \) by a function \( f(\cdot): \)

\[ q(z|\lambda) = h_z(z) \exp \left[ f(z, \lambda) - A_z(\lambda) \right]. \tag{25} \]

Then we divide the vector \( \lambda := \{\lambda_1, \lambda_2, \ldots, \lambda_K\} \) into \( K \) blocks with \( \lambda_j \in \Omega_j \) being the \( j \)-th block of parameters. In EF, the function \( f \) is just linear in \( \lambda_j \) at (1). We can generalize the notion of linearity to multiple blocks of parameters by considering \( f \) to be a multilinear function.

**Definition 4 (Minimal Multilinear-EF)** We call \( f \) a multilinear function when, for each block \( j \), there exist functions \( \phi_j \) and \( r_j \) such that \( f \) is linear with respect to \( \lambda_j \), i.e.,

\[ f(z, \lambda) = (\lambda_j, \phi_j(z, \lambda_j)) + r_j(z, \lambda_{-j}), \tag{26} \]

where \( \lambda_{-j} \) is the parameter vector containing all \( \lambda \) except \( \lambda_j \). A distribution \( q(z|\lambda) \) defined as in (25), but with a multilinear \( f \), is called a multilinear EF. Additionally, when \( \Omega_j \) is open and the following expectation parameters \( \mu_j(\lambda) := \mathbb{E}_{q(z)}[\phi_j(z, \lambda_j)] \) are one-to-one, we call the distribution a minimal multilinear EF distribution.

Clearly, minimal EFs are minimal multilinear EFs. The following theorem give a result about a block NGD update performed on individual blocks of parameters \( \lambda_j \).

**Theorem 4** For approximations with multilinearly-minimal EF representation, the following updates are equivalent:

\[
\lambda_j \leftarrow \lambda_j + \beta \nabla_{\lambda_j} \mathcal{L}(\lambda) \tag{27}
\]

\[
\lambda_j \leftarrow \lambda_j + \beta \nabla_{\mu_j} \mathcal{L}(\lambda) \tag{28}
\]

The proof of this theorem is similar to Theorem 3. We now give an example and demonstrate the simplicity of the NGD update. Let’s consider the Matrix-Variate Gaussian (MVG) distribution defined as follows:

\[
\mathcal{M}(Z|W, U, V) := \mathcal{N}(\text{vec}(Z)|\text{vec}(W), U \otimes V). \]

This distribution has been used for Bayesian neural networks (Lourizos & Welling, 2016; Sun et al., 2017). An approximate NGD update is also derived by Zhang et al. (2018) where the FIM is approximated by a block-diagonal matrix and K-FAC approximation. Our update have a similar block-diagonal approximation, but the update for the each block is an exact NGD unlike Zhang et al. (2018) where the steps are approximated by K-FAC.

In Appendix I, we show that the MVG distribution \( \mathcal{M}(Z|W, U, V) \) can be written in the minimal multilinear form. The NGD update, derived in Appendix I, is summarized below to optimize the lower bound as \( \mathcal{L}(\lambda) = E_{q}[-h(Z)] \) where \( h(Z) := -\log p(D, Z) + \log q(Z) \). To simplify our implementation, we use the Gauss-Newton approximation (Graves, 2011) although it is not necessary to do so. The resulting block NGD update is shown below,

\[
W \leftarrow W - \beta_1 UGV, \tag{29}
\]

\[
U^{-1} \leftarrow U^{-1} + \beta_2 GV G^T, \tag{30}
\]

\[
V^{-1} \leftarrow V^{-1} + \beta_2 G^T U G, \tag{31}
\]
where we sample $Z$ from the MVG distribution and evaluate the gradient $G := \nabla_{Z} h(Z)$. These updates extend the VON update obtained in Khan et al. (2018) to MVG approximations. The gradient $G$ is pre-conditioned, which is very similar to other preconditioned algorithms, such as K-FAC (Martens & Grosse, 2015; Zhang et al., 2018) and Shampoo (Gupta et al., 2018). The update can be extended to Tensor-Variate Gaussian (Ohlson et al., 2013).

6. Experimental Results

The code is available at: https://github.com/yorkerlin/VB-MixEF.

6.1. Qualitative Results on Synthetic Examples

First, we show qualitative results on three toy examples and visualize the results obtained by structured approximations.

The first toy example is the Gaussian mixture example from Wang et al. (2018). In this example, the true distribution is a finite mixture of Gaussians (MOG) $p(z) = \sum_{j=1}^{C} \frac{1}{2} \mathcal{N}(z|\mu_j, I)$, where each element of $\mu_j$ is uniformly drawn from the interval $[-s, s]$. We approximate the posterior distribution by an MOG approximation described in Section 4.1. We consider a case with $K = 20$, $C = 10$, $s = 20$, and $d = 20$. We initialize $\pi_c = \frac{1}{K}$ and $\Sigma_c = 100I$. Each element of $\mu_c$ is randomly initialized by Gaussian noise with mean 0 and variance 100. We use 10 Monte Carlo samples to compute the gradients. The leftmost plot in Figure 2 shows the first 9 marginal distributions of the true distribution and its approximations, where we clearly see that MOG closely matches the marginals. All 20 marginal distributions are in Figure 6 in Appendix B.5.

In the second toy example we approximate the beta-binomial model for overdispersion considered in Salimans & Knowles (2013); Salimans et al. (2015) by using MOG ($N = 20$, $d = 2$). The model is to used to estimate the rates of death from stomach cancer for cities in Missouri. The exact posterior of the model is non-standard and extremely skewed. In the middle plot in Figure 2, we see that our MOG approximation approximates the true posterior better and better as we increase the number of mixture components.

In the last toy example, we visualize the skew-Gaussian approximations for the two-dimensional Bayesian Logistic regression example taken from Murphy (2013) ($N = 60$, $d = 2$). In the rightmost plot in Figure 2, we can see that the skewness of the true posterior is captured well by the skew-Gaussian distribution. The Gaussian approximation results in a worse approximation than the skew-Gaussian.

6.2. Results on Real Data

Next, we show results on real-world datasets. We consider two models in our experiments. We start with Bayesian Logistic regression (BLR) and present results for MOG approximations on two small UCI datasets. The ‘Breast-Cancer’ dataset has $N = 683$, $d = 10$ with 341 chosen for training, and regularization parameter is set to 1.0. The ‘Sonar’ dataset has $N = 208$, $d = 6$ with 100 chosen for training, and regularization parameter is set to 0.204. We vary the number of mixture components to $K = 1, 3, 5, 10$. In Figure 3, we plot the KL divergence between the true posterior and the MOG approximation, and compare our method (referred to as ‘NGVI’) proposed in Section 4.1 to the black-box gradient method (referred to as ‘BBVI’) with the re-parametrization trick (Salimans & Knowles, 2013;
Fast and Simple Natural-Gradient Variational Inference with Mixture of Exponential-family Approximations

For both methods, we use a full batch for each update. We observe that NGVI always converges faster than BBVI. We also see that MoG is a better approximation than the single Gaussian, and the quality of the posterior approximation improves as the number of mixture increases.

Next, we show results on a larger dataset using two other kinds of variational approximation: Skew-Gaussian and Student’s t. We use the UCI dataset “covtype-binary-scale” with $d = 54$, $N = 581,012$ with 464,809 chosen for training and regularization parameter 0.002. We use the algorithm discussed in Section 4.2 and 4.3. For black-box methods, we use the Adam optimizer and refer to it as BBVI. In the skew-Gaussian case, we use a Gaussian prior, and, for the Student’s t-distribution, we use a Student’s t-prior as shown in (18). Figure 4 demonstrates the fast convergence of our method compared to BBVI.

Finally, we discuss results on Bayesian neural network (BNN) with a standard normal prior on weights. We use one hidden layer, 50 hidden units, and ReLU activation functions. We approximate the posterior by a skew-Gaussian distribution using NGVI. We also compare to two other methods where we used BBVI to fit a skew-Gaussian approximation as well as a Gaussian approximation. For scalability reasons, we use of a diagonal covariance for all methods. We use 10 Monte Carlo (MC) samples and mini-batch size of 32. For NGVI, we use the gradient magnitude-approximation as explained in Appendix J. Figure 5 shows the performance of all methods in terms of the test RMSE. We can see that our method converges faster than BBVI, although the performance of skew-Gaussian methods seem to be similar to a Gaussian.

7. Discussion

In this paper, we present fast and simple NGD for VI with structured approximations. The approximations we have considered are currently beyond the reach of existing methods, and our approach extends these existing approaches to perform NGD updates with a simple update which can also be implemented efficiently in some cases. Our current proposal is limited to a certain class of approximations, and further work is needed to generalize our results to many other types of structured approximations. The minimalism condition we proposed uses one-to-one mappings of the expectation parameterization. We believe that this condition can be relaxed which will enable simple NGD update for many types of approximations.

Our main focus has been on the derivation of simple updates. We have presented examples where the updates can also be implemented efficiently. There are however implementation bottlenecks in existing software frameworks to implement some of the reparameterization tricks used in our algorithms. It is important to find ways to enable efficient updates by modifying the existing software frameworks. Another issue is that the NGD update needs to make sure that the parameters stay inside $\Omega$, and this issue deserves further exploration. Another important direction is to apply structured approximations to large problems, especially those involving deep networks. We hope to perform such extensive experiments in the future to establish the benefits obtained by our NGD update for Bayesian deep learning.
Acknowledgements

We would like to thank Voot Tangkaratt for useful discussions during this work. WL is supported by a UBC International Doctoral Fellowship.

References

Andrews, D. F. and Mallows, C. L. Scale mixtures of normal distributions. *Journal of the Royal Statistical Society. Series B (Methodological)*, pp. 99–102, 1974.

Arellano-Valle, R. B., Contreras-Reyes, J. E., and Genton, M. G. Shannon Entropy and Mutual Information for Multivariate Skew-Elliptical Distributions. *Scandinavian Journal of Statistics*, 40(1):42–62, 2013.

Azzalini, A. The skew-normal distribution and related multivariate families. *Scandinavian Journal of Statistics*, 32(2):159–188, 2005.

Azzalini, A. *The skew-normal and related families*, volume 3. Cambridge University Press, 2013.

Azzalini, A. and Valle, A. D. The multivariate skew-normal distribution. *Biometrika*, 83(4):715–726, 1996.

Eltoft, T., Kim, T., and Lee, T.-W. Multivariate scale mixture of Gaussians modeling. In *International Conference on Independent Component Analysis and Signal Separation*, pp. 799–806. Springer, 2006.

Feigin, P. D. Conditional Exponential Families and a Representation Theorem for Asymptotic Inference. *The Annals of Statistics*, pp. 597–603, 1981.

Figurnov, M., Mohamed, S., and Mnih, A. Implicit Reparameterization Gradients. 2018.

Furmston, T. and Barber, D. Variational methods for reinforcement learning. In *Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics*, pp. 241–248, 2010.

Genton, M. G. *Skew-elliptical distributions and their applications: a journey beyond normality*. CRC Press, 2004.

Graves, A. Practical variational inference for neural networks. In *Advances in neural information processing systems*, pp. 2348–2356, 2011.

Grushka, E. Characterization of exponentially modified Gaussian peaks in chromatography. *Analytical Chemistry*, 44(11):1733–1738, 1972.

Gupta, V., Koren, T., and Singer, Y. Shampoo: Preconditioned Stochastic Tensor Optimization. In *Proceedings of the 35th International Conference on Machine Learning*, pp. 1842–1850, 2018.

Hensman, J., Rattray, M., and Lawrence, N. D. Fast variational inference in the conjugate exponential family. In *Advances in neural information processing systems*, pp. 2888–2896, 2012.

Hensman, J., Fusi, N., and Lawrence, N. D. Gaussian processes for big data. *arXiv preprint arXiv:1309.6835*, 2013.

Hoffman, M. D. and Blei, D. M. Structured stochastic variational inference. In *Artificial Intelligence and Statistics*, 2015.
Hoffman, M. D., Blei, D. M., Wang, C., and Paisley, J. Stochastic variational inference. The Journal of Machine Learning Research, 14(1):1303–1347, 2013.

Honkela, A., Tornio, M., Raiko, T., and Karhunen, J. Natural conjugate gradient in variational inference. In International Conference on Neural Information Processing, pp. 305–314. Springer, 2007.

Honkela, A., Raiko, T., Kuusela, M., Tornio, M., and Karhunen, J. Approximate Riemannian Conjugate Gradient Learning for Fixed-form Variational Bayes. Journal of Machine Learning Research (JMLR), 11:3235–3268, 2011.

Johansen, S. Introduction to the Theory of Regular Exponential Families. 1979.

Jørgensen, B., Seshadri, V., and Whitmore, G. On the mixture of the inverse Gaussian distribution with its complementary reciprocal. Scandinavian Journal of Statistics, pp. 77–89, 1991.

Khan, M. and Lin, W. Conjugate-computation variational inference: Converting variational inference in non-conjugate models to inferences in conjugate models. In Artificial Intelligence and Statistics, pp. 878–887, 2017.

Khan, M. E. and Nielsen, D. Fast yet Simple Natural-Gradient Descent for Variational Inference in Complex Models. arXiv preprint arXiv:1807.04489, 2018.

Khan, M. E., Babanezhad, R., Lin, W., Schmidt, M., and Sugiyama, M. Faster stochastic variational inference using Proximal-Gradient methods with general divergence functions. In Proceedings of the Thirty-Second Conference on Uncertainty in Artificial Intelligence, pp. 319–328. AUAI Press, 2016.

Kingma, D. P. and Welling, M. Auto-encoding variational bayes. arXiv preprint arXiv:1312.6114, 2013.

Kotz, S. and Nadarajah, S. Multivariate t-distributions and their applications. Cambridge University Press, 2004.

Kumar, S. and Tsvetkov, Y. Von Mises-Fisher Loss for Training Sequence to Sequence Models with Continuous Outputs. arXiv preprint arXiv:1812.04616, 2018.

Lin, W., Khan, M. E., and Schmidt, M. Stein’s Lemma for the Reparameterization Trick with Exponential-family Mixtures. https://github.com/yorkerlin/VB-MixEF/blob/master/report.pdf, 2019. Accessed: 2019/06.

Lindsey, J. K. Parametric statistical inference. Oxford University Press, 1996.

Louizos, C. and Welling, M. Structured and efficient variational deep learning with matrix gaussian posteriors. In International Conference on Machine Learning, pp. 1708–1716, 2016.

Mishkin, A., Kunstner, F., Nielsen, D., Schmidt, M., and Khan, M. E. SLANG: Fast Structured Covariance Approximations for Bayesian Deep Learning with Natural Gradient. In Advances in Neural Information Processing Systems, pp. 6246–6256, 2018.

Murphy, K. P. Machine learning : a probabilistic perspective. MIT Press, Cambridge, Mass. [u.a.], 2013. ISBN 9780262018029 0262018020.

Nguyen, C. V., Li, Y., Bui, T. D., and Turner, R. E. Variational Continual Learning. arXiv preprint arXiv:1710.10628, 2017.

Oh, C., Adamczykowski, K., and Park, M. Radial and Directional Posteriors for Bayesian Neural Networks. arXiv preprint arXiv:1902.02603, 2019.

Ohlson, M., Ahmad, M. R., and Von Rosen, D. The multilinear normal distribution: Introduction and some basic properties. Journal of Multivariate Analysis, 113:37–47, 2013.

Opper, M. and Archambeau, C. The variational Gaussian approximation revisited. Neural computation, 21(3):786–792, 2009.

Price, R. A useful theorem for nonlinear devices having Gaussian inputs. IRE Transactions on Information Theory, 4(2):69–72, 1958.

Ranganath, R., Gerrish, S., and Blei, D. Black box variational inference. In Artificial Intelligence and Statistics, pp. 814–822, 2014.

Ranganath, R., Tran, D., and Blei, D. Hierarchical variational models. In International Conference on Machine Learning, pp. 324–333, 2016.
Rezende, D. J., Mohamed, S., and Wierstra, D. Stochastic backpropagation and approximate inference in deep generative models. *arXiv preprint arXiv:1401.4082*, 2014.

Ruiz-Antolín, D. and Segura, J. A new type of sharp bounds for ratios of modified Bessel functions. *Journal of Mathematical Analysis and Applications*, 443(2):1232–1246, 2016.

Salimans, T. and Knowles, D. Fixed-form variational posterior approximation through stochastic linear regression. *Bayesian Analysis*, 8(4):837–882, 2013.

Salimans, T., Kingma, D., and Welling, M. Markov chain monte carlo and variational inference: Bridging the gap. In *International Conference on Machine Learning*, pp. 1218–1226, 2015.

Salimbeni, H., Eleftheriadis, S., and Hensman, J. Natural Gradients in Practice: Non-Conjugate Variational Inference in Gaussian Process Models. *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2018.

Sato, M.-A. Online model selection based on the variational Bayes. *Neural computation*, 13(7):1649–1681, 2001.

Staines, J. and Barber, D. Variational optimization. *arXiv preprint arXiv:1212.4507*, 2012.

Sun, S., Chen, C., and Carin, L. Learning Structured Weight Uncertainty in Bayesian Neural Networks. In *Proceedings of the 20th International Conference on Artificial Intelligence and Statistics, AISTATS*, pp. 1283–1292, 2017.

Titsias, M. and Lázaro-Gredilla, M. Doubly stochastic variational Bayes for non-conjugate inference. In *International Conference on Machine Learning*, pp. 1971–1979, 2014.

Titsias, M. K. and Ruiz, F. J. Unbiased Implicit Variational Inference. *arXiv preprint arXiv:1808.02078*, 2018.

Wainwright, M. J. and Jordan, M. I. Graphical models, exponential families, and variational inference. *Foundations and Trends in Machine Learning*, 1–2:1–305, 2008.

Wang, D., Liu, H., and Liu, Q. Variational Inference with Tail-adaptive f-Divergence. In *Advances in Neural Information Processing Systems*, pp. 5742–5752, 2018.

Xing, E. P., Jordan, M. I., and Russell, S. A generalized mean field algorithm for variational inference in exponential families. In *Proceedings of the Nineteenth conference on Uncertainty in Artificial Intelligence*, pp. 583–591. Morgan Kaufmann Publishers Inc., 2002.

Yang, Z.-H. and Chu, Y.-M. On approximating the modified Bessel function of the second kind. *Journal of Inequalities and Applications*, 2017(1):41, 2017.

Yin, M. and Zhou, M. Semi-Implicit Variational Inference. *arXiv preprint arXiv:1805.11183*, 2018.

Zhang, G., Sun, S., Duvenaud, D., and Grosse, R. Noisy Natural Gradient as Variational Inference. In *Proceedings of the 35th International Conference on Machine Learning*, 2018.
A. Proof of Theorem 2

In this section, we provide a proof for Theorem 2:

For an MCEF representation given in Definition 3, the FIM $F_{w,z}(\lambda)$ given in (9) is positive-definite and invertible for all $\lambda \in \Omega$.

We prove this using a sequence of lemmas.

**Lemma 1** $\log q(w, z|\lambda)$ is twice differentiable with respect to $\lambda$.

**Proof:** From Definition 2, we see that the $\log q(z, w)$ is differentiable when $A_w(\lambda_w)$ and $A_z(\lambda_z, w)$ are twice differentiable for each $w$ sampled from $q(w)$. Since $q(w)$ is an EF, $A_w(\lambda_w)$ is twice differentiable (Johansen, 1979). Similarly, since conditioned on $w$, $q(z|w)$ is also an EF, $A_z(\lambda_z, w)$ is twice differentiable too. Therefore, the log of the joint distribution is twice differentiable. \hfill \Box

**Lemma 2** The FIM $F_{w,z}(\lambda)$ is block-diagonal with two blocks:

$$F_{w,z}(\lambda) = \begin{bmatrix} F_z(\lambda) & 0 \\ 0 & F_w(\lambda_w) \end{bmatrix}, \quad (32)$$

where $F_w(\lambda_w)$ is the FIM of $q(w)$ and $F_z(\lambda)$ is the expected of the FIM of $q(z|w)$ where expectation is taken under $q(w)$ as shown below:

$$F_w(\lambda_w) := -E_{q(w)} \left[ \nabla_{\lambda_w}^2 \log q(w|\lambda_w) \right]$$

$$F_z(\lambda) := -E_{q(w)} \left[ E_{q(z|w)} \left[ \nabla_{\lambda}^2 \log q(z|w, \lambda_z) \right] \right]$$

**Proof:** By Lemma 1, $\log q(w, z|\lambda)$ is twice differentiable, so the FIM is well defined. Below, we simplify the FIM to show that it has a block-diagonal structure. The first step below follows from the definition of the FIM. The second step is simply writing the FIM in a $2 \times 2$ block corresponding to $\lambda_z$ and $\lambda_w$. In the third step, we write the joint as the product of $q(z|w)$ and $q(w)$. The fourth step is obtained since the two blocks are separable in $\lambda_z$ and $\lambda_w$. In the fifth step, we take the expectation inside which gives us the desired result in the last step.

$$F_{w,z}(\lambda) = -E_{q(z,w|\lambda)} \left[ \nabla_{\lambda_z}^2 \log q(z,w|\lambda) \right]$$

$$= -E_{q(z,w|\lambda)} \left[ \begin{bmatrix} \nabla_{\lambda_z}^2 \log q(z,w|\lambda) & \nabla_{\lambda_z} \nabla_{\lambda_w} \log q(z,w|\lambda) \\ \nabla_{\lambda_z} \nabla_{\lambda_w} \log q(z,w|\lambda) & \nabla_{\lambda_w}^2 \log q(z,w|\lambda) \end{bmatrix} \right]$$

$$= -E_{q(z,w|\lambda)} \left[ \begin{bmatrix} \nabla_{\lambda_z}^2 \log q(z,w|\lambda_z) + \nabla_{\lambda_z} \nabla_{\lambda_w} \log q(z,w|\lambda_z) + \nabla_{\lambda_w}^2 \log q(z,w|\lambda_w) \\ \nabla_{\lambda_z} \nabla_{\lambda_w} \log q(z,w|\lambda_z) + \nabla_{\lambda_w}^2 \log q(z,w|\lambda_w) \end{bmatrix} \right]$$

$$= -E_{q(z,w|\lambda)} \left[ \begin{bmatrix} \nabla_{\lambda_z}^2 \log q(z,w|\lambda_z) & 0 \\ 0 & \nabla_{\lambda_w}^2 \log q(w|\lambda_w) \end{bmatrix} \right]$$

$$= \begin{bmatrix} F_z(\lambda) & 0 \\ 0 & F_w(\lambda_w) \end{bmatrix}, \quad \Box$$

**Lemma 3** The first block of the FIM matrix $F_z$ is equal to the derivative of the expectation parameter $m_z(\lambda)$:

$$F_z(\lambda) := \nabla_{\lambda} m_z^T(\lambda)$$
The steps below establish the positive-definite nature of the mapping \( \lambda \) as discussed in Section 2, we conclude that the second block \( F_{\lambda,w}(\lambda) \) is positive-definite in \( \Omega \times \Omega_w \).

Proof: When the mapping \( m_w \) is one-to-one, \( q(w|\lambda_w) \) is a minimal EF, and given that \( \Omega_w \) is relatively open, using the result discussed in Section 2, we conclude that the second block \( F_{\lambda,w}(\lambda) \) of \( F_{\lambda,w}(\lambda) \) given in (32) is positive definite and invertible for all \( \lambda \). Now we prove that the first block \( F_{\lambda}(\lambda) \) is also positive definite.

The steps below establish the positive-semi definiteness first. The first step is simply the definition of the FIM, while the second step is obtained by using the fact that \( \nabla \log f(\lambda) = \nabla f(\lambda) / f(\lambda) \). The third step is obtained by using the chain-rule, and the fourth step simply uses the log-trick above to simplify the second term. In the fifth step, we take the derivative of the first term which cancels out. The last step is straightforward since the outer products are always nonnegative.

\[
\nabla_{\lambda_z} \bar{A}_z(\lambda_z, w) = -\mathbb{E}_{q(z|w)} \left[ \nabla_{\lambda_z} \log q(z|w, \lambda_z) \right], \\
= -\mathbb{E}_{q(z|w)} \left[ \nabla_{\lambda_z} \left( \frac{\nabla_{\lambda_z} q(z|w, \lambda_z)}{q(z|w, \lambda_z)} \right) \right], \\
= -\mathbb{E}_{q(z|w)} \left[ \nabla_{\lambda_z} q(z|w, \lambda_z) q(z|w, \lambda_z) \nabla_{\lambda_z} q(z|w, \lambda_z) \right] \\
= \mathbb{E}_{q(z|w)} \left[ -\nabla_{\lambda_z} q(z|w, \lambda_z) \right] + \mathbb{E}_{q(z|w)} \left[ \nabla_{\lambda_z} \log q(z|w, \lambda_z) \nabla_{\lambda_z} \log q(z|w, \lambda_z) \right], \\
= \int -\nabla_{\lambda_z} q(z|w, \lambda_z) dz + \mathbb{E}_{q(z|w)} \left[ \nabla_{\lambda_z} \log q(z|w, \lambda_z) \nabla_{\lambda_z} \log q(z|w, \lambda_z) \right], \\
= -\frac{1}{\lambda_z} \int q(z|w, \lambda_z) dz + \mathbb{E}_{q(z|w)} \left[ \nabla_{\lambda_z} \log q(z|w, \lambda_z) \nabla_{\lambda_z} \log q(z|w, \lambda_z) \right], \\
= \mathbb{E}_{q(z|w)} \left[ \nabla_{\lambda_z} \log q(z|w, \lambda_z) \nabla_{\lambda_z} \log q(z|w, \lambda_z) \right] \geq 0.
\]
Using Lemma 3 and (35), we see that FIM is positive semi-definite:

$$ F_z(\lambda) = \nabla_\lambda, m_z^T = \nabla_\lambda, E_{q(w|\lambda_w)} [ \nabla_{\lambda_z} A_z(\lambda_z, w)] = E_{q(w)} [ \nabla^2_{\lambda_z} A_z(\lambda_z, w)] \succeq 0 $$

Now, we prove the final claim that, for every $\lambda_w \in \Omega_w$, if the conditional mapping $m_z(\cdot, \lambda_w)$ is one-to-one, then $F_z(\lambda)$ is positive definite. We will prove this statement by contradiction. Suppose there exists $\lambda$ such that $F_z(\lambda)$ is positive semi-definite, since $F_z(\lambda)$ is positive semi-definite, there exists a non-zero vector $a$ such that $a^T F_z(\lambda) a = 0$. Simplifying below, we show that this leads to a contradiction. The first and second step are obtained by simply plugging (36), while the third step is obtained by using the definition of $q(z|w, \lambda_z)$ and the fourth step is obtained by using (34). The last step is obtained by noting that the quantity is simply the variance of $a^T \phi_z(z, w)$ conditioned on $w$. 

$$ a^T F_z(\lambda) a = E_{q(w)} [a^T \nabla_{\lambda_z} A_z(\lambda_z, w)] a $$

$$ = E_{q(w)} [a^T E_{q(z|w)} \{ \nabla_{\lambda_z} \log q(z|w, \lambda_z) \nabla_{\lambda_z} \log q(z|w, \lambda_z) \} a] $$

$$ = E_{q(w)} [a^T (\phi_z(z, w) - \nabla_{\lambda_z} A_z(\lambda_z, w)) (\phi_z(z, w) - \nabla_{\lambda_z} A_z(\lambda_z, w))^T a] $$

$$ = E_{q(w)} [a^T (\phi_z(z, w) - E_{q(z|w)} [\phi_z(z, w)] (\phi_z(z, w) - E_{q(z|w)} [\phi_z(z, w)])^T a] $$

The expectation of a function positive quantity is equal to zero only when each function value is equal to zero, therefore for the above to be zeros, we need $a^T \phi_z(z, w) = 0$. However, as we show below, this is not possible since the representation $q(z|w)$ is minimal conditioned on $w$.

Since $\Omega_z$ is relatively open, there exists a small $\delta > 0$ to always be able to obtain a perturbed version $\lambda'_z = \lambda_z + \delta a$, such that $\lambda'_z \in \Omega_z$. Since the conditional mapping is one-to-one, $m_z(\lambda'_z, \lambda_w) \neq m_z(\lambda_z, \lambda_w)$. By using (35) and (33), when $a^T \phi_z(z, w) = 0$, we get a contradiction:

$$ m_z(\lambda'_z, \lambda_w) = E_{q(w|\lambda_w)} [\nabla_{\lambda_z} A_z(\lambda'_z, w)] $$

$$ = E_{q(w|\lambda_w)} \left[ \int \phi_z(z, w) h_z(z, w) \exp [\langle \phi_z(z, w), \lambda'_z \rangle] dz \right] $$

$$ = E_{q(w|\lambda_w)} \left[ \int \phi_z(z, w) h_z(z, w) \exp [\langle \phi_z(z, w), \lambda_z \rangle] dz \right] $$

$$ = m_z(\lambda_z, \lambda_w) $$

where we can move from (37) to (38), since $\langle \phi_z(z, w), \lambda'_z \rangle = \langle \phi_z(z, w), \lambda_z + \delta a \rangle = \langle \phi_z(z, w), \lambda_z \rangle$. Due to the contradiction, $F_z(\lambda)$ must be positive definite. This proves that both the blocks are positive definite and invertible.

\[ \square \]

**Lemma 5** The gradient with respect to $\lambda$ can be expressed as the gradient with respect to $m$:

$$ \nabla_\lambda \mathcal{L} = [\nabla_\lambda m^T] \nabla_m \mathcal{L} = [F_{wz}(\lambda)] \nabla_m \mathcal{L} $$

**Proof:** Using Lemma 3, and chain rule, we can establish the results for $\lambda_z$:

$$ \nabla_{\lambda_z} \mathcal{L} = \nabla_{\lambda_z} m_z^T(\lambda) [\nabla_m \mathcal{L}] = F_z(\lambda) [\nabla_m \mathcal{L}] $$

For $\lambda_w$, this result holds trivially, which proves the statement. \[ \square \]
B. Finite Mixture of Gaussians

The finite mixture of EF distribution has the following conditional distribution \( q(z|w) \):

\[
q(z|w) = \sum_{c=1}^{K} \mathbb{I}_c(w) q(z|\lambda_c) = \sum_{c=1}^{K} \mathbb{I}_c(w) h_z(z) \exp \left[ (\lambda_c, \phi_z(z)) - A_z(\lambda_c) \right]
\]

\[
= h_z(z) \exp \left\{ \sum_{c=1}^{K} (\mathbb{I}_c(w) \phi_z(z), \lambda_c) - \sum_{c' \neq c}^{K} \mathbb{I}_{c'}(w) A_z(\lambda_{c'}) \right\}
\]

where we assume each component admits the same parametric form.

From the above expression and using the EF form for the multinomial distribution, we can write the sufficient statistics, natural parameters, and expectation parameters as shown below, where \( m_c := \mathbb{E}_{q(z|w=c)} [\phi_z(z)] \) is the expectation parameter of a component \( q(z|w = c) \).

\[
\begin{bmatrix}
\mathbb{I}_1(w) \\
\mathbb{I}_2(w) \\
\vdots \\
\mathbb{I}_{K-1}(w) \\
\mathbb{I}_1(w) \phi_z(z) \\
\mathbb{I}_2(w) \phi_z(z) \\
\vdots \\
\mathbb{I}_K(w) \phi_z(z)
\end{bmatrix}
\begin{bmatrix}
\log(\pi_1/\pi_K) \\
\log(\pi_2/\pi_K) \\
\vdots \\
\log(\pi_{K-1}/\pi_K) \\
\lambda_1 \\
\lambda_2 \\
\vdots \\
\lambda_K
\end{bmatrix}
= \begin{bmatrix}
\pi_1 \\
\pi_2 \\
\vdots \\
\pi_{K-1} \\
\pi_1 m_1 \\
\pi_2 m_2 \\
\vdots \\
\pi_K m_K
\end{bmatrix}
\]

From the last two vectors, we can see that the mapping between \( \lambda \) and \( m \) is going to be one-to-one, when each EF \( q(z|\lambda_c) \) is minimal (which makes sure that mapping \( \lambda_c \) and \( m_c \) is one-to-one), and all \( \lambda_c \) are distinct.

B.1. The Model and ELBO

We consider the following model: \( p(D, z) = \prod_{n=1}^{N} p(D_n|z) p(z) \). We approximate the posterior by using the finite mixture of EFs whose marginal is denoted by \( q(z) \) as given in (15). The variational lower bound is given by the following:

\[
\mathcal{L}(\lambda) = \sum_{n=1}^{N} \left[ \log p(D_n|z) \right] + \log \frac{p(z)}{q(z)}
\]

\[
= \mathbb{E}_{q(z)} \left[ -h(z) \right], \text{ where } h(z) := - \left[ \log \frac{p(z)}{q(z)} + \sum_{n} \log p(D_n|z) \right].
\]

Note that the lower bound is defined with the marginal \( q(z) \) and the variable \( w \) is not part of the model but only the variational approximation \( q(z, w) \).

B.2. Finite Mixture of Gaussians Approximation

We now give details about the NGD update for finite mixture of Gaussians. Note that the NGD update for \( \lambda_z \) and \( \lambda_w \) can be computed separately since the FIM is block-diagonal. We first derive the NGD update for each component \( q(z|w = c) \), and then give an update for \( \lambda_w \).

As shown in Table 1, the natural and expectation parameters of the \( c \)'th component is given as follows:

\[
\Lambda_c := -\frac{1}{2} \Sigma_c^{-1} \quad M_c := \pi_c (\mu_c \mu_c^T + \Sigma_c) \\
\lambda_c := \Sigma_c^{-1} \mu_c \quad m_c := \pi_c \mu_c
\]

The expectation parameters \( m_c \) and \( M_c \) are functions of \( \pi_c, \mu_c, \Sigma_c \) and its gradient can be obtained in terms of the gradient
with respect to these quantities by using the chain rule. The final expressions are shown below:

\[
\nabla_m \mathcal{L} = \frac{1}{\pi_c} (\nabla_{\mu_c} \mathcal{L} - 2 [\nabla_{\Sigma_c} \mathcal{L}] \mu_c)
\]

\[
\nabla_M \mathcal{L} = \frac{1}{\pi_c} (\nabla_{\Sigma_c} \mathcal{L})
\]

We can compute gradients with respect to \( \mu_c \) and \( \Sigma_c \) by using the gradient and Hessian of \( h(z) \) at a sample \( z \) from \( q(z) \).

This can be done by using the Bonnet’s and Price’s theorems (Bonnet, 1964; Price, 1958; Opper & Archambeau, 2009; Rezende et al., 2014). Staines & Barber (2012) and Lin et al. (2019) discuss the conditions of the target function \( h(z) \) when it comes to applying these theorems. Firstly, we define \( \delta_c = q(z | w = c) / q(z) : = \mathcal{N}(z | \mu_c, \Sigma_c) / \sum_{c'=1}^{C} \pi_{c'} \mathcal{N}(z | \mu_{c'}, \Sigma_{c'}) \).

Using these theorems, we obtain the following stochastic-gradient estimations for the mixture of Gaussian case:

\[
\nabla_{\mu_c} \mathcal{L}(\lambda) = - \mathbb{E}_{q(c)} [q(w = c | z) \nabla_z h(z)] \approx - \pi_c \delta_c \nabla_z h(z)
\]

\[
\nabla_{\Sigma_c} \mathcal{L}(\lambda) = - \mathbb{E}_{q(c)} [q(w = c | z) \nabla^2 h(z)] \approx - \frac{\pi_c \delta_c}{2} \nabla^2 h(z).
\]

where \( q(w = c | z) = \pi_c \delta_c \) and \( z \) is sampled from \( q(z) \).

We can then plug these gradient estimations in the natural-gradient update for \( \Lambda_c \):

\[
\frac{1}{2} \left[ \Sigma_c^{(\text{new})} \right]^{-1} \left[ \mu_c^{(\text{new})} \right] \leftarrow \frac{1}{2} \Sigma_c^{-1} \mu_c + \beta \nabla_m \mathcal{L} \Rightarrow \left[ \Sigma_c^{(\text{new})} \right]^{-1} \left[ \mu_c^{(\text{new})} \right] \leftarrow \Sigma_c^{-1} \mu_c + \beta \delta_c \nabla^2 h(z)
\]

Similar for \( \lambda_c \):

\[
\left[ \Sigma_c^{(\text{new})} \right]^{-1} \left[ \mu_c^{(\text{new})} \right] \leftarrow \Sigma_c^{-1} \mu_c + \beta \nabla_m \mathcal{L} \leftarrow \Sigma_c^{-1} \mu_c + \frac{1}{\pi_c} (\nabla_{\mu_c} \mathcal{L} - 2 [\nabla_{\Sigma_c} \mathcal{L}] \mu_c)
\]

\[
\left[ \Sigma_c^{(\text{new})} \right]^{-1} \left[ \mu_c^{(\text{new})} \right] \leftarrow \left[ \Sigma_c^{-1} - \frac{\beta}{\pi_c} [\nabla_{\Sigma_c} \mathcal{L}] \right] \mu_c + \frac{1}{\pi_c} (\nabla_{\mu_c} \mathcal{L})
\]

\[
\left[ \Sigma_c^{(\text{new})} \right]^{-1} \left[ \mu_c^{(\text{new})} \right] \leftarrow \left[ \Sigma_c^{-1} + \beta \delta_n [\nabla^2 h(z)] \right] \mu_c + \frac{1}{\pi_c} (\nabla_{\mu_c} \mathcal{L})
\]

This gives the following update (by using the stochastic gradients):

\[
\mu_c^{(\text{new})} \leftarrow \mu_c - \beta \delta_c \Sigma_c^{(\text{new})} \nabla^2 h(z)
\]

B.3. Natural Gradients for \( q(w) \)

Now, we give the update for \( q(w | \lambda_w) \). Its natural parameter and expectation parameter are

\[
\lambda_w = \left\{ \log \left( \frac{\pi_c}{\pi_K} \right) \right\}_{c=1}^{K-1} \quad \mathbf{m}_w = \{ \mathbb{E}_{q(w)} [\mathbb{E}_c(w)] \}_{c=1}^{K-1} = \{ \pi_c \}_{c=1}^{K-1}
\]

To derive the gradients, we note that only \( q(z) \) depends on \( \pi \) since the model does not contain this as a parameter. Therefore, we need the gradient of the variational approximation which can be written as follows:

\[
\nabla_{\pi_c} q(z) = \nabla_{\pi_c} \sum_{k=1}^{K} \pi_k q(z | \lambda_k) = q(z | \lambda_c) - q(z | \lambda_K).
\]

The second term appears because the last \( \pi_K \) depends on \( \pi_c \).
For the convenience of our derivation, we will separate the lower bound into terms that depend on $q(z)$ and the rest of the terms, as shown below:

$$\nabla_{\pi_c} \mathcal{L}(\lambda) = \nabla_{\pi_c} \mathbb{E}_{q(z)} \left[ \sum_{n=1}^{N} \log p(D_n|z) + \log p(z) - \log q(z) \right]$$

$$= \int \nabla_{q(z)} \mathbb{E}_{q(z)} \left[ \sum_{n=1}^{N} \log p(D_n|z) + \log p(z) - \log q(z) \right] \, dz - \int q(z) \mathbb{E}_{q(z)} \log q(z) \, dz$$

$$= \int \left[ q(z|\lambda_c) - q(z|\lambda_K) \right] \left[ \sum_{n=1}^{N} \left( \log p(D_n|z) + \log \frac{p(z)}{q(z)} \right) \right] \, dz$$

$$= \mathbb{E}_{q(z)} \left[ (\delta_c - \delta_K) \left[ \sum_{n=1}^{N} \left( \log p(D_n|z) + \log \frac{p(z)}{q(z)} \right) \right] \right] - h(z)$$

$$\approx -(\delta_c - \delta_K) h(z)$$

where $z$ is a sample from $q(z)$.

Using this, we can perform the following NGD update:

$$\log \left( \frac{\pi_c}{\pi_K} \right) \leftarrow \log \left( \frac{\pi_c}{\pi_K} \right) - \beta(\delta_c - \delta_K) h(z)$$

### B.4. Extension to Finite Mixture of EFs

The algorithm presented in Section 4.1 can be extended to handle generic minimal EF components. We now present a general gradient estimator to do so. The update of $\pi_c$ remains unaltered, so we do not discuss them here. We only discuss how to update natural parameters $\lambda_c$ of $q(z|\lambda_c)$.

The natural parameter and sufficient statistics are $\lambda_c$ and $\mathbb{E}_c(w) \phi_z(z)$ respectively. We wish to perform the following update: $\lambda_c \leftarrow \lambda_c + \beta_c \nabla_{\lambda_c} \mathcal{L}(\lambda)$. In general, we can compute the gradient $\nabla_{m_c} \mathcal{L}(\lambda)$ by computing the FIM of each component as shown below:

$$\nabla_{m_c} \mathcal{L}(\lambda) = (\nabla_{\lambda_c} m_c)^{-1} \nabla_{\lambda_c} \mathcal{L}(\lambda) = (\nabla_{\lambda_c} \mathbb{E}_{q(w,z)} [\mathbb{E}_c(w) \phi_z(z)])^{-1} \nabla_{\lambda_c} \mathcal{L}(\lambda),$$

Both of these gradients can be obtained given $\nabla_{\lambda_c} z$, where $z$ is a sample from $q(z)$ as shown below.

$$\nabla_{\lambda_c} \mathbb{E}_{q(w,z)} [\mathbb{E}_c(w) \phi_z(z)] = \nabla_{\lambda_c} \int \pi_c q(z|w = c) \phi_z(z) \, dz = \int \pi_c q(z|w = c) \nabla_z [\phi_z(z)] \, dz$$

$$\nabla_{\lambda_c} \mathcal{L}(\lambda) = \int \pi_c \nabla_{\lambda_c} q(z|w = c) \, dz = \int q(z|w = c) \nabla \mathcal{L}(\lambda) \, dz$$

If we assume that $q(z|w)$ is an univariate continuous exponential family distribution, we can use the implicitly reparameterization trick (Salimans & Knowles, 2013; Figurnov et al., 2018) to get the following gradient. Lin et al. (2019) discuss the trick under a weaker assumption than Salimans & Knowles (2013); Figurnov et al. (2018).

$$\nabla_{\lambda_c} z = -\frac{\nabla_{\lambda_c} Q_c(z|\lambda_c)}{q(z|w = c)}.$$
where \( Q_c(z|\lambda_c) \) is the cumulative distribution function (CDF) of \( q(z|w = c) \). Therefore, we now can compute the required gradient as below:

\[
\nabla_{\lambda_c} \mathcal{L}(\lambda) = \int \pi_c q(z|w = c) \left[ -\nabla_z h(z) \right] \left[ -\frac{\nabla_{\lambda_c} Q_c(z|\lambda_c)}{q(z|w = c)} \right] dz
\]

\[
= \mathbb{E}_{q(z)} \left[ \pi_c \frac{q(z|w = c)}{q(z)} \left[ -\nabla_{\lambda_c} Q_c(z|\lambda_c) \right] \nabla_z h(z) \right],
\]

and

\[
\nabla_{\lambda_c} \mathbb{E}_{q(w,z)} \left[ I_c(w) \phi_z(z) \right] = \int \pi_c q(z|w = c) \nabla_z \left[ \phi_z(z) \right] \left[ -\frac{\nabla_{\lambda_c} Q_c(z|\lambda_c)}{q(z|w = c)} \right] dz
\]

\[
= \mathbb{E}_{q(z)} \left[ -\pi_c \nabla_{\lambda_c} Q_c(z|\lambda_c) \nabla_z \left[ \phi_z(z) \right] \right].
\]

This is not the most efficient way to compute NGDs, however, for the specific cases (e.g., Gaussian, exponential distribution, inverse Gaussian), we can get simplifications whenever gradient with respect to the expectation parameters are easy to compute.

The Birnbaum-Saunders distribution, which is a finite mixture of inverse Gaussians, is presented in Appendix C. This example is different from examples given in this section since we allow each mixing component takes a distinct but tied parametric form.

### B.5. Result for the Toy Example

See Figure 6

### C. Birnbaum-Saunders Distribution

Firstly, we denote the inverse Gaussian distribution by \( \text{InvGauss}(z; \mu, v) = \left( \frac{v}{2\pi z^3} \right)^{1/2} \exp \left[ -\frac{v}{2\mu^2} - \frac{v}{2z} + \frac{v}{\mu} \right] \), where \( z > 0, v > 0, \text{and } \mu > 0 \). We consider the following mixture distribution.

\[
q(w) = p I(w = 0) \left( 1 - p \right) I(w = 1)
\]

\[
q(z|w) = I(w = 0) \text{InvGauss}(z; \mu, v) + I(w = 1) \frac{\text{InvGauss}(z; \mu, v)}{\mu}, \tag{40}
\]

where \( \frac{1}{\mu} \text{InvGauss}(z; \mu, v) \) is a normalized distribution since it is the distribution of \( z = y^{-1} \) where \( y \) is distributed by \( \text{InvGauss}(y; \mu^{-1}, v/\mu^2) \).

As we can observe from Eq (40), each mixing component has a distinct parametric form and variational parameters are shared between the components, which is different from examples discussed in Appendix B. According to Desmond (1986); Jorgensen et al. (1991); Balakrishnan & Kundu (2019), the marginal distribution is known as the Birnbaum-Saunders distribution (Birnbaum & Saunders, 1969) shown as below, where \( p = \frac{1}{2} \).

\[
q(z|\mu) = \sum_w q(w) q(z|w)
\]

\[
= \frac{1}{2} \left\{ \left( \frac{v}{2\pi z^3} \right)^{1/2} \exp \left[ -\frac{vz}{2\mu^2} - \frac{v}{2z} + \frac{v}{\mu} \right] \right\}
\]

\[
= \frac{\sqrt{\nu}}{2\pi^{3/2}} \left[ \frac{1}{z^{3/2}} + \frac{1}{\mu z^{1/2}} \right] \exp \left[ -\frac{vz}{2\mu^2} - \frac{v}{2z} + \frac{v}{\mu} \right]
\]

\[
= \frac{\sqrt{\nu}}{2\mu \sqrt{2\pi}} \left[ \left( \frac{\mu}{z} \right)^{1/2} + \left( \frac{v}{z} \right)^{3/2} \right] \exp \left\{ -\frac{v(\frac{\mu}{2} + \frac{z}{2} - 2)}{2\mu} \right\}
\]

**Lemma 6** The joint distribution of the Birnbaum-Saunders distribution given in (40) can be written in a conditional EF form.
Figure 6. This is a complete version of the leftmost figure in Figure 2. The figure shows MOG approximation (with $K = 20$) to fit an MOG model with 10 components in a 20 dimensional problem.

Proof: It is obvious that $q(w)$ is Bernoulli distribution with $p = \frac{1}{2}$, which is an EF distribution. Now, we show that $q(z|w)$ is a conditional EF distribution as below.

$$q(z|w) = \exp \left\{ \mathbb{I}(w = 0) \left[ -\frac{vz}{2\mu^2} - \frac{v}{2z} + \frac{v}{\mu} + \frac{1}{2} \log \frac{v}{2\pi z^3} \right] + \mathbb{I}(w = 1) \left[ -\frac{vz}{2\mu^2} - \frac{v}{2z} + \frac{v}{\mu} + \frac{1}{2} \log \frac{v}{2\pi z} - \log \mu \right] \right\}$$

$$= \exp \left\{ -\frac{vz}{2\mu^2} - \frac{v}{2z} + \frac{v}{\mu} + \mathbb{I}(w = 0) \left[ \frac{1}{2} \log \frac{v}{2\pi z^3} \right] + \mathbb{I}(w = 1) \left[ \frac{1}{2} \log \frac{v}{2\pi z} - \log \mu \right] \right\}$$

$$= \frac{1}{\sqrt{2\pi}} e^{-3\mathbb{I}(w=0)/2 - 1/(w=1)/2} \exp \left\{ -\frac{vz}{2\mu^2} - \frac{v}{2z} + \frac{v}{\mu} + \frac{1}{2} \log(v) - \mathbb{I}(w = 1) \log(\mu) \right\}$$

The natural parameters and sufficient statistics are $\left\{ -\frac{v}{2\mu^2}, -\frac{v}{2z} \right\}$ and $\left\{ z, \frac{1}{z} \right\}$ respectively. \qed
According to Balakrishnan & Kundu (2019), the expectation parameters are

\[
m_1 = \mathbb{E}_{q(z)}[z] = \mu + \frac{\mu^2}{2v}
\]
\[
m_2 = \mathbb{E}_{q(z)}[z^{-1}] = \mu^{-1} + \frac{1}{2v}
\]

The sufficient statistics, natural parameters, and expectation parameters are summarized below:

\[
\begin{bmatrix}
    z \\
    \frac{1}{z}
\end{bmatrix}
= \begin{bmatrix}
    -\frac{v}{2\pi^2} \\
    -\frac{v}{2}
\end{bmatrix}
\begin{bmatrix}
    \mu + \frac{\mu^2}{2v} \\
    \mu^{-1} + \frac{1}{2v}
\end{bmatrix}
\]

**Lemma 7** The joint distribution given in (40) is a minimal conditional-EF.

**Proof:** Since \(\Lambda_m\) is known in this case, we only need to show there exists an one-to-one mapping between the natural parameter and the expectation parameter. Just by observing the parameters given above, we can see that there exists an one-to-one mapping between the natural parameter and \(\{\mu, v\}\) since \(\mu > 0\) and \(v > 0\). Furthermore, we know that \(m_1m_2 > 1\) and \(m_1 > 0\). We can show that there also exists an one-to-one mapping between \(\{\mu, v\}\) and the expectation parameter by noticing that

\[
\mu = \sqrt{m_1/m_2}
\]
\[
v = \frac{1}{2(m_2 - \sqrt{m_1/m_2})}
\]

Since one-to-one mapping is transitive, we know that mapping between natural and expectation parameters is one-to-one. Hence proved.

Note that we can use the implicitly re-parametrization trick to compute the gradient w.r.t. \(\mu\) and \(v\). Furthermore, the expectation parameters \(m_1\) and \(m_2\) are functions of \(\mu, v\) and the gradients can be obtained in terms of the gradient with respect to \(\mu\) and \(v\) by using the chain rule.

**D. Studnet’s t-distribution**

**Lemma 8** The joint distribution \(\mathcal{N}(z|\mu, w\Sigma)\mathcal{IG}(w|a, a)\), where \(z \in \mathbb{R}^d\), is a curved exponential family distribution.

**Proof:** The joint-distribution can be expressed as a four-parameter exponential form as shown below:

\[
\mathcal{N}(z|\mu, w\Sigma)\mathcal{IG}(w|a, a) = \det(2\pi w\Sigma)^{-d/2} \exp\left\{-\frac{1}{2} (z - \mu)^T (w\Sigma)^{-1} (z - \mu) - \frac{1}{2} \log \det(\Sigma) - a \log w + a \log(\Gamma(a) - a \log a)\right\}
\]
\[
= (2\pi w)^{-d/2} w^{-1} \exp\left\{-\frac{1}{2} (z - \mu)^T (w\Sigma)^{-1} (z - \mu) - \frac{1}{2} \log \det(\Sigma) - a \log w - a \log(\Gamma(a) - a \log a)\right\}
\]
\[
= (2\pi w)^{-d/2} w^{-1} \exp\left\{(\tilde{\Lambda}_1, wz) + (\tilde{\Lambda}_2, wz) + (\tilde{\Lambda}_3, w^T) + \tilde{\Lambda}_4 + \log w\right\} - \log(\Gamma(a) - a \log(a + \frac{1}{2} \log \det(\Sigma))\right\}
\]
\[
= (2\pi w)^{-d/2} w^{-1} \exp\left\{\langle\Lambda_1, wzz^T\rangle + \langle\Lambda_2, wz\rangle + \langle\Lambda_3, w^T\rangle + \langle\Lambda_4, w^{-1}\rangle\right\} - \log(\Gamma(a) - a \log(a + \frac{1}{2} \log \det(\Sigma))\right\}
\]

where the following are the natural parameters:

\[
\Lambda_1 := -\frac{1}{2} \Sigma^{-1}, \quad \Lambda_2 := \Sigma^{-1} \mu, \quad \Lambda_3 := -\frac{1}{2} \mu^T \Sigma^{-1} \mu, \quad \Lambda_4 := -a
\]

We can see that \(\Lambda_3\) is fully determined by \(\Lambda_1\) and \(\Lambda_2\), i.e.,

\[
\Lambda_3 = -\frac{1}{2} \mu^T \Sigma^{-1} \mu = -\frac{1}{2} (\Sigma \Sigma^{-1} \mu)^T (\Sigma^{-1} \mu) = -\frac{1}{2} \left(\frac{1}{2} (\Sigma \Sigma^{-1} \mu)\right)^T \Lambda_2
\]
In a minimal representation we can specify all four parameters freely, but in this case we have less degree of freedom. Therefore, this is a curved EF representation.

Instead of using the above 4 parameter form, we can write the distribution in the conditional EF form given in Definition 2.

**Lemma 9** The joint distribution of Studnet’s t-distribution given in (17) can be written in a conditional EF form.

**Proof:** We can rewrite the conditional \( q(z|w) \) in an EF-form as follows:

\[
q(z|w) = \mathcal{N}(z|\mu, w\Sigma)
\]

\[
= (2\pi)^{-d/2} \exp\left\{ \operatorname{Tr}\left( -\frac{1}{2} \Sigma^{-1} w^{-1} zz^T \right) + \mu^T \Sigma^{-1} w^{-1} z - \frac{1}{2} \left( w^{-1} \mu^T \Sigma^{-1} \mu + \log \det(w\Sigma) \right) \right\}
\]

The sufficient statistics \( \phi_z(z, w) = \{ w^{-1} z, w^{-1} zz^T \} \). The natural parameter is \( \lambda_z = \{ \Sigma^{-1} \mu, -\frac{1}{2} \Sigma^{-1} \} \). Since \( q(w) \) is an inverse Gamma distribution, which is an EF distribution as shown below, the joint \( q(z, w) \) is a conditional EF. The EF form of the inverse gamma distribution is shown below:

\[
q(w|a, a) = w^{-1} \exp(-((\log(w) + \frac{1}{w})a - (\log(\Gamma(a)) - a \log(a)))
\]

We can read the sufficient statistics \( \phi_w(w) = -\log(w) - \frac{1}{w} \) and the natural parameter \( \lambda_w = a \) from this form.

Using the fact that \( E_{q(w|a)}[1/w] = a/a = a = 1 \), and \( E_{q(w|a)}[\log w] = \log a - \psi(a) \), we can derive the expectation parameter shown below:

\[
m := E_{q(w|a)}[q(z|w, \Sigma)] \left[ w^{-1} z \right] = \mu,
\]

\[
M := E_{q(w|a)}[q(z|w, \Sigma)] \left[ w^{-1} zz^T \right] = \mu \mu^T + \Sigma,
\]

\[
m_a := E_{q(w|a)} \left[ -\frac{1}{w} - \log(w) \right] = -1 - \log a + \psi(a)
\]

The sufficient statistics, natural parameters, and expectation parameters are summarized below:

\[
\begin{bmatrix}
-1/w - \log w \\
\frac{a}{w} \\
\frac{zz^T}{w}
\end{bmatrix}
\begin{bmatrix}
\Sigma^{-1} \mu \\
\frac{1}{2} \Sigma^{-1} \\
\mu \mu^T + \Sigma
\end{bmatrix}
\]

The following lemma shows that the Student’s t-distribution is an MCEF obtained by establishing one-to-one mapping between natural and expectation parameters.

**Lemma 10** The joint distribution of Studnet’s t-distribution shown in (17) is a minimal conditional EF.

**Proof:** The proof is rather simple. First we note that the expectation parameters for \( q(z|w) \) do not depend on \( \lambda_w := a \). In fact, the mapping between the last two natural and expectation parameters is one-to-one since they correspond to a Gaussian distribution which has a minimal representation.

The only thing remaining is to show that the mapping between \( a \) and \( m_w(a) := -1 - \log a + \psi(a) \) is one-to-one. Since \( \nabla_a m_w(a) \) is the Fisher information of \( q(w) \), we can show this when \( \nabla_a m_w(a) > 0 \). The gradient \( \nabla_a m_w(a) = \nabla_a \psi(a) - 1/a - 1/(2a^2) > 0 \) when \( a > 0 \). Therefore, \( \nabla_a \psi(a) - 1/a > 0 \) which establishes that the Fisher information is positive, therefore the distribution is a minimal EF. This completes the proof.

**D.1. Derivation of the NGD Update**

Let’s consider \( q(w) = \mathcal{IG}(w|a, a) \) and \( q(z|w) = \mathcal{N}(z|\mu, w\Sigma) \). We denote the log-likelihood for the \( n \)’th data point by \( f_n(z) := -\log p(D_n|z) \) with a Student’s t-prior on \( z \) expressed as a scale mixture of Gaussians \( p(z, w) = \)
Fast and Simple Natural-Gradient Variational Inference with Mixture of Exponential-family Approximations

$I_G(w|a_0, a_0)\mathcal{N}(\mathbf{z}|\mathbf{0}, w\mathbf{I})$. We use the lower bound defined in the joint-distribution $p(D, z, w)$:

$$L(\lambda) = \mathbb{E}_{q(z,w)} \left[ \log p(D, z, w) - \log q(D, z, w) \right]$$

$$= \mathbb{E}_{q(z,w)} \left[ \sum_{n=1}^{N} \log p(D_n|z) + \log \mathcal{N}(\mathbf{z}|\mathbf{0}, w\Sigma) + \log \frac{I_G(w|a_0, a_0)}{I_G(w|a, a)} \right],$$

Our goal is to compute the gradient of this ELBO with respect to the expectation parameters.

Since the expectation parameters $m_\lambda$ only depend on $\mu$ and $\Sigma$, we can write the gradient with respect to them using the chain rule (similar to the finite mixture of Gaussians case):

$$\nabla_m L(\lambda) = \nabla_\mu L(\lambda) = 2 \nabla_\Sigma L(\lambda) \mu$$

$$\nabla_M L(\lambda) = \nabla_\Sigma L(\lambda)$$

These gradients of the lower bound can be obtained as follows:

$$\nabla_\mu L(\lambda) = - \sum_{n=1}^{N} \nabla_\mu \mathbb{E}_{q(z,w)} [f_n(z)] - \mu$$

$$\nabla_\Sigma L(\lambda) = - \sum_{n=1}^{N} \nabla_\Sigma \mathbb{E}_{q(z,w)} [f_n(z)] - \frac{1}{2} \mathbf{I} + \frac{1}{2} \Sigma^{-1}$$

Plugging these in the natural-gradient updates (14), we get the following updates (we have simplified these in the same way as explained in Appendix B.2; more details in Khan et al. (2018)):

$$\Sigma^{-1} \leftarrow (1 - \beta) \Sigma^{-1} + 2 \beta \sum_{n=1}^{N} \nabla_\Sigma \mathbb{E}_{q(z,w)} [f_n(z)] + \beta \mathbf{I}$$

$$\mu \leftarrow \mu - \beta \sum_{n=1}^{N} \nabla_\mu \mathbb{E}_{q(z,w)} [f_n(z)] + \mu$$

To compute the gradients, the reparametrization trick (Kingma & Welling, 2013) can be used. However, we can do better by using the extended Bonnet’s and Price’s theorems for Student’s t-distribution (Lin et al., 2019). Assuming that $f_n(z)$ satisfies the assumptions needed for these two theorems, we can use the following stochastic-gradient approximations for the gradients:

$$\nabla_\mu \mathbb{E}_{q(w)} \mathcal{N}(z|\mu, w\Sigma) \left[ f(z) \right] \approx \mathbb{E}_{q(z)} \left[ \nabla_z f(z) \right] \approx \nabla_z f(z),$$

$$\nabla_\Sigma \mathbb{E}_{q(w)} \mathcal{N}(z|\mu, w\Sigma) \left[ f(z) \right] \approx \frac{1}{2} \mathbb{E}_{q(z)} \left[ u(z) \nabla_z^2 f(z) \right] \approx \frac{1}{2} u(z) \nabla_z^2 f(z),$$

$$= \frac{1}{2} \mathbb{E}_{q(z,w)} \left[ w \nabla_z^2 f(z) \right] \approx \frac{1}{2} w \nabla_z^2 f(z),$$

where $z \in \mathcal{R}^d$ is generated from $q(z)$, $w$ is generated from $q(w)$, and

$$u(z) := \frac{a + \frac{1}{2} (z - \mu)^T \Sigma^{-1} (z - \mu)}{(a + d/2 - 1)}.$$

Using these gradients, we get the following update:

$$\Sigma^{-1} \leftarrow (1 - \beta) \Sigma^{-1} + \beta \left[ u(z) \nabla_z^2 f_n(z) + \mathbf{I} / N \right],$$

$$\mu \leftarrow \mu - \beta \Sigma \left[ \nabla_z f_n(z) + \mu / N \right].$$

Now we derive the NGD update for $\alpha$. Recall that the natural parameter is $\alpha$ and the expectation parameter is $m_\alpha = -1 - \log \alpha + \psi(\alpha)$. The gradient of the lower bound can be expressed as

$$\nabla_{m_\alpha} L(\lambda) = - \sum_{n=1}^{N} \nabla_{m_\alpha} \mathbb{E}_{q(z,w)} [f_n(z)] + a_0 - a$$
We then use stochastic approximation to get the desired update.

\[ a \leftarrow (1 - \beta) a + \beta \left( a_0 - \sum_{n=1}^{N} \nabla_{m_n} E_{q(z,w)} [f_n(z)] \right) \]  

(41)

While the gradient with respect to the expectation parameter does not admit a closed-form expression, we can compute the gradient using the re-parametrization trick. According to (39), the gradient \( \nabla_{m_a} E_{q(z,w)} [f_n(z)] \) can be computed as

\[ \nabla_{m_a} E_{q(z,w)} [f_n(z)] = (\nabla_a m_a)^{-1} \nabla_a E_{q(z,w)} [f_n(z)] = (\nabla_a E_{q(w)} [\phi_w(w)])^{-1} \nabla_a E_{q(z,w)} [f_n(z)] \]

Note that \( \nabla_a E_{q(w)} [\phi_w(w)] = \nabla_a (m_a) \) has a closed-form expression. However we have found that using stochastic approximation for both the numerator and denominator works better. Salimans & Knowles (2013) show that such approximation reduces the variance but introduce a bit bias. We use the reparameterization trick for both terms. Since \( q(w) \) is (implicitly) re-parameterizable (Salimans & Knowles, 2013; Figurnov et al., 2018), the gradient can be computed as

\[ \nabla_a E_{q(w)} [\phi_w(w)] = - \int I \mathcal{G}(w|a, \alpha) (\nabla_w [w^{-1} + \log w]) (\nabla_a w) dw \approx (w^{-2} - w^{-1}) \nabla_a w \]

where \( w \) is generated from \( I \mathcal{G}(w|a, \alpha) \). Similarly,

\[ \nabla_a E_{q(z,w)} [f_n(z)] = \int \int q(w) (\nabla_w q(z|w)) (\nabla_a w) f_n(z) dw dz = \int \int I \mathcal{G}(w|a, \alpha) (\nabla_w N(z|\mu, w \Sigma)) (\nabla_a w) f_n(z) dw dz \]

For stochastic approximation, we generate \( w \) from \( q(w) \) and let \( \hat{\Sigma} = w \Sigma \). The above expression can be approximated as below.

\[ \nabla_a E_{q(z,w)} [f_n(z)] \approx \int (\nabla_w N(z|\mu, w \Sigma)) (\nabla_a w) f_n(z) dz \]

\[ = \int \text{Tr} \left( \Sigma \nabla \Sigma N(z|\mu, \hat{\Sigma}) \right) (\nabla_a w) f_n(z) dz \]

\[ = \nabla_a w \text{Tr} \left( \Sigma \nabla \Sigma E_{N(z|\mu, \hat{\Sigma})} [f_n(z)] \right) \]

\[ = \frac{\nabla_a w}{2} \text{Tr} \left( \Sigma \nabla \Sigma f_n(z) \right) \],

where we use the Price’s theorem \( \nabla \Sigma E_{N(z|\mu, \hat{\Sigma})} [f_n(z)] = \frac{1}{2} E_{N(z|\mu, \hat{\Sigma})} [\nabla^2 f_n(z)] \).

We then use stochastic approximation to get the desired update.

\[ \nabla_a E_{q(z,w)} [f_n(z)] \approx \frac{\nabla_a w}{2} \text{Tr} \left( \Sigma \nabla \Sigma f_n(z) \right) \]

where \( z \) is generated from \( q(z) \) and \( w \) is generated from \( q(w) \).

Anther example is the symmetric normal inverse-Gaussian distribution, which can be found at Appendix H.

### E. Multivariate Skew-Gaussian Distribution

We consider the following variational distribution.

\[ q(z, w) = N(z|\mu + |w|\alpha, \Sigma)N(w|0, 1) \]  

(42)

The marginal distribution is known as the multivariate skew Gaussian distribution (Azzalini, 2005) as shown in the following lemma.

**Lemma 11** The marginal distribution \( q(z) \) is \( 2\Phi \left( \frac{(z - \mu)^T \Sigma^{-1} \alpha}{\sqrt{1 + |\alpha| \Sigma^{-1} \alpha}} \right) N(z|\mu, \Sigma + \alpha \alpha^T), \) where \( \Phi(\cdot) \) is the CDF of the standard univariate Gaussian distribution.
where we move from the first step to the second step using the fact that

\[ q(z) = 2 \int_0^{+\infty} \mathcal{N}(w|0, 1) \mathcal{N}(z|\mu + w\alpha, \Sigma) dw \]

By grouping terms related to \( w \) together and completing a Gaussian form for \( w \), we obtain the following expression

\[ q(z) = 2 \int_0^{+\infty} \mathcal{N}(w|0, 1) \mathcal{N}(z - w\alpha|\mu, \Sigma) dw \]

Proof: The marginal distribution \( z \) is

\[ q(z) = 2 \int_0^{+\infty} \mathcal{N}(w|0, 1) \mathcal{N}(z|\mu + w\alpha, \Sigma) dw \]

\[ = 2 \int_0^{+\infty} \mathcal{N}(w|0, 1) \mathcal{N}(z - w\alpha|\mu, \Sigma) dw \]

Lemma 13 **Multivariate skew Gaussians is a minimal conditional-EF.**

Proof: We first rewrite \( q(z|w) \) in a EF-form as follows:

\[ q(z|w) = \mathcal{N}(z|\mu + |w|\alpha, \Sigma) \]

\[ = (2\pi)^{-d/2} \exp \left\{ \text{Tr} \left( -\frac{1}{2} \Sigma^{-1}zz^T \right) + |w|\alpha^T \Sigma^{-1}z + \mu^T \Sigma^{-1}z - \frac{1}{2} (|w|\alpha^T \Sigma^{-1} + |w|\alpha + \log \det(\Sigma)) \right\} \]

The sufficient statistics \( \phi_z(z, w) = \{ z, |w|z, zz^T \} \) and the natural parameter \( \lambda_z = \{ \Sigma^{-1}\mu, \Sigma^{-1}\alpha, -\frac{1}{2}\Sigma^{-1} \} \) can be read from the form. Since \( q(w) \) is a univariate Gaussian distribution with known parameters, which is a EF distribution. Therefore, the joint distribution \( q(z, w) \) is a conditional EF.

Lemma 12 **The joint distribution of skew-Gaussian distribution given at Eq. (42) can be written in a conditional EF form.**

Proof: Let \( c = \sqrt{\frac{2}{\pi}} \). Using the fact that \( \mathbb{E}_{q(w|0, 1)} [|w|] = c \), we can derive the expectation parameter shown below:

\[ m := \mathbb{E}_{q(z|w, 0, 1)\mathcal{N}(z|\mu + |w|\alpha, \Sigma)} [z] = \mu + c\alpha, \]

\[ m_\alpha := \mathbb{E}_{q(z|w, 0, 1)\mathcal{N}(z|\mu + |w|\alpha, \Sigma)} [|w|z] = c\mu + \alpha, \]

\[ M := \mathbb{E}_{q(z|w, 0, 1)\mathcal{N}(z|\mu + |w|\alpha, \Sigma)} [zz^T] = \mu\mu^T + \alpha\alpha^T + c (\mu\alpha^T + \alpha\mu^T) + \Sigma \]

The following lemma shows that the skew-Gaussian distribution is indeed a minimal conditional-EF.

**Lemma 13** **Multivariate skew Gaussians is a minimal conditional-EF.**
We use the lower bound defined in the following distribution

\[ L(\lambda) = \mathbb{E}_{q(z|\lambda)} \left[ \sum_{n=1}^{N} \log p(D_n|z) + \log \mathcal{N}(z|0, \delta^{-1}I) - \log q(z|\lambda) \right], \]

where \( q(z) = 2\Phi \left( \frac{z-\mu}{\sqrt{1+\alpha^2 \Sigma^{-1}}} \right) \mathcal{N}(z|\mu, \Sigma + \alpha \alpha^T) \) and recall that \( \Phi(\cdot) \) denotes the CDF of the standard univariate normal distribution.

Our goal is to compute the gradient of this ELBO with respect to the expectation parameters.

**E.2. Natural Gradient for \( q(z|w) \)**

We do not need to compute these gradients with respect to the expectation parameters directly. The gradients can be computed in terms of \( \{\mu, \alpha, \Sigma\} \).

Using the mapping at (43)-(45) and the chain rule, we can express the following gradients with respect to the expectation parameters in terms of the gradients with respect to \( \mu \), \( \alpha \), and \( \Sigma \):

\[
\nabla_m L = \frac{1}{1 - c^2} \nabla_\mu L - \frac{c}{1 - c^2} \nabla_\alpha L - 2 \langle \nabla_\Sigma L \rangle \mu
\]

\[
\nabla_{\alpha} L = \frac{1}{1 - c^2} \nabla_\alpha L - \frac{c}{1 - c^2} \nabla_\mu L - 2 \langle \nabla_\Sigma L \rangle \alpha
\]

\[
\nabla_{\Sigma} L = \nabla_\Sigma L
\]

By plugging the gradients into the update in (14) and then re-expressing the update in terms of \( \mu \), \( \alpha \), \( \Sigma \) (we have simplified these in the same way as explained in Appendix B.2), we obtain the natural gradient update in terms of \( \mu \), \( \alpha \), and \( \Sigma \).

\[
\Sigma^{-1} \leftarrow \Sigma^{-1} - 2\beta \nabla_\Sigma L
\]

\[
\mu \leftarrow \mu + \beta \Sigma \left( \frac{1}{1 - c^2} \nabla_\mu L - \frac{c}{1 - c^2} \nabla_\alpha L \right)
\]

\[
\alpha \leftarrow \alpha + \beta \Sigma \left( \frac{1}{1 - c^2} \nabla_\alpha L - \frac{c}{1 - c^2} \nabla_\mu L \right)
\]
Recall that the lower bound is

\[
\mathcal{L}(\lambda) = \mathbb{E}_{q(z|\lambda)} \left[ -\sum_{n=1}^{N} f_n(z) + \log \mathcal{N}(z|0, \delta^{-1} I) - \log q(z|\lambda) \right],
\]

For the prior term, there is a closed-form expression for gradient computation.

\[
\mathbb{E}_{q(z)} \left[ \log \mathcal{N}(z|0, \delta^{-1} I) \right] = -\frac{d}{2} \log(2\pi) + \frac{d\delta}{2} - \frac{\delta}{2} (\lambda^T \lambda + 2c\mu^T \lambda + \text{Tr}(\Sigma) + \mu^T \Sigma \mu)
\]

It is easy to show that the gradients about the prior term are

\[
\begin{align*}
\mathbf{g}_{\mu}^{\text{prior}} &= -\delta (\mu + c\lambda) \\
\mathbf{g}_{\lambda}^{\text{prior}} &= -\delta (\lambda + c\mu) \\
\mathbf{g}_{\Sigma}^{\text{prior}} &= -\frac{d}{2} I
\end{align*}
\]

For the entropy term, by Contreras-Reyes & Arellano-Valle (2012); Arellano-Valle et al. (2013), it can be expressed as follows.

\[
\mathbb{E}_{q(z)} \left[ -\log q(z|\lambda) \right] = \frac{d}{2} (\log(2\pi) + 1) + \frac{1}{2} \log |\Sigma + \lambda \lambda^T| - 2\mathbb{E}_{q(z|\lambda)} \left[ \Phi(z_3) \log(\Phi(z_3)) \right] - \log(2)
\]

We can use the re-parametrization trick to compute the gradients about the entropy term. However, we can found out the exact gradients usually works better. Using the expression in (49), the gradients of the entropy term are given as follows:

\[
\begin{align*}
\mathbf{g}_{\mu}^{\text{entropy}} &= 0 \\
\mathbf{g}_{\lambda}^{\text{entropy}} &= (\Sigma + \lambda \lambda^T)^{-1} \lambda - \mathbb{E}_{q(z|\lambda)} \left[ \frac{\log(\Phi(z_3))}{\sqrt{2\pi} (1 + \lambda^T \Sigma^{-1} \lambda)} \right] + \frac{2z_3 \Sigma^{-1} \lambda}{\sqrt{2\pi} (1 + \lambda^T \Sigma^{-1} \lambda)} \\
\mathbf{g}_{\Sigma}^{\text{entropy}} &= \frac{1}{2} (\Sigma + \lambda \lambda^T)^{-1} + \mathbb{E}_{q(z|\lambda)} \left[ \frac{\log(\Phi(z_3))}{\sqrt{2\pi} (1 + \lambda^T \Sigma^{-1} \lambda)} \right] + \frac{z_3 \Sigma^{-1} \lambda \lambda^T \Sigma^{-1} \lambda}{\sqrt{2\pi} (1 + \lambda^T \Sigma^{-1} \lambda)}
\end{align*}
\]

where the expectations involve 1d integrations, which can be computed by Gauss-Hermite quadrature.

The remaining thing is to compute the gradients about \( \mathbb{E}_{q(z)} [f_n(z)] \). To compute the gradients, the reparametrization trick can be used. However, we can do better by using the extended Bonnet’s and Price’s theorems for skew-Gaussian distribution (Lin et al., 2019). Assuming that \( f_n(z) \) satisfies the assumptions needed for these two theorems, we obtain the following gradient expression:

\[
\begin{align*}
g_1^n &= \nabla_\mu \mathbb{E}_{q(z)} [f_n(z)] = \mathbb{E}_{q(z)} [\nabla_z f_n(z)] \approx \nabla_z f_n(z) \\
g_2^n &= \nabla_\lambda \mathbb{E}_{q(z)} [f_n(z)] \\
&= \mathbb{E}_{q(z)} \left[ u(z) \nabla_z f_n(z) + v\mathbb{E}_{q(z|w)} [\nabla_z f_n(z)] \right] \approx u(z) \nabla_z f_n(z) + v\nabla_z f_n(z) \\
&= \mathbb{E}_{q(w,z)} \left[ |w| \nabla_z f_n(z) \right] \approx |w| \nabla_z f_n(z) \\
g_3^n &= 2\nabla_\Sigma \mathbb{E}_{q(z)} [f_n(z)] = \mathbb{E}_{q(z)} \left[ \nabla_z^2 f_n(z) \right] \approx \nabla_z^2 f_n(z)
\end{align*}
\]

where \( v = \frac{c}{(1 + \lambda^T \Sigma^{-1} \lambda)} \), \( u(z) := \frac{(z - \mu)^T \Sigma^{-1} \alpha}{1 + \lambda^T \Sigma^{-1} \lambda} \), and \( w \sim \mathcal{N}(0, 1) \), \( \tilde{z} \sim \mathcal{N}(\tilde{z}|\mu, \Sigma) \), \( z = \tilde{z} + |w| \alpha \).

Putting together, we can express the gradients in the following form, which will be used for deriving the extended variational
Adam update.

\[
\nabla_{\mu} L(\lambda) = -\sum_{n=1}^{N} \left( \frac{g_{1}^{n} - g_{\text{entropy}}^{\mu}}{0} \right) - \delta(\mu + c\alpha) \\
= -\sum_{n=1}^{N} g_{1}^{n} - \delta(\mu + c\alpha) \\
\n\nabla_{\alpha} L(\lambda) = -\sum_{n=1}^{N} \left( \frac{g_{2}^{n} - g_{\text{entropy}}^{\alpha}}{\alpha} \right) - \delta(\alpha + c\mu) \\
= -\sum_{n=1}^{N} g_{2}^{n} - \delta(\alpha + c\mu) \\
\n\nabla_{\Sigma} L(\lambda) = -\frac{1}{2} \sum_{n=1}^{N} \left( g_{3}^{n} - 2g_{\text{entropy}}^{\alpha} / N \right) - \delta I + \frac{1}{2} (\Sigma^{-1} - \Sigma^{-1}) \\
= -\frac{1}{2} \sum_{n=1}^{N} \left( g_{3}^{n} - 2g_{\text{entropy}}^{\alpha} / N + \Sigma^{-1} / N \right) - \delta I + \frac{1}{2} \Sigma^{-1} \\
\]

(53) (54) (55)

For stochastic approximation, we can sub-sampling a data point \( n \) and use MC samples to approximate \( g_{1}, g_{2}, \) and \( g_{3} \).

Plugging these stochastic gradients into (46)-(48), we obtain the NGD update:

\[
\Sigma^{-1} \leftarrow (1 - \beta)\Sigma^{-1} + \beta(\delta I + Ng_{3}^{n}) \\
\mu \leftarrow \mu - \beta\Sigma \left( \frac{N}{1 - c^{2}} (g_{\mu}^{n} - cg_{\mu}^{n}) + \delta \mu \right) \\
\alpha \leftarrow \alpha - \beta\Sigma \left( \frac{N}{1 - c^{2}} (g_{\alpha}^{n} - cg_{\alpha}^{n}) + \delta \alpha \right) \\
\]

F. Multivariate Exponentially Modified Gaussian Distribution

We consider the following mixture distribution.

\[
q(z, w) = \mathcal{N}(z|\mu + w\alpha, \Sigma)\text{Exp}(w|1) \\
\]

The marginal distribution is a multivariate extension of the exponentially modified Gaussian distribution (Grushka, 1972) and the Gaussian minus exponential distribution (Carr & Madan, 2009) due to the following lemma.

**Lemma 14** The marginal distribution \( q(z) (\alpha \neq 0) \) is

\[
q(z) = \frac{\sqrt{2\pi} \det(2\pi \Sigma)^{-\frac{1}{2}}}{\sqrt{\alpha^{T} \Sigma^{-1} \alpha}} \Phi \left( \frac{(z - \mu)^{T} \Sigma^{-1} \alpha - 1}{\sqrt{\alpha^{T} \Sigma^{-1} \alpha}} \right) \exp \left\{ \frac{1}{2} \left[ \frac{(z - \mu)^{T} \Sigma^{-1} \alpha - 1}{\alpha^{T} \Sigma^{-1} \alpha} - (z - \mu)^{T} \Sigma^{-1} (z - \mu) \right] \right\} , \\
\]

where \( \Phi(\cdot) \) is the CDF of the standard univariate Gaussian distribution.

In the univariate case, the marginal distribution becomes the exponentially modified Gaussian distribution when \( \alpha > 0 \) and the Gaussian minus exponential distribution when \( \alpha < 0 \).
where we move from Eq. (56) to Eq. (57) using the fact that \( \Phi(\cdot) \) call that as below:

\[
\frac{\text{det} (2\pi \Sigma)}{\sqrt{\alpha^t \Sigma^{-1} \alpha}} \int_0^{+\infty} \mathcal{N}(w|\mu + w\alpha, \Sigma) dw
\]

By grouping terms related to \( w \) together and completing a Gaussian form for \( w \), we obtain the following expression.

\[
\frac{\text{det} (2\pi \Sigma)}{\sqrt{\alpha^t \Sigma^{-1} \alpha}} \int_0^{+\infty} \mathcal{N}(w|\mu + w\alpha, \Sigma) \exp \left\{ \frac{1}{2} \left[ \frac{(z - \mu)^T \Sigma^{-1} \alpha - 1}{\alpha^T \Sigma^{-1} \alpha} - (z - \mu)^T \Sigma^{-1} (z - \mu) \right] \right\} \]

\[
\left( \frac{z - \mu)^T \Sigma^{-1} \alpha - 1}{\alpha^T \Sigma^{-1} \alpha} \right)
\]

\[
\frac{\sqrt{2\pi \text{det} (2\pi \Sigma)}}{\sqrt{\alpha^t \Sigma^{-1} \alpha}} \Phi \left( \frac{(z - \mu)^T \Sigma^{-1} \alpha - 1}{\alpha^T \Sigma^{-1} \alpha} \right) \exp \left\{ \frac{1}{2} \left[ \frac{(z - \mu)^T \Sigma^{-1} \alpha - 1}{\alpha^T \Sigma^{-1} \alpha} - (z - \mu)^T \Sigma^{-1} (z - \mu) \right] \right\}
\]

(56)

(57)

where we move from Eq. (56) to Eq. (57) using the fact that \( \int_0^{+\infty} \mathcal{N}(w|u, \sigma^2) dw = \Phi(u/\sigma) \).

Similar to the skew-Gaussian case, in this example, the sufficient statistics \( \phi(z, w) = \{z, w, z^T \} \) and the natural parameter \( \lambda_z = \{ \Sigma^{-1} \mu, \Sigma^{-1} \alpha, -\frac{1}{2} \Sigma^{-1} \} \) can be read from \( q(z|w) = \mathcal{N}(z|\mu + w\alpha, \Sigma) \). The joint distribution \( q(z, w) \) is a conditional EF since \( q(w) \) is an exponential distribution with known parameters, which is an EF distribution. Likewise, we can show that the joint distribution is also a minimal conditional EF. We can derive the expectation parameter shown below:

\[
m := \mathbb{E}_{\mathcal{N}(\mu, \Sigma)} [z] = \mu + \alpha,
\]

\[
m_\alpha := \mathbb{E}_{\mathcal{N}(\mu, \Sigma)} [w] = \mu + 2\alpha,
\]

\[
M := \mathbb{E}_{\mathcal{N}(\mu, \Sigma)} [zz^T] = \mu\mu^T + 2\alpha\alpha^T + (\mu\alpha^T + \alpha\mu^T) + \Sigma
\]

The sufficient statistics, natural parameters, and expectation parameters are summarized below:

\[
\begin{bmatrix}
z \\
w \\
z^T
\end{bmatrix}
\]

\[
\begin{bmatrix}
\Sigma^{-1} \\
\Sigma^{-1}
\end{bmatrix}
\]

\[
\begin{bmatrix}
\mu + \alpha \\
\mu + 2\alpha
\end{bmatrix}
\]

F.1. Derivation of the NGD Update

As shown in Appendix E.1, we consider the variational approximation using the exponentially modified Gaussian distribution \( q(z|\lambda) \). We consider the same model as Appendix E.1 with a Gaussian-prior \( \mathcal{N}(z|0, \delta^{-1} I) \) on \( z \). The lower bound is defined as below:

\[
\mathcal{L} (\lambda) = \mathbb{E}_{q(z|\lambda)} \left[ \sum_{n=1}^{N} \log p(D_n|z) + \log \mathcal{N}(z|0, \delta^{-1} I) - \log q(z|\lambda) \right],
\]

where \( q(z) = \frac{\sqrt{2\pi \text{det}(2\pi \Sigma)}}{\sqrt{\alpha^t \Sigma^{-1} \alpha}} \Phi \left( \frac{(z - \mu)^T \Sigma^{-1} \alpha - 1}{\alpha^T \Sigma^{-1} \alpha} \right) \exp \left\{ \frac{1}{2} \left[ \frac{(z - \mu)^T \Sigma^{-1} \alpha - 1}{\alpha^T \Sigma^{-1} \alpha} - (z - \mu)^T \Sigma^{-1} (z - \mu) \right] \right\} \) and recall that \( \Phi(\cdot) \) denotes the CDF of the standard univariate normal distribution.

Our goal is to compute the gradient of this ELBO with respect to the expectation parameters.

F.2. Natural Gradient for \( q(z|w) \)

We do not need to compute these gradients with respect to the expectation parameters directly. The gradients can be computed in terms of \( \{\mu, \alpha, \Sigma\} \).
Similarly, by the chain rule, we can express the following gradients with respect to the expectation parameters in terms of the gradients with respect to $\mu$, $\alpha$, and $\Sigma$.

\[
\begin{align*}
\nabla_m \mathcal{L} &= 2\nabla_\mu \mathcal{L} - \nabla_\alpha \mathcal{L} - 2 (\nabla_\Sigma \mathcal{L}) \mu \\
\nabla_{m\alpha} \mathcal{L} &= \nabla_\alpha \mathcal{L} - \nabla_\mu \mathcal{L} - 2 (\nabla_\Sigma \mathcal{L}) \alpha \\
\nabla_M \mathcal{L} &= \nabla_\Sigma \mathcal{L}
\end{align*}
\]

By plugging the gradients into the update in (14) and then re-expressing the update in terms of $\mu$, $\alpha$, $\Sigma$, we obtain the natural gradient update in terms of $\mu$, $\alpha$, and $\Sigma$.

\[
\begin{align*}
\Sigma^{-1} &\leftarrow \Sigma^{-1} - 2 \beta \nabla_\Sigma \mathcal{L} \\
\mu &\leftarrow \mu + \beta \Sigma (2 \nabla_\mu \mathcal{L} - \nabla_\alpha \mathcal{L}) \\
\alpha &\leftarrow \alpha + \beta \Sigma (\nabla_\alpha \mathcal{L} - \nabla_\mu \mathcal{L})
\end{align*}
\] (58) (59) (60)

Recall that the lower bound is

\[
\mathcal{L}(\lambda) = \mathbb{E}_{q(z)} \left[ -\frac{1}{2} \log \frac{1}{2\pi} + \log \left( \frac{\alpha^T \Sigma^{-1} \alpha}{2\pi} \right) - \frac{1}{\alpha^T \Sigma^{-1} \alpha} + (d + 1) \right] - \mathbb{E}_{\text{Exp}([\alpha, \Sigma], \lambda)} \left[ \log \phi \left( z_2 - \frac{1}{\sqrt{\alpha^T \Sigma^{-1} \alpha}} \right) \right]
\] (61)

For the prior term, there is a closed-form expression for gradient computation.

\[
\mathbb{E}_{q(z)} \left[ \log \mathcal{N}(z; 0, \delta^{-1} I) \right] = -\frac{d}{2} \log(2\pi) + \frac{d \delta}{2} - \frac{\delta}{2} (2\alpha^T \alpha + 2\mu^T \alpha + \text{Tr}(\Sigma) + \mu^T \mu)
\]

It is easy to show that the gradients about the prior term are

\[
\begin{align*}
\nabla_{\mu}^{\text{prior}} &= -\delta (\mu + \alpha) \\
\nabla_{\alpha}^{\text{prior}} &= -\delta (2\alpha + \mu) \\
\nabla_{\Sigma}^{\text{prior}} &= -\frac{\delta}{2} I
\end{align*}
\]

For the entropy term, it can be expressed as follows.

\[
\mathbb{E}_{q(z)} \left[ -\log q(z) \right] = \frac{1}{2} \left\{ \log \det(2\pi \Sigma) + \log \left( \frac{\alpha^T \Sigma^{-1} \alpha}{2\pi} \right) - \frac{1}{\alpha^T \Sigma^{-1} \alpha} + (d + 1) \right\} - \mathbb{E}_{\text{Exp}([\alpha, \Sigma], \lambda)} \left[ \log \phi \left( z_2 - \frac{1}{\sqrt{\alpha^T \Sigma^{-1} \alpha}} \right) \right]
\] (61)

Using the expression in (61), the gradients of the entropy term are given as follows:

\[
\begin{align*}
\nabla_{\mu}^{\text{entropy}} &= 0 \\
\nabla_{\alpha}^{\text{entropy}} &= \frac{\Sigma^{-1} \alpha}{\alpha^T \Sigma^{-1} \alpha} + \Sigma^{-1} \alpha \left( \frac{\alpha^T \Sigma^{-1} \alpha}{2} \right)^2 - \mathbb{E}_{\text{Exp}([\alpha, \Sigma], \lambda)} \left[ \frac{\exp \left( -\frac{t^2}{2} - \log \phi(t) \right)}{\sqrt{2\pi}} \left( w + \frac{1}{\alpha^T \Sigma^{-1} \alpha} \right) \left( \frac{\Sigma^{-1} \alpha}{\sqrt{\alpha^T \Sigma^{-1} \alpha}} \right) \right]
\end{align*}
\] (62)

\[
\begin{align*}
\nabla_{\Sigma}^{\text{entropy}} &= \frac{\Sigma^{-1} - \Sigma^{-1} \alpha \alpha^T \Sigma^{-1} - \Sigma^{-1} \alpha \alpha^T \Sigma^{-1}}{2 \alpha^T \Sigma^{-1} \alpha} + \frac{\exp \left( -\frac{t^2}{2} - \log \phi(t) \right)}{\sqrt{2\pi}} \left( w + \frac{1}{\alpha^T \Sigma^{-1} \alpha} \right) \left( \frac{\Sigma^{-1} \alpha \alpha^T \Sigma^{-1}}{2 \sqrt{\alpha^T \Sigma^{-1} \alpha}} \right)
\end{align*}
\] (63)

where $t = z_2 + \frac{w \alpha^T \Sigma^{-1} \alpha}{\sqrt{\alpha^T \Sigma^{-1} \alpha}}$ and the expectations involve 2d integrations, which can be computed by Gauss-Hermite quadrature and Gauss-Laguerre quadrature.
The remaining thing is to compute the gradients about $E_{q(z)}[f_n(z)]$. To compute the gradients, the reparameterization trick can be used. However, we can use the extended Bonnet’s and Price’s theorems (Lin et al., 2019). Assuming that $f_n(z)$ satisfies the assumptions needed for these two theorems, we obtain the following gradient expression:

$$
g_1^n := \nabla_\mu E_{q(z)}[f_n(z)] = E_{q(z)}[\nabla_z f_n(z)] \approx \nabla_z f_n(z)$$

$$
g_2^n := \nabla_\lambda E_{q(z)}[f_n(z)]$

$$
= E_{q(z)}[u(z)\nabla_z f_n(z)] + vE_{N(\mu,\Sigma)}[\nabla_z f_n(\hat{z})] \approx u(z)\nabla_z f_n(z) + v\nabla_{\hat{z}} f_n(\hat{z})$$

$$
g_3^n := 2\nabla_{\Sigma} E_{q(z)}[f_n(z)] = E_{q(z)}[\nabla^2_z f_n(z)] \approx \nabla^2_z f_n(z)$$

where $v = \frac{1}{(\alpha^2 + \Sigma^{-1})}$, $u(z) := \frac{(z - \mu)^T \Sigma^{-1}}{\alpha^2\Sigma^{-1}}$, and $w \sim \text{Exp}(w|1)$, $\hat{z} \sim N(\hat{z}|\mu, \Sigma)$, $z = \hat{z} + w\alpha$.

Putting together, we can express the gradients in the following form, which will be used for deriving the extended variational Adam update.

$$
\nabla_\mu L(\lambda) = -\sum_{n=1}^N \left( \frac{g_1^n - g_{\mu\text{entropy}}}{\text{entropy}} \right) - \delta(\mu + \alpha) = -\sum_{n=1}^N \left( \frac{g_1^n}{\text{entropy}} \right) - \delta(\mu + \alpha) \tag{65}
$$

$$
\nabla_\alpha L(\lambda) = -\sum_{n=1}^N \left( \frac{g_2^n - g_{\alpha\text{entropy}}}{\text{entropy}} \right) - \delta(2\alpha + \mu) = -\sum_{n=1}^N \left( \frac{g_2^n}{\text{entropy}} \right) - \delta(2\alpha + \mu) \tag{66}
$$

$$
\nabla_\Sigma L(\lambda) = -\frac{1}{2} \sum_{n=1}^N \left( \frac{g_3^n - 2g_{\Sigma\text{entropy}}}{\text{entropy}} \right) - \frac{\delta}{2} I + \frac{1}{2} (\Sigma^{-1} - \Sigma^{-1}) = -\frac{1}{2} \sum_{n=1}^N \left( \frac{g_3^n - 2g_{\Sigma\text{entropy}}}{\text{entropy}} \right) - \frac{\delta}{2} I + \frac{1}{2} \Sigma^{-1} \tag{67}
$$

Similarly, for stochastic approximation, we can sub-sampling a data point $n$ and use MC samples to approximate $g_1^n$, $g_2^n$, and $g_3^n$. Plugging these stochastic gradients into (58)-(60), we obtain the NGD update:

$$
\Sigma^{-1} \leftarrow (1 - \beta)\Sigma^{-1} + \beta(\delta I + Ng_3^n)$$

$$
\mu \leftarrow \mu - \beta \Sigma(N(2g_1^n - g_{\mu\text{entropy}}) + \delta\mu)$$

$$
\alpha \leftarrow \alpha - \beta \Sigma(N(g_2^n - g_{\alpha\text{entropy}}) + \delta\alpha)$$

**G. Multivariate Normal Inverse-Gaussian Distribution**

We consider the following mixture distribution (Barndorff-Nielsen, 1997), which is a Gaussian variance-mean mixture distribution. For simplicity, we assume $\lambda$ is known.

$$
q(w, z) = N(z|\mu + w\alpha, w\Sigma)\text{InvGauss}(w|1, \lambda)
$$

where $\text{InvGauss}(w|1, \lambda) = \left( \frac{\lambda}{2\pi\pi^w} \right)^{\frac{1}{2}} \exp \left\{ -\frac{1}{2} (w + w^{-1}) + \lambda \right\}$ denotes the inverse Gaussian distribution.
Lemma 15 The marginal distribution is

\[ q(z) = \frac{\lambda^{\frac{1}{2}}}{(2\pi)^{\frac{d+1}{2}}} \det(\Sigma)^{-1/2} \exp \left[ (z - \mu)^T \Sigma^{-1} \alpha + \lambda \right] \]

\[ \frac{2K_{\frac{d+1}{2}} \left( \sqrt{(\alpha^T \Sigma^{-1} \alpha + \lambda) \left( (z - \mu)^T \Sigma^{-1} (z - \mu) + \lambda \right)} \right)}{\sqrt{(\alpha^T \Sigma^{-1} \alpha + \lambda) \left( (z - \mu)^T \Sigma^{-1} (z - \mu) + \lambda \right)}} \]

where \( K_v(x) \) denotes the modified Bessel function of the second kind.

Proof: By definition, we can compute the marginal distribution as follows.

\[ q(z) = \int_0^{+\infty} q(z|w)q(w)dw \]

\[ = \int_0^{+\infty} \det(2\pi\Sigma)^{-1/2} \exp \left\{ -\frac{1}{2} \left[ (z - \mu - w\alpha)^T (w\Sigma)^{-1} (z - \mu - w\alpha) \right] \right\} \left( \frac{\lambda}{2\pi w^3} \right)^{1/2} \exp \left\{ -\frac{\lambda}{2} \left( w + \frac{1}{w} \right) + \lambda \right\} dw \]

By grouping all terms related to \( w \) together, we have

\[ = \frac{\lambda^\frac{1}{2}}{(2\pi)^{\frac{d+1}{2}}} \det(\Sigma)^{-1/2} \exp \left[ (z - \mu)^T \Sigma^{-1} \alpha + \lambda \right] \int_0^{+\infty} w^{-\frac{d+3}{2}} \exp \left\{ -\frac{1}{2} w \left( \alpha^T \Sigma^{-1} \alpha + \lambda + \frac{(z - \mu)^T \Sigma^{-1} (z - \mu) + \lambda}{w} \right) \right\} dw \]

By completing a generalized inverse Gaussian form, we have

\[ = \frac{\lambda^\frac{1}{2}}{(2\pi)^{\frac{d+1}{2}}} \det(\Sigma)^{-1/2} \exp \left[ (z - \mu)^T \Sigma^{-1} \alpha + \lambda \right] \frac{2K_{\frac{d+1}{2}} \left( \sqrt{(\alpha^T \Sigma^{-1} \alpha + \lambda) \left( (z - \mu)^T \Sigma^{-1} (z - \mu) + \lambda \right)} \right)}{\sqrt{(\alpha^T \Sigma^{-1} \alpha + \lambda) \left( (z - \mu)^T \Sigma^{-1} (z - \mu) + \lambda \right)}} \]

We obtain the last step by the fact that \( K_v(x) = K_{-v}(x) \)

Similarly, the sufficient statistics \( \phi(z, w) = \{ z/w, z, zwT/w \} \) and the natural parameter \( \lambda_z = \{ \Sigma^{-1} \mu, \Sigma^{-1} \alpha, -\frac{1}{2} \Sigma^{-1} \} \) can be read from \( q(z|w) = \mathcal{N}(z|\mu + w\alpha, w\Sigma) \). The joint distribution \( q(z, w) \) is a conditional EF because \( q(w) \) is an inverse Gaussian distribution with known parameters, which is an EF distribution. Likewise, we can show that the joint distribution is also a minimal conditional EF.

We can derive the expectation parameter shown below:

\[ m := \mathbb{E}_{\text{InvGauss}(w,\lambda_z) N(z|\mu + w\alpha, w\Sigma)} [w^{-1}z] = (1 + \lambda^{-1}) \mu + \alpha, \]

\[ m_{\alpha} := \mathbb{E}_{\text{InvGauss}(w,\lambda_z) N(z|\mu + w\alpha, w\Sigma)} [z] = \mu + \alpha, \]

\[ M := \mathbb{E}_{\text{InvGauss}(w,\lambda_z) N(z|\mu + w\alpha, w\Sigma)} [w^{-1}zzT] = (1 + \lambda^{-1}) \mu \mu^T + \alpha \alpha^T + \mu \alpha^T + \alpha \mu^T + \Sigma \]

The sufficient statistics, natural parameters, and expectation parameters are summarized below:

\[
\begin{bmatrix}
\frac{z}{w} \\
\frac{z}{w} \\
\frac{zz^T}{w}
\end{bmatrix} =
\begin{bmatrix}
\Sigma^{-1} \mu \\
\Sigma^{-1} \alpha \\
-\frac{1}{2} \Sigma^{-1}
\end{bmatrix} =
\begin{bmatrix}
(1 + \lambda^{-1}) \mu + \alpha \\
\mu + \alpha \\
(1 + \lambda^{-1}) \mu \mu^T + \alpha \alpha^T + \mu \alpha^T + \alpha \mu^T + \Sigma
\end{bmatrix}
\]
G.1. Derivation of the NGD Update

We consider the variational approximation using the normal inverse Gaussian distribution \( q(z|\lambda) \). We consider the same model as Appendix B.1 with a Gaussian-prior \( N(z|0, \delta^{-1}I) \) on \( z \). The lower bound is defined as below:

\[
L(\lambda) = E_{q(z|\lambda)} \left[ \sum_{n=1}^{N} \log p(D_n|z) + \log N(z|0, \delta^{-1}I) - \log q(z|\lambda) \right] = E_{q(z)} [-h(z)], \text{ where } h(z) := -\left[ \log \frac{N(z|0, \delta^{-1}I)}{q(z)} + \sum_{n} \log p(D_n|z) \right].
\]

Our goal is to compute the gradient of this ELBO with respect to the expectation parameters.

G.2. Natural Gradient for \( q(z|w) \)

Likewise, we do not need to compute these gradients with respect to the expectation parameters directly. The gradients can be computed in terms of \( \{\mu, \alpha, \Sigma\} \). Similarly, by the chain rule, we can express the following gradients with respect to the expectation parameters in terms of the gradients with respect to \( \mu, \alpha, \) and \( \Sigma \).

\[
\nabla_{\mu} L = \lambda \nabla_{\mu} L - \lambda \nabla_{\alpha} L - 2 (\nabla_{\Sigma} L) \mu \\
\nabla_{\alpha} L = (1 + \lambda) \nabla_{\alpha} L - \lambda \nabla_{\mu} L - 2 (\nabla_{\Sigma} L) \alpha \\
\n\nabla_{\Sigma} L = \nabla_{\Sigma} L
\]

By plugging the gradients into the update in (14) and then re-expressing the update in terms of \( \mu, \alpha, \Sigma \), we obtain the natural gradient update in terms of \( \mu, \alpha, \) and \( \Sigma \).

\[
\Sigma^{-1} \leftarrow \Sigma^{-1} - 2 \beta \nabla_{\Sigma} L \tag{68}
\]

\[
\mu \leftarrow \mu + \beta \Sigma (\lambda \nabla_{\mu} L - \lambda \nabla_{\alpha} L) \tag{69}
\]

\[
\alpha \leftarrow \alpha + \beta \Sigma (1 + \lambda) \nabla_{\alpha} L - \lambda \nabla_{\mu} L \tag{70}
\]

We can compute gradients with respect to \( \mu, \alpha, \) and \( \Sigma \) by the extended Bonnet’s and Price’s theorem (Lin et al., 2019). In Lin et al. (2019), they discuss the conditions of the target function \( h(z) \) when it comes to applying these theorems.

\[
\nabla_{\mu} L(\lambda) = -E_{q(z)} [\nabla_{z} h(z)] \approx -\nabla_{z} h(z) \\
\nabla_{\alpha} L(\lambda) = -E_{q(w,z)} [w \nabla_{z} h_n(z)] \approx -w \nabla_{z} h_n(z) \\
\quad = -E_{q(z)} [u(z) \nabla_{z} h_n(z)] \approx -u(z) \nabla_{z} h_n(z) \\
\nabla_{\Sigma} L(\lambda) = -\frac{1}{2} E_{q(z)} [w \nabla_{z}^2 h(z)] \approx -\frac{w}{2} \nabla_{z}^2 h(z). \\
\quad = -\frac{1}{2} E_{q(z)} [u(z) \nabla_{z}^2 h(z)] \approx -\frac{u(z)}{2} \nabla_{z}^2 h(z).
\]

where \( u(z) := \sqrt{\frac{(z-\mu)^T \Sigma^{-1} (z-\mu)+\lambda}{\alpha^T \Sigma^{-1} \alpha + \lambda}} K_{\alpha,\lambda} \frac{\sqrt{\left(\alpha^T \Sigma^{-1} \alpha + \lambda\right) \left((z-\mu)^T \Sigma^{-1} (z-\mu)+\lambda\right)}}{K_{\alpha,\lambda} \frac{\sqrt{\left(\alpha^T \Sigma^{-1} \alpha + \lambda\right) \left((z-\mu)^T \Sigma^{-1} (z-\mu)+\lambda\right)}}} \) and \( w \sim \text{InvGauss}(w|1, \lambda), z \sim N(z|\mu + w \alpha, \Sigma). \)

Directly calculating the ratio between the modified Bessel functions of the second kind is expensive and numerically unstable when \( \nu \) is large. However, the ratio between consecutive order has a tight and algebraic bound (Ruiz-Antolín & Segura, 2016) as given below. When \( \nu \in \mathcal{R} \) and \( \nu \geq \frac{1}{2} \), the bound of the ratio is

\[
D_{2\nu - 1}(\nu, x) \leq \frac{K_{\nu - 1}(x)}{K_{\nu}(x)} \leq D_{\nu}(\nu, x)
\]
where function $D_\alpha(v, x)$ is defined as below.

$$D_\alpha(v, x) := \frac{x}{\psi_\alpha(v, x) + \sqrt{(\psi_\alpha(v, x))^2 + x^2}}$$

$$\psi_\alpha(v, x) := (v - \frac{1}{2}) - \frac{\tau_\alpha(v)}{2\sqrt{(\tau_\alpha(v))^2 + x^2}}, \ \tau_\alpha(v) := v - \frac{\alpha + 1}{2}$$

For natural number $v \in \mathbb{N}$, a tighter bound (see Eq (3.10) at Yang & Chu (2017)) with higher computation cost can be used, where we make use of the following relationship due to Eq (72) and (73).

$$\frac{K_{v-1}(x)}{K_v(x)} = \frac{K_{v+1}(x)}{K_v(x)} - \frac{2v}{x}$$

To compute the ratio, we propose to use the following approximation when $v \geq \frac{1}{2}$. A similar approach to approximate the ratio between two modified Bessel functions of the first kind is used in Oh et al. (2019) and Kumar & Tsvetkov (2018).

$$\frac{K_{v-1}(x)}{K_v(x)} \approx \frac{D_{2v-1}(v, x) + D_0(v, x)}{2} \quad (71)$$

Now, we discuss how to compute $\nabla_x \log K_v(x)$ and $\nabla_x^2 \log K_v(x)$. The first term appears when we compute $\nabla_x h(z)$. Similarly, the second term appears when we compute $\nabla_x^2 h(z)$.

First, we make use of the recurrence forms of the modified Bessel function of the second kind for $v \in \mathcal{R}$ (see page 20 at Culham (2004)).

$$\nabla_x K_v(x) = -K_{v-1}(x) - \frac{v}{x} K_v(x) \quad (72)$$

$$\nabla_x K_v(x) = \frac{v}{x} K_v(x) - K_{v+1}(x) \quad (73)$$

Using these recurrence forms, we have

$$\frac{\nabla_x K_v(x)}{K_v(x)} = -\frac{K_{v-1}(x)}{K_v(x)} - \frac{v}{x} \quad (74)$$

Furthermore, we have the following result due to the recurrence forms.

$$\nabla_x^2 K_v(x) = \nabla_x \left[ \nabla_x K_v(x) \right]$$

$$= -\nabla_x K_{v-1}(x) - \frac{v}{x} \nabla_x K_v(x) + \frac{v}{x^2} K_v(x)$$

$$= -\nabla_x K_{v-1}(x) - \frac{v}{x} \left[ -K_{v-1}(x) - \frac{v}{x} K_v(x) \right]$$

$$= -\frac{v - 1}{x} \nabla_x K_{v-1}(x) + \frac{v + x^2}{x^2} K_v(x) - \frac{v}{x} \nabla_x K_v(x)$$

$$= \frac{1}{x} K_{v-1}(x) + \frac{v + x^2}{x^2} K_v(x)$$
Fast and Simple Natural-Gradient Variational Inference with Mixture of Exponential-family Approximations

which implies that

\[
\frac{\nabla^2 K_v(x)}{K_v(x)} = \frac{1}{x} K_{v-1}(x) + \frac{v + x^2 + v^2}{x^2}
\]  

(75)

Using Eq (74) and (75), we have

\[
\nabla_x \log K_v(x) = \nabla_x K_v(x)
\]

\[
= \frac{K_{v-1}(x)}{K_v(x)} - \frac{v}{x}
\]

\[
\nabla^2_x \log K_v(x) = \nabla_x \left[ \frac{\nabla_x K_v(x)}{K_v(x)} \right]
\]

\[
= \frac{1}{x} K_{v-1}(x) + \frac{v + x^2 + v^2}{x^2} - \left( \frac{K_{v-1}(x)}{K_v(x)} - \frac{v}{x} \right)^2
\]

\[
= 1 - 2v \left( \frac{K_{v-1}(x)}{K_v(x)} \right) - \left( \frac{K_{v-1}(x)}{K_v(x)} \right)^2 + \frac{v}{x^2} + 1
\]

where the ratio can be approximated by Eq (71).

H. Multivariate Symmetric Normal Inverse-Gaussian Distribution

The symmetric normal inverse-Gaussian distribution is a scale mixture distribution. A difference between the distribution at Appendix G is shown in red. Such difference allows this distribution to have heavy tails.

\[
q(w, z) = \mathcal{N}(z|\mu, w^{-1} \Sigma) \operatorname{InvGauss}(w|1, \lambda)
\]

where we assume \(\lambda\) is fixed for simplicity and \(\operatorname{InvGauss}(w|1, \lambda) = \left( \frac{\lambda}{2\pi w^3} \right)^{1/2} \exp \left\{ -\frac{\lambda}{2} \left( w + w^{-1} \right) \right\} \).

Similarly, we can show that the marginal distribution is

\[
q(z) = \frac{\lambda^{1/2}}{(2\pi)^{d+1/2} \det(\Sigma)^{1/2}} \exp(\lambda) \frac{2K_{d+1}}{(2\pi)^{d+1/2}} \left( \frac{\lambda (z - \mu)^T \Sigma^{-1} (z - \mu) + \lambda}{(z - \mu)^T \Sigma^{-1} (z - \mu) + \lambda} \right) \]

Furthermore, the mixture distribution is a minimal conditional EF distribution. The sufficient statistics, natural parameters, and expectation parameters are summarized below:

\[
\begin{bmatrix}
w z \\
w z z^T
\end{bmatrix} = \begin{bmatrix}
\Sigma^{-1} \mu \\
-\frac{1}{2} \Sigma^{-1}
\end{bmatrix} + \begin{bmatrix}
\mu \\
\mu \mu^T + \Sigma
\end{bmatrix}
\]

Likewise, we can derive the natural-gradient update in terms of \(\mu\) and \(\Sigma\) as shown below.

\[
\Sigma^{-1} \leftarrow \Sigma^{-1} - 2\beta \nabla_\Sigma \mathcal{L}
\]

\[
\mu \leftarrow \mu + \beta \nabla_\mu \mathcal{L}
\]

Now, we discuss the gradient computation of the following lower bound.

\[
\mathcal{L}(\lambda) = \mathbb{E}_{q(z)} \left[ \sum_{n=1}^{N} \log p(D_n|z) + \log \mathcal{N}(z|0, \delta^{-1} \mathbf{I}) - \log q(z|\lambda) \right]
\]
For the prior term, we have
\[
E_{q(z)} \left[ \log \mathcal{N}(z|0, \delta^{-1}I) \right] = - \frac{d}{2} \log(2\pi) + \frac{d\delta}{2} - \frac{\delta}{2} (\mu^T \mu + (1 + \lambda^{-1}) \text{Tr}(\Sigma))
\] (76)

Due to Eq (76), the closed-form gradients are given below.
\[
g^\text{prior}_\mu = -\delta \mu \\
g^\text{prior}_\Sigma = -\frac{\delta (1 + \lambda^{-1})}{2} I
\]

In this example, we can re-express the entropy term as below.
\[
E_{q(z)} \left[ -\log q(z) \right] = \frac{(d + 1) \log(2\pi)}{2} + \frac{\log \det(\Sigma)}{2} - \lambda - \frac{d + 1}{4} \log(\lambda) - E_{\text{InvGauss}(w|1, \lambda)^2}(z_i) \left[ \log \left( \frac{2K_{d-1} \left( \sqrt{\lambda (w^{-1}z_1 + \lambda)} \right)}{(w^{-1}z_1 + \lambda)^{\frac{d-1}{2}}} \right) \right]
\] (77)

where \(\chi^2(z_1|d)\) denotes the chi-squared distribution with \(d\) degrees of freedom. The expectation can be computed by the inverse Gaussian quadrature (Choi et al., 2018) and the generalized Gauss-Laguerre quadrature.

By Eq (77), the closed-form gradients of the entropy term are shown below.
\[
g^\text{entropy}_\mu = 0 \\
g^\text{entropy}_\Sigma = \frac{\Sigma^{-1}}{2}
\]

The remaining step is to compute the gradients about \(E_{q(z)} \left[ f_n(z) \right]\). To compute the gradients, we use the extended the Bonnet’s and Price’s theorems (Lin et al., 2019). Assuming that \(f_n(z)\) satisfies the assumptions needed for these two theorems, we obtain the following gradient expression:
\[
g_n^\mu := \nabla_\mu E_{q(z)} \left[ f_n(z) \right] = E_{q(z)} \left[ \nabla_\mu f_n(z) \right] \approx \nabla_\mu f_n(z) \\
g_n^\Sigma := 2 \nabla_\Sigma E_{q(z)} \left[ f_n(z) \right] \\
= E_{q(z)} \left[ u(z) \nabla_\Sigma^2 f_n(z) \right] \approx u(z) \nabla_\Sigma^2 f_n(z) \\
= E_{q(w,z)} \left[ u(w) \nabla_\Sigma^2 f_n(z) \right] \approx w^{-1} \nabla_\Sigma^2 f_n(z)
\]

where \(u(z) := \sqrt{(z-\mu)^T \Sigma^{-1} (z-\mu) + \lambda} K_{\frac{d-1}{2}} \left( \sqrt{\frac{\lambda (z-\mu)^T \Sigma^{-1} (z-\mu) + \lambda}{(z-\mu)^T \Sigma^{-1} (z-\mu) + \lambda}} \right)\), where the ratio between the Bessel functions

\(K_{\frac{d-1}{2}} \left( \sqrt{\frac{\lambda (z-\mu)^T \Sigma^{-1} (z-\mu) + \lambda}{(z-\mu)^T \Sigma^{-1} (z-\mu) + \lambda}} \right)\)

can be approximated by Eq (71) when \(d \geq 2\), and \(w \sim \text{InvGauss}(w|1, \lambda), z \sim \mathcal{N}(z|\mu, w^{-1} \Sigma)\).

Putting together, we can express the gradients in the following form:
\[
\nabla_\mu \mathcal{L}(\lambda) = - \sum_{n=1}^N g_n^\mu - \delta \mu \\
\nabla_\Sigma \mathcal{L}(\lambda) = - \frac{1}{2} \sum_{n=1}^N g_n^\Sigma - \frac{\delta (1 + \lambda^{-1})}{2} I + \frac{1}{2} \Sigma^{-1}
\] (78) (79)

Similarly, for stochastic approximation, we can sub-sampling a data point \(n\) and use MC samples to approximate \(g_n^\mu\) and \(g_n^\Sigma\). Plugging these stochastic gradients into
\[
\Sigma^{-1} \leftarrow (1 - \beta) \Sigma^{-1} + \beta (1 + \lambda^{-1}) I + N g_n^\mu \\
\mu \leftarrow \mu - \beta \Sigma (N g_n^\mu + \delta \mu)
\]
I. Matrix-Variate Gaussian Distribution

We first show that MVG is a multi-linear exponential-family distribution.

**Lemma 16** Matrix Gaussian distribution is a member of the multi-linear exponential family.

**Proof:** Let $\Lambda_1 = W$, $\Lambda_2 = U^{-1}$, and $\Lambda_3 = V^{-1}$. The distribution on $Z \in \mathcal{R}^{d \times p}$ can be expressed as follows.

$$
\mathcal{MNV}(Z|W, U, V) = (2\pi)^{-dp/2} \exp \left[ -\frac{1}{2} \text{Tr} \left( V^{-1}(Z - W)^T U^{-1}(Z - W) \right) - \left( \frac{d}{2} \log \det(V) + \frac{p}{2} \log \det(U) \right) \right]
$$

We will now express the gradients in terms of the gradient of the function $\phi_1, \phi_2,$ and $\phi_3$ from the multi-linear function

$$
f(Z, \Lambda) := \text{Tr} \left( \Lambda_3 \left( -\frac{1}{2}Z + \Lambda_1 \right)^T \Lambda_2 Z \right).
$$

For example, we can obtain function $\phi_1$ from $f(Z, \Lambda)$ as shown below:

$$
f(Z, \Lambda) = \langle \Lambda_1, \frac{\Lambda_2 Z \Lambda_3}{\phi_1(Z, \Lambda_{-1})} \rangle - \frac{1}{2} \text{Tr} \left( \Lambda_3 Z^T \Lambda_2 Z \right).
$$

Similarly, we can obtain functions $\phi_2$ and $\phi_3$. The corresponding expectation parameters of the Matrix Gaussian distribution can then be derived as below:

$$
M_1 = \mathbb{E}_{\mathcal{MNV}(z|W,U,V)} \left[ \Lambda_2 Z \Lambda_3 \right] = \Lambda_2 \Lambda_1 \Lambda_3
$$

$$
M_2 = \mathbb{E}_{\mathcal{MNV}(z|W,U,V)} \left[ -\frac{1}{2} Z \Lambda_3 Z^T + Z \Lambda_3 \Lambda_1^T \right] = \frac{1}{2} \left( \Lambda_1 \Lambda_3 \Lambda_1^T - p \Lambda_2^{-1} \right)
$$

$$
M_3 = \mathbb{E}_{\mathcal{MNV}(z|W,U,V)} \left[ -\frac{1}{2} Z^T \Lambda_2 Z + \Lambda_1^T \Lambda_2 Z \right] = \frac{1}{2} \left( \Lambda_1^T \Lambda_2 \Lambda - d \Lambda_3^{-1} \right)
$$

We can then compute the gradient with respect to the expectation parameters using chain-rule:

$$
\nabla_{M_i} \mathbb{E}_{\mathcal{M}(z|\lambda)} \left[ h(Z) \right] = (\Lambda_2)^{-1} \nabla_W \mathbb{E}_{\mathcal{MNV}(z|W,U,V)} \left[ h(Z) \right] (\Lambda_3)^{-1}
$$

$$
\nabla_{M_2} \mathbb{E}_{\mathcal{M}(z|\lambda)} \left[ h(Z) \right] = -\frac{2}{p} \nabla_U \mathbb{E}_{\mathcal{MNV}(z|W,U,V)} \left[ h(Z) \right]
$$

$$
\nabla_{M_3} \mathbb{E}_{\mathcal{M}(z|\lambda)} \left[ h(Z) \right] = -\frac{2}{d} \nabla_V \mathbb{E}_{\mathcal{MNV}(z|W,U,V)} \left[ h(Z) \right]
$$

We will now express the gradients in terms of the gradient of the function $h(Z)$. This leads to a simple update because gradient of $h(Z)$ can be obtained using automatic gradients (or backpropagation when using a neural network). Let $z = \text{vec}(Z)$ and $Z = \text{Mat}(z)$. The distribution can be re-expressed as a multivariate Gaussian distribution $\mathcal{N}(z|\mu, \Sigma)$, where $\mu = \text{vec}(W \Sigma U)$, $\Sigma = V \otimes U$, and $\otimes$ denotes the Kronecker product. Furthermore, the lower bound can be re-expressed as $\mathbb{E}_{\mathcal{N}(z|\mu, \Sigma)} \left[ -\hat{h}(z) \right]$, where $\hat{h}(z) = h(Z)$. We make use of the Bonnet’s and Price’s theorems (Oppen & Archambeau, 2009):

$$
\nabla_{\mu} \mathbb{E}_{\mathcal{N}(z|\mu, \Sigma)} \left[ \hat{h}(z) \right] = \mathbb{E}_{\mathcal{N}(z|\mu, \Sigma)} \left[ \nabla_{\mu} \hat{h}(z) \right]
$$

$$
\nabla_{\Sigma} \mathbb{E}_{\mathcal{N}(z|\mu, \Sigma)} \left[ \nabla_{z} \hat{h}(z) \right] = \frac{1}{2} \mathbb{E}_{\mathcal{N}(z|\mu, \Sigma)} \left[ \nabla_{z} \hat{h}(z) \right]
$$
These identities can be used to express the gradient with respect to the expectation parameters in terms of the gradient with respect to $Z$:

$$\nabla_W \mathbb{E}_{MN(Z|W,U,V)} [h(Z)] = \text{Mat} \left( \mathbb{E}_{N(\mu,\Sigma)} \left[ \nabla_z \hat{h}(z) \right] \right)$$

$$= \mathbb{E}_{MN(Z|W,U,V)} [\nabla_Z h(Z)]$$

$$\nabla_U \mathbb{E}_{MN(Z|W,U,V)} [h(Z)] = (\nabla_U \Sigma) \nabla_Z \mathbb{E}_{N(\mu,\Sigma)} \left[ \nabla_z \hat{h}(z) \right]$$

$$= \frac{1}{2} (\nabla_U \Sigma) \mathbb{E}_{N(\mu,\Sigma)} \left[ \nabla_z^2 \hat{h}(z) \right]$$

$$\approx \frac{1}{2} (\nabla_U \Sigma) \mathbb{E}_{N(\mu,\Sigma)} \left[ \nabla_z \hat{h}(z) \nabla_z \hat{h}(z)^T \right]$$

$$= \frac{1}{2} \mathbb{E}_{MN(Z|W,U,V)} [\nabla_Z h(Z) \nabla_Z h(Z)^T]$$

$$\nabla_V \mathbb{E}_{MN(Z|W,U,V)} [h(Z)] = (\nabla_V \Sigma) \nabla_Z \mathbb{E}_{N(\mu,\Sigma)} \left[ \nabla_z \hat{h}(z) \right]$$

$$= \frac{1}{2} (\nabla_V \Sigma) \mathbb{E}_{N(\mu,\Sigma)} \left[ \nabla_z^2 \hat{h}(z) \right]$$

$$\approx \frac{1}{2} (\nabla_V \Sigma) \mathbb{E}_{N(\mu,\Sigma)} \left[ \nabla_z \hat{h}(z) \nabla_z \hat{h}(z)^T \right]$$

$$= \frac{1}{2} \mathbb{E}_{MN(Z|W,U,V)} [\nabla_Z h(Z)^T \nabla_Z h(Z)] .$$

To avoid computation of the Hessian, we have used the Gauss-Newton approximation (Khan et al., 2018) in Eq (80) and Eq. (81).

We choose the step-size as $\beta = \{ \beta_1, p\beta_2, d\beta_2 \}$. The update with the Gauss-Newton approximation can be expressed as

$$\Lambda_1 \leftarrow \Lambda_1 - \beta_1 (\Lambda_2)^{-1} \mathbb{E}_{MN(Z|W,U,V)} [\nabla_Z h(Z)] (\Lambda_3)^{-1}$$

$$\Lambda_2 \leftarrow \Lambda_2 + \beta_2 \mathbb{E}_{MN(Z|W,U,V)} [\nabla_Z h(Z) \nabla_Z h(Z)^T]$$

$$\Lambda_3 \leftarrow \Lambda_3 + \beta_2 \mathbb{E}_{MN(Z|W,U,V)} [\nabla_Z h(Z)^T \nabla_Z h(Z)]$$

We can re-express these in terms of $\{ W, U^{-1}, V^{-1} \}$ to get the final updates:

$$W \leftarrow W - \beta_1 U \mathbb{E}_{MN(Z|W,U,V)} [\nabla_Z h(Z)] V$$

$$(U)^{-1} \leftarrow (U)^{-1} + \beta_2 \mathbb{E}_{MN(Z|W,U,V)} [\nabla_Z h(Z) \nabla_Z h(Z)^T]$$

$$(V)^{-1} \leftarrow (V)^{-1} + \beta_2 \mathbb{E}_{MN(Z|W,U,V)} [\nabla_Z h(Z)^T \nabla_Z h(Z)]$$

### J. Extensions to Variational Adam

For simplicity, we consider a case when variational parameters of $q(w|\lambda_w)$ are fixed. Since $\lambda_w$ is fixed, using the same derivation as Khan et al. (2018), we obtain the following natural-gradient update with the natural momentum ($0 \leq m < 1$).

$$\lambda_{z}^{t+1} = \frac{1}{1-m} \lambda_{z}^{t} - \frac{m}{1-m} \lambda_{z}^{t-1} + \frac{\beta}{1-m} \nabla_{m_z} \mathcal{L}(\lambda_z)$$

We assume the model prior is a Gaussian prior $p(z) = \mathcal{N}(z|0, \delta^{-1}I)$ to derive extensions of the variational Adam update, where the variational distribution is a Gaussian mixture distribution such as skew Gaussian, exponentially modified Gaussian, symmetric normal inverse-Gaussian, and Student’s t-distribution.
J.1. Extension for Skew Gaussian

Re-expressing the update (82) in terms of $\mu$, $\alpha$, $\Sigma$ (the same derivation as Khan et al. (2018)), we obtain the following update:

$$
\Sigma_{t+1}^{-1} = \Sigma_t^{-1} - 2 \frac{\beta}{1-m} \nabla \Sigma_t \mathcal{L} + \frac{m}{1-m} (\Sigma_t^{-1} - \Sigma_{t-1}^{-1})
$$

$$
\mu_{t+1} = \mu_t + \frac{\beta}{1-m} \Sigma_t \nabla \mu_t \mathcal{L} - \frac{c}{1-c^2} \nabla \alpha_t \mathcal{L} + \frac{m}{1-m} \Sigma_{t+1} \Sigma_{t-1}^{-1} (\mu_t - \mu_{t-1})
$$

$$
\alpha_{t+1} = \alpha_t + \frac{\beta}{1-m} \Sigma_t \nabla \alpha_t \mathcal{L} - \frac{c}{1-c^2} \nabla \mu_t \mathcal{L} + \frac{m}{1-m} \Sigma_{t+1} \Sigma_{t-1}^{-1} (\alpha_t - \alpha_{t-1})
$$

where we use a skew Gaussian distribution as the variational distribution, $\nabla \mu_t \mathcal{L}$, $\nabla \alpha_t \mathcal{L}$, and $\nabla \Sigma_t \mathcal{L}$ are defined at (53)-(55).

We make use of the same approximations as Khan et al. (2018) such as the square root approximation, $\Sigma_{t-1} \approx \Sigma_t$, and a diagonal covariance structure in $\Sigma$ to obtain an extension of the variational skew-Adam update. Recall that $g_\alpha^{\text{entropy}}$ and $g_\Sigma^{\text{entropy}}$ are defined at (51) and (52) and $c = \sqrt{\frac{2}{\pi}}$.

Using the same algebra manipulation used in Khan et al. (2018), we obtain the variational Adam update with Gaussian prior $p(z) = \mathcal{N}(z|\mathbf{0}, \delta^{-1} \mathbf{I})$, where $\Sigma^{-1} = \text{Diag}(Ns + \delta)$, $v = \frac{c}{(1+\alpha^2 \Sigma^{-1} \alpha)}$, and $u(z) = \frac{(z-\mu)^T \Sigma^{-1} \alpha}{1+\alpha^2 \Sigma^{-1} \alpha}$.

**Skew Gaussian extension**

1: while not converged do
2: \[ \hat{z} \leftarrow \mu + \sigma \circ \epsilon, \text{ where } \epsilon \sim \mathcal{N}(0, \mathbf{I}), \sigma \leftarrow 1/\sqrt{Ns + \delta} \]
3: \[ z \leftarrow \hat{z} + |w| \alpha, \text{ where } w \sim \mathcal{N}(0, 1) \]
4: Randomly sample a data example $D_i$
5: \[ g_\mu \leftarrow -\nabla \log p(D_i | z) \]
6: \[ \text{option I: } \hat{g}_\alpha \leftarrow -|w| \nabla \log p(D_i | z) \]
7: \[ \text{option II: } \hat{g}_\alpha \leftarrow -[v \nabla \log p(D_i | \hat{z}) + u(z) \nabla \log p(D_i | z)] \]
8: \[ g_\alpha \leftarrow \hat{g}_\alpha - g_\alpha^{\text{entropy}} / N \]
9: \[ g_s \leftarrow g_\mu \odot g_\mu - \text{diag}(2g_\Sigma^{\text{entropy}}) / N + (s + \delta / N) \]
10: \[ m_\mu \leftarrow g_\mu \cdot \nabla \mathcal{L} \leftarrow (1 - \gamma_1) \left( \frac{g_\mu - g_\Sigma^{\text{entropy}}} {1-c^2} \right) + \delta \mu / N \]
11: \[ m_\alpha \leftarrow g_\alpha \cdot \nabla \mathcal{L} \leftarrow (1 - \gamma_1) \left( \frac{g_\alpha - g_\Sigma^{\text{entropy}}} {1-c^2} \right) + \delta \alpha / N \]
12: \[ s \leftarrow g_\Sigma \odot s + (1 - \gamma_2) g_s \]
13: \[ \hat{m}_\mu \leftarrow m_\mu / (1 - \gamma_1^2), \quad \hat{m}_\alpha \leftarrow m_\alpha / (1 - \gamma_1^2), \quad \hat{s} \leftarrow (s + \delta / N) / (1 - \gamma_2^2) \]
14: \[ \mu \leftarrow \mu - \beta \hat{m}_\mu / \sqrt{s}, \quad \alpha \leftarrow \alpha - \beta \hat{m}_\alpha / \sqrt{s} \]
15: \[ t \leftarrow t + 1 \]
16: end while

J.2. Extension for Exponentially Modified Gaussian

Similarly, re-expressing the update (82) in terms of $\mu$, $\alpha$, $\Sigma$, we obtain the following update:

$$
\Sigma_{t+1}^{-1} = \Sigma_t^{-1} - 2 \frac{\beta}{1-m} \nabla \Sigma_t \mathcal{L} + \frac{m}{1-m} (\Sigma_t^{-1} - \Sigma_{t-1}^{-1})
$$

$$
\mu_{t+1} = \mu_t + \frac{\beta}{1-m} \Sigma_t \nabla \mu_t \mathcal{L} - \frac{c}{1-c^2} \nabla \alpha_t \mathcal{L} + \frac{m}{1-m} \Sigma_{t+1} \Sigma_{t-1}^{-1} (\mu_t - \mu_{t-1})
$$

$$
\alpha_{t+1} = \alpha_t + \frac{\beta}{1-m} \Sigma_t \nabla \alpha_t \mathcal{L} - \frac{c}{1-c^2} \nabla \mu_t \mathcal{L} + \frac{m}{1-m} \Sigma_{t+1} \Sigma_{t-1}^{-1} (\alpha_t - \alpha_{t-1})
$$

where we use an exponentially modified Gaussian distribution as the variational distribution, $\nabla \mu_t \mathcal{L}$, $\nabla \alpha_t \mathcal{L}$, and $\nabla \Sigma_t \mathcal{L}$ are defined at (65)-(67).

Likewise, we can obtain the variational Adam update with Gaussian prior $p(z) = \mathcal{N}(z|\mathbf{0}, \delta^{-1} \mathbf{I})$ as shown below, where $g_\alpha^{\text{entropy}}$ and $g_\Sigma^{\text{entropy}}$ are defined at (63) and (64), $\Sigma^{-1} = \text{Diag}(Ns + \delta)$, $v = \frac{1}{(\alpha^2 \Sigma^{-1} \alpha)}$, and $u(z) = \frac{(z-\mu)^T \Sigma^{-1} \alpha}{\alpha^2 \Sigma^{-1} \alpha}$.
### Exponentially Modified Gaussian extension

1: while not converged do  
2: \( \hat{z} \leftarrow \mu + \sigma \circ \epsilon, \) where \( \epsilon \sim \mathcal{N}(0, I), \sigma \leftarrow 1/\sqrt{Ns + \delta} \)  
3: \( z \leftarrow \hat{z} + w\alpha, \) where \( w \sim \text{Exp}(1) \)  
4: Randomly sample a data example \( D_i \)  
5: \( g_\alpha \leftarrow -\nabla \log p(D_i|z) \)  
6: **option I:** \( g_\alpha \leftarrow -w\nabla \log p(D_i|z) \)  
7: **option II:** \( g_\alpha \leftarrow -[v\nabla \log p(D_i|\hat{z}) + u(z)\nabla \log p(D_i|z)] \)  
8: \( g_\alpha \leftarrow \bar{g}_\alpha - g_\text{entropy} / N \)  
9: \( g_\alpha \leftarrow g_\mu \circ g_\alpha - \text{diag}(2g_\text{entropy}) / N + (s + \delta) / N \)  
10: \( m_\mu \leftarrow \gamma_1 m_\mu + (1 - \gamma_1) (2g_\mu - g_\alpha + \delta \mu / N) \)  
11: \( m_\alpha \leftarrow \gamma_1 m_\alpha + (1 - \gamma_1) (g_\alpha - g_\mu + \delta \alpha / N) \)  
12: \( s \leftarrow \gamma_2 s + (1 - \gamma_2) g_\alpha \)  
13: \( \bar{m}_\mu \leftarrow m_\mu / (1 - \gamma_1), \quad \bar{m}_\alpha \leftarrow m_\alpha / (1 - \gamma_1), \quad \bar{s} \leftarrow (s + \delta) / (1 - \gamma_2) \)  
14: \( \mu \leftarrow \mu - \beta \bar{m}_\mu / \sqrt{\bar{s}}, \quad \alpha \leftarrow \alpha - \beta \bar{m}_\alpha / \sqrt{\bar{s}} \)  
15: \( t \leftarrow t + 1 \)  
16: end while

#### J.3. Extension for Student’s t-distribution

Likewise, re-expressing the update (82) in terms of \( \mu, \Sigma \), we obtain the following update:

\[
\Sigma_{t+1} = \Sigma_t^{-1} - 2 - \frac{\beta}{1 - m} \nabla_{\Sigma_t} L + \frac{m}{1 - m} (\Sigma_t^{-1} - \Sigma_{t-1}^{-1})
\]

\[
\mu_{t+1} = \mu_t + \frac{\beta}{1 - m} \nabla_{\mu_t} L + \frac{m}{1 - m} \Sigma_{t+1}^{-1} (\mu_t - \mu_{t-1})
\]

where we use a Student’s t-distribution with fixed \( \alpha > 1 \) as the variational distribution, \( \nabla_{\mu_t} L \) and \( \nabla_{\Sigma_t} L \) are defined at (83) - (84).

Now, we consider the following lower bound (\( z \in \mathbb{R}^d \)).

\[
L(\lambda) = \mathbb{E}_{q(z|\lambda)} \left[ \sum_{n=1}^{N} \log p(D_n|z) + \log \mathcal{N}(z, 0, \delta^{-1}I) - \log q(z|\lambda) \right].
\]

where

\[
q(z) = \frac{\det (\pi \Sigma)^{-1/2} \Gamma(\alpha + d/2)}{(\Gamma(\alpha) (2\alpha)^{-\alpha})} \left( 2\alpha + (z - \mu)^T \Sigma^{-1} (z - \mu) \right)^{-\alpha-d/2}.
\]

We use the results from Kotz & Nadarajah (2004).

\[
\mathbb{E}_{q(z|\lambda)} [-\log q(z|\lambda)] = \frac{1}{2} \log |\Sigma| + \log \left( \frac{2a\pi)^{d/2}}{\Gamma(d/2)} + \log \frac{\Gamma(d/2)\Gamma(a)}{\Gamma(d/2 + a)} + (a + d/2) (\psi (a + d/2) - \psi (a)) \right)
\]

\[
\mathbb{E}_{q(z|\lambda)} [\log \mathcal{N}(z, 0, \delta^{-1}I)] = \frac{d}{2} \log (2\pi) + \frac{d\log(\delta)}{2} - \frac{1}{2} \mu^T \mu - \frac{\delta}{2a - 1} \text{Tr} (\Sigma)
\]

where \( \psi(\cdot) \) is the digamma function.

The remaining thing is to compute the gradients about \( \mathbb{E}_{q(z)} [f_n(z)] \). To compute the gradients, the reparametrization trick can be used. However, we can do better by the extended Bonnet’s and Price’s theorems for Student’s t-distribution (Lin et al., 2019). Assuming that \( f_n(z) \) satisfies the assumptions needed for these two theorems, we obtain the following gradient...
expression:

\[ g_n^1 := \nabla_\mu E_{q(z)}[f_n(z)] = E_{q(z)}[\nabla z f_n(z)] \approx \nabla z f_n(z) \]

\[ g_s^1 := 2\nabla \Sigma E_{q(z)}[f_n(z)] \]

\[ = E_{q(z)}[u(z)\nabla^2 f_n(z)] \approx u(z)\nabla^2 f_n(z) \]

\[ = E_{q(\nu, z)}[w\nabla^2 f_n(z)] \approx w\nabla^2 f_n(z) \]

where \( z \in \mathcal{R}^d \) is generated from \( q(z) \), \( w \) is generated from \( q(w) \), and

\[ u(z) := \frac{a + \frac{1}{2} (z - \mu)^T \Sigma^{-1} (z - \mu)}{(a + d/2 - 1)} \]

The gradients of \( L(\lambda) \) can be expressed as

\[ \nabla_\mu L(\lambda) = -\sum_{n=1}^{N} g_n^1 - \delta \mu \]  

\[ \nabla_\Sigma L(\lambda) = -\frac{1}{2} \sum_{n=1}^{N} g_s^1 - \delta \frac{a}{2} \frac{\mu}{a-1} I + \frac{1}{2} \Sigma^{-1} \]  

(83)

(84)

Likewise, we can obtain the variational Adam update with Gaussian prior \( p(z) = \mathcal{N}(z|0, \delta^{-1} I) \) as shown below, where \( z \in \mathcal{R}^d, \Sigma^{-1} = \text{Diag}(Ns + \frac{\alpha \delta}{\alpha-1}) \), and \( u(z) = \frac{a + \frac{1}{2} (z - \mu)^T \Sigma^{-1} (z - \mu)}{(a + d/2 - 1)} \).

**Student’s t \( (\alpha > 1) \) extension**

1. while not converged do
2. \( z \leftarrow \mu + \sigma \circ \epsilon \), where \( w \sim \mathcal{G}(\alpha, \alpha), \epsilon \sim \mathcal{N}(0, I), \sigma \leftarrow \sqrt{w/(Ns + \frac{\alpha \delta}{\alpha-1})} \)
3. Randomly sample a data example \( D_i \)
4. \( g_\mu \leftarrow -\nabla \log p(D_i | z) \)
5. **option I**: \( g_\mu \leftarrow w g_\mu \circ g_\mu \)
6. **option II**: \( g_\mu \leftarrow u(z) g_\mu \circ g_\mu \)
7. \( m_\mu \leftarrow \gamma_1 m_\mu + (1 - \gamma_1) \left( g_\mu + \delta \mu / N \right) \)
8. \( s \leftarrow \gamma_2 s + (1 - \gamma_2) g_\beta \)
9. \( \tilde{m}_\mu \leftarrow m_\mu / (1 - \gamma_1), \tilde{s} \leftarrow (s + \frac{\alpha \delta}{N(\alpha-1)}) / (1 - \gamma_2) \)
10. \( \mu \leftarrow \mu - \beta \tilde{m}_\mu / \sqrt{\tilde{s}} \)
11. \( t \leftarrow t + 1 \)
12. end while

**J.4. Extension for Symmetric Normal Inverse-Gaussian Distribution**

Re-expressing the update (82) in terms of \( \mu \) and \( \Sigma \) (the same derivation as Khan et al. (2018)), we obtain the following update:

\[ \Sigma_{t+1} = \Sigma_t - 2 \beta \frac{1}{1 - m} \nabla_\Sigma \mathcal{L} + \frac{m}{1 - m} (\Sigma_t - \Sigma_{t-1}) \]

\[ \mu_{t+1} = \mu_t + \beta \frac{1}{1 - m} \nabla_\mu \mathcal{L} + \frac{m}{1 - m} \Sigma_{t+1} \Sigma_{t-1}^{-1} (\mu_t - \mu_{t-1}) \]

where we use a symmetric normal inverse-Gaussian distribution with fixed \( \lambda > 0 \) as the variational distribution, \( \nabla_\mu \mathcal{L} \) and \( \nabla_\Sigma \mathcal{L} \) are defined at (78) - (79).

Likewise, we can obtain the variational Adam update with Gaussian prior \( p(z) = \mathcal{N}(z|0, \delta^{-1} I) \) as shown below, where
$z \in \mathbb{R}^d$, $\Sigma^{-1} = \text{Diag}(N\delta + \delta(1 + \lambda^{-1}))$, and

$$u(z) = \sqrt{(z - \mu)^T \Sigma^{-1} (z - \mu) + \lambda \frac{K_{d-1}}{\lambda} \left( \sqrt{\lambda \left( (z - \mu)^T \Sigma^{-1} (z - \mu) + \lambda \right)} \right)}$$

Recall that the ratio about the Bessel functions can be approximated by Eq (71) when $d \geq 2$.

**Symmetric Normal Inverse-Gaussian ($\lambda > 0$) extension**

1: while not converged do  
2: $z \leftarrow \mu + \sigma \circ \epsilon$, where $w \sim \text{InvGauss}(1, \lambda)$, $\epsilon \sim \mathcal{N}(0, I)$, $\sigma \leftarrow \sqrt{1/\left[w(N\delta + \delta(1 + \lambda^{-1}))\right]}$  
3: Randomly sample a data example $D_i$  
4: $g_\mu \leftarrow -\nabla \log p(D_i|z)$  
5: option I: $g_s \leftarrow w^{-1} g_\mu \circ g_\mu$  
6: option II: $g_s \leftarrow u(z) g_\mu \circ g_\mu$  
7: $m_\mu \leftarrow \gamma_1 m_\mu + (1 - \gamma_1) (g_\mu + \delta \mu / N)$  
8: $s \leftarrow \gamma_2 s + (1 - \gamma_2) g_s$  
9: $\tilde{m}_\mu \leftarrow m_\mu / (1 - \gamma_1)$, $\tilde{s} \leftarrow (s + \delta(1 + \lambda^{-1}) / N) / (1 - \gamma_2)$  
10: $\mu \leftarrow \mu - \beta \tilde{m}_\mu / \sqrt{\tilde{s}}$  
11: $t \leftarrow t + 1$  
12: end while