Handling the Positive-Definite Constraint in the Bayesian Learning Rule

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Abstract

The Bayesian learning rule is a recently proposed variational inference method, which not only contains many existing learning algorithms as special cases but also enables the design of new algorithms. Unfortunately, when posterior parameters lie in an open constraint set, the rule may not satisfy the constraints and requires line-searches which could slow down the algorithm. In this paper, we fix this issue for the positive-definite constraint by proposing an improved rule that naturally handles the constraint. Our modification is obtained using Riemannian gradient methods, and is valid when the approximation attains a block-coordinate natural parameterization (e.g., Gaussian distributions and their mixtures). Our method outperforms existing methods without any significant increase in computation. Our work makes it easier to apply the learning rule in the presence of positive-definite constraints in parameter spaces.

1. Introduction

Bayesian learning rule, a recently proposed method, enables derivation of learning algorithms from Bayesian principles (Khan & Rue, 2019). It is a natural-gradient variational inference method (Khan & Lin, 2017; Zhang et al., 2018) where, by carefully choosing a posterior approximation, we can derive a variety of algorithms in fields such as probabilistic graphical models, continuous optimization, and deep learning. For example, Khan & Lin (2017) derive approximate inference methods, such as stochastic variational inference and variational message passing; Khan et al. (2018) derive connections to deep-learning algorithms; and Khan & Rue (2019) derive many classical algorithms such as least-squares, gradient descent, Newton’s method, and forward-backward algorithm. Not only this, but we can also design new algorithms using this rule, e.g., for uncertainty estimation in deep learning (Osawa et al., 2019).

An issue with the rule is that when the parameters of the posterior approximation lie in an open constraint set, the update may not always satisfy the constraints, e.g., for Gaussian approximations, the posterior covariance needs to be positive definite but the rule may violate this; see Appendix D.1 in Khan et al. (2018) for an example. A straightforward solution is to use line-search to keep the iterations within the constraint set (Khan & Lin, 2017), but this can lead to slow convergence. In some cases, we can find an approximate update which always satisfies the constraints, e.g., for Gaussian approximations (Graves, 2011; Osawa et al., 2019). However, in general, it is difficult to come up with such approximations that are both fast and reasonably accurate. Our goal in this paper is to modify the Bayesian learning rule so that it can naturally handle such constraints.

We propose an improved Bayesian learning rule to handle the positive-definite constraints without any line search. This is obtained by using a generalization of natural-gradient methods called the Riemannian-gradient methods. We show that, for approximations with a specific block-diagonal structure on the Fisher information matrix (FIM), the constraints are satisfied when an additional term is added to the rule. Such a structure is always possible when the parameters of the approximation are partitioned in what we call the block-coordinate natural (BCN) parameterizations. Fortunately, for many approximations with such parameterizations, the improved rule requires almost the same computation as the original rule. An example is shown in Figure 1 where our improved rule fixes an implementation issue with an algorithm for uncertainty estimation in deep learning (Osawa et al., 2019). We present such examples where the improved rule converges faster than the original rule and many existing variational inference methods. Our work makes it easier to handle constraints with the learning rule.

1.1. Related Works

Our work is closely related to the method of Tran et al. (2019). They propose a method based on a retraction map very similar to ours in Gaussian cases. Their retraction map does not directly generalize to other distributions, while ours does. They also do not provide a justification or derivation of the map. We also fix this gap by deriving the map from first principles, justifying its use, and obtaining an Adam-like update by choosing a proper parametrization for...
### Variational Online Gauss-Newton (VOGN) Algorithm

1. $z \leftarrow \mu + (N\hat{s})^{-1/2} \odot \epsilon$, where $\epsilon \sim \mathcal{N}(0, I)$
2. Randomly sample a minibatch $M$ of size $M$
3. Compute and store individual $g_i, \forall i \in M$
4. $g_\mu \leftarrow \frac{1}{N} \mu + \frac{1}{M} \sum_{i=1}^M g_i$
5. $m \leftarrow r_1 m + (1 - r_1) g_\mu$, $\bar{m} \leftarrow m/(1 - r_1^k)$
6. $g_s \leftarrow \frac{1}{N} - \hat{s} + \frac{1}{M} \sum_{i=1}^M (g_i \odot g_i)$
7. $\tilde{s} \leftarrow \hat{s} + (1 - r_1) g_s$
8. $\mu \leftarrow \mu - t \bar{m}/\tilde{s}$, where $\hat{s} \leftarrow \tilde{s}/(1 - r_1^k)$

### Our Adam-like Optimizer

1. $z \leftarrow \mu + (N\hat{s})^{-1/2} \odot \epsilon$, where $\epsilon \sim \mathcal{N}(0, I)$
2. Randomly sample a minibatch $M$ of size $M$
3. Compute minibatch $\bar{g} \leftarrow \frac{1}{M} \sum_{i=1}^M g_i$
4. $g_\mu \leftarrow \frac{1}{N} \mu + \bar{g}$
5. $m \leftarrow r_1 m + (1 - r_1) g_\mu$, $\bar{m} \leftarrow m/(1 - r_1^k)$
6. $g_s \leftarrow \frac{1}{N} - \bar{s} + \frac{1}{M} \sum_{i=1}^M (g_i \odot g_i)$
7. $\tilde{s} \leftarrow \bar{s} + (1 - r_2) g_s + \frac{1}{2} (1 - r_2)^2 g_s \odot \hat{s}^{-1} \odot g_s$

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**Figure 1.** Our improved Bayesian learning rule solves an implementation issue with an existing algorithm known as VOGN (Khan et al., 2018) (shown in the left). VOGN is an Adam-like optimizer which gives state-of-the-art results on large deep learning problems (Osawa et al., 2019). However, it requires us to store individual gradients in a minibatch which makes the algorithm slow (show with blue in line 3 and 6). This is necessary for the scaling vector $\hat{s}$ to obtain a good estimate of uncertainty. Our work in this paper fixes this issue using the improved Bayesian learning rule. Our Adam-like optimizer (shown in the right) only requires average over the minibatch (see line 3). Line 6 is simply changed to use the averaged gradient. The additional terms added to the Bayesian learning rule is highlighted in red in line 8. These changes do not increase the computation cost significantly while fixing the implementation issue of VOGN. Due to our modification, the scaling vector $\hat{s}$ always remains positive. A small difference is that the mean $\mu$ is updated before in our optimizer (see line 7 and 8), while in VOGN it is the opposite.

Gaussian cases (see Appendix E). Furthermore, in Tran et al. (2019), retraction map and Riemannian gradient used in neural network cases are not derived from the same Riemannian metric. In our work, the retraction map induced by the proposed rule and Riemannian gradient are naturally derived from the same metric. Hosseini & Sra (2015) use a similar Riemannian method to ours but for the specific case of Gaussian mixture model. It is unclear if this approach generalizes to other models or loss functions. Song et al. (2018) derive a similar update in a non-Bayesian context, but their update does not always satisfy the constraints even for univariate Gaussians (see Appendix A). Their update is neither simple nor efficient for multivariate Gaussians. Our method applies to more general settings than these methods.

### 2. Bayesian Learning Rule

Given a dataset $D$, it is common in machine learning to estimate unknown variables $z$ of a statistical model by minimizing $\ell(z) \equiv \ell(D, z) + R(z)$ where $\ell(D, z)$ is a loss function and $R(z)$ is a regularizer. Many estimation strategies can be used, giving rise to various type of learning algorithms, e.g., maximum-likelihood approaches use gradient-based algorithms such as gradient descent and Newton’s method, while Bayesian approaches use Bayesian inference algorithms such as message passing.

Recently, Khan & Rue (2019) show that many existing learning algorithms can be obtained from Bayesian principles. The main idea is to utilize the following Bayesian formulation where, instead of minimizing over $z$, we minimize over a distribution $q(z)$:

$$\min_{q(z) \in Q} \mathbb{E}_{q(z)}[\ell(D, z)] + D_{KL}[q(z) \parallel p(z)] = L(q).$$  \hspace{1cm} (1)

Here, $q(z)$ is an approximation of the posterior of $z$ given $D, Q$ is the set of approximation distributions, $p(z) \propto \exp(-R(z))$ is the prior, and $D_{KL}$ denotes the Kullback-Leibler divergence. To obtain existing learning algorithms from the above formulation, we need to carefully choose the approximation family $Q$. Khan & Rue (2019) consider the following minimal exponential family (EF) distribution:

$$q(z|\lambda) := h(z) \exp\left[\langle \phi(z), \lambda \rangle - A(\lambda) \right]$$  \hspace{1cm} (2)

where $\phi(z)$ is a vector containing sufficient statistics, $h(z)$ is the base measure, $\lambda \in \Omega$ is the natural parameter, $\Omega$ is the set of valid natural-parameters so that the log-partition function $A(\lambda)$ is finite, and $\langle \cdot, \cdot \rangle$ denotes an inner product.

Khan & Rue (2019) present the Bayesian learning rule to optimize (1), which is in fact a natural-gradient algorithm originally proposed by Khan & Lin (2017) for variational inference. The algorithm takes the following form in its simplest form (Khan & Nielsen, 2018):

$$\lambda \leftarrow \lambda - t \hat{g}, \text{ with } \hat{g} := \mathbf{F}(\lambda)^{-1} \nabla_{\lambda} L(\lambda)$$  \hspace{1cm} (3)

where $t > 0$ is a scalar step-size and $\hat{g}$ is the natural gradient defined using the Fisher information matrix $\mathbf{F}(\lambda) := -\mathbb{E}_q[\nabla^2_{\lambda} \log q(z|\lambda)]$ of $q$ and $L(\lambda)$ which is equal to $L(q)$ but defined in terms of $\lambda$. Khan & Rue (2019) proposed further simplifications, e.g., for approximations with base measure $h(z) \equiv 1$, we can write (3) as,

$$\lambda \leftarrow (1 - t)\lambda - t \nabla_{\lambda} \mathbb{E}_q[\ell(z)]$$  \hspace{1cm} (4)
where $\mathbf{m} := \mathbb{E}_{q(z)}[\phi(z)]$ denotes the expectation parameter.

Existing learning algorithms can be derived as special cases by choosing an approximate form for $q(z)$. For example, when $q(z) := \mathcal{N}(z|\mu, S^{-1})$ is a multivariate Gaussian approximation with mean $\mu$ and precision matrix $S$, the learning rule (4) can be expressed as follows:

$$S \leftarrow (1 - t)S + t \mathbb{E}_q[\nabla^2 \bar{\ell}(z)] \quad (5)$$

$$\mu \leftarrow \mu - t S^{-1} \mathbb{E}_q[\nabla \bar{\ell}(z)] \quad (6)$$

This algorithm uses the Hessian to update $S$ which is then used to scale the update for $\mu$, in a similar fashion as Newton’s method. The update for $\mu$ in (3) and (4) is not only used to derive the Hessian but also to improve them and design new ones.

### 2.1. Positive-Definite Constraints

An issue with updates (3) and (4) is that they do not take the constraint $\lambda \in \Omega$ into account. Recall that $\Omega$ is the set of valid natural parameters. The update is valid when $\Omega$ is unconstrained (e.g., a real-coordinate space), but otherwise it may violate the constraints. The simplest example is the multivariate Gaussian of dimension $d$ where the precision matrix $S \in \mathbb{S}^{d \times d}$ is required to be real, symmetric positive-definite, while $\mu \in \mathbb{R}^d$ is unconstrained. In such cases, the update may violate the constraint, e.g., in the update (5), the precision $S$ can become indefinite, when the loss $\bar{\ell}(z)$ is nonconvex. A similar issue appears when flexible approximations are used such as mixtures of Gaussians.

Another example is gamma distribution: $q(z|\alpha, \beta) \propto z^{\alpha-1}e^{-z\beta}$ where both $\alpha, \beta > 0$. We denote the positivity constraint using $\mathbb{S}^+_{++}$. The rule takes the following form:

$$\alpha \leftarrow (1 - t)\alpha - t \hat{g}_\alpha, \quad \beta \leftarrow (1 - t)\beta - t \hat{g}_\beta \quad (7)$$

where $\hat{g}_\alpha$ and $\hat{g}_\beta$ are gradient of $\mathbb{E}_{q(z)}[\bar{\ell}(z) - \log z]$ with respect to the expectation parameters $m_\alpha = \mathbb{E}_{q(z)}[\log z]$ and $m_\beta = \mathbb{E}_{q(z)}[-z]$ respectively; see a detailed derivation in Appendix E.3 in Khan & Lin (2017). Here again the learning rule does not ensure that $\alpha$ and $\beta$ are always positive.

In general, a backtracking line search, as original proposed in Khan & Lin (2017), can be used to ensure that the iterates stay within the constraint set. However, this could be very slow in practice. Khan et al. (2018) discuss this issue for the Gaussian case; see Appendix D.1 in their paper. They found that using line-search is computationally expensive and also not trivial to implement for deep-learning problems. They address this issue by approximating the Hessian in (5) with a positive-definite matrix. This ensures that $S$ is always positive-definite. This works well in practice and obtains state-of-the-art results on large deep-learning problems (Osawa et al., 2019). Unfortunately, such approximations are difficult to come up for a general case, e.g., for the gamma approximation, there is no such straight-forward approximation in update (7) to ensure positivity of $\alpha$ and $\beta$. Handling constraints within the Bayesian learning rule is an open issue which limits its application.

In this paper, we focus on the positive-definite constraint and show that, in many cases, such constraints can be naturally handled by adding an additional term to the Bayesian learning rule. We show that, for this to happen, the approximation needs to follow a specific parameterization. We will now describe the modification in the next section, followed by its derivation using Riemannian gradient methods.

### 3. An Improved Bayesian Learning Rule

In this section, we will derive an improved Bayesian learning rule which can naturally handle the positive-definite constraints on the parameters of the approximation. Our key idea is to partition the parameter vector into blocks such that the constraints in each block are mutually-exclusive. This is formally stated in the following assumption.

**Assumption 1 [Mutually-Exclusive Constraints]**: We assume parameter $\lambda = \{\lambda^{[1]}, \ldots, \lambda^{[m]}\}$ can be partitioned into $m$ blocks with mutually-exclusive constraints $\Omega = \Omega_1 \times \cdots \times \Omega_m$, where square bracket $[i]$ denotes the $i$-th block and each block $\lambda^{[i]}$ is either unconstrained or positive-definite. If $\lambda^{[i]}$ is positive-definite, it has all degrees of freedom.

As an example, consider multivariate Gaussian approximation with the following two blocks: one block containing the mean $\mu$ and another containing the full precision $S$. This satisfies the above assumption because the first block is unconstrained and the second block is positive definite with all degrees of freedom. In $d$-dimensional diagonal Gaussian cases, we consider $2d$ blocks: one block containing the mean $\mu$, and one block containing the precision $s_i$ for each dimension $i$, where each $s_i$ is positive. Other distributions such as gammas and inverse Gaussians can also be partitioned to two blocks, where each block is positive.
Handling the Positive-Definite Constraint in the Bayesian Learning Rule

Now, we define the BCN parameterization.

**Assumption 2 [Block Coordinate Parameterization]:** A parameterization is block coordinate (BC) if the Fisher Information Matrix (FIM) under this parameterization is block-diagonal according to the block structure of the parameterization.

As an example, the mean and the covariance/precision in Gaussian approximation as two different blocks is a BC parameterization, while the natural parameterization is not (see Appendix E for a proof and Barfoot (2020)).

**Assumption 3 [Block Natural Parameterization for Exponential-Family]:** For an exponential-family distribution \( q(z|\lambda) \) and each block \( \lambda^{[i]} \), there exist function \( \phi_i \) and \( h_i \) such that \( q(z|\lambda) \) can be re-expressed as a minimal exponential family distribution given that the rest of blocks \( \lambda^{[\neq i]} \) are known.

\[
q(z|\lambda) \equiv h_i \left( z, \lambda^{[\neq i]} \right) \exp \left( \langle \phi_i \left( z, \lambda^{[\neq i]} \right), \lambda^{[i]} \rangle - A(\lambda) \right)
\]

We illustrate this on the Gaussian distribution which can be written as following exponential form:

\[
q(\mu, S|\lambda) = \exp \left( -\frac{1}{2} z^T S z + z^T S \mu - A(\lambda, S) \right)
\]

where the log-partition function is equal to \( A(\lambda, S) = \frac{1}{2} \left[ \mu^T S - \log |S|/(2\pi) \right] \). Considering two blocks with parameters \( \lambda \) and \( S \) respectively, we can express this distribution in the following two ways where the first equation is for the \( \mu \) block while the second equation is for the \( S \) block:

\[
q(\mu, S|\lambda) = \frac{1}{h_1(z, S)} \exp \left( -\frac{1}{2} z^T S z + z^T S \mu - A(\lambda, S) \right)
\]

\[
q(\mu, S|\lambda) = \frac{1}{h_2(\mu, S)} \exp \left( -\frac{1}{2} \mu^T S + \mu S \mu - A(\lambda, S) \right)
\]

We define the block-coordinate natural (BCN) parameterization as the parameterization of an exponential-family distribution which satisfies Assumptions 1 to 3. Therefore, Gaussian distribution with \( \mu \) and \( S \) as blocks can be expressed in a BCN parameterization.

Before, we present the improved rule, we need to define our indexing notation. A list is given in Table 1. We will use the Einstein notation to omit summation symbols, e.g., \( F^{ca} F_{ab} := \sum_a F^{ca} F_{ab} \). Another example is that natural gradient \( \tilde{g} = F^{-1} g \) can be rewritten as \( \tilde{g} = F^{ca} g_a \), where \( g_a := \partial_a \ell(\lambda) \)

We will now present the rule (a detailed derivation is in Section 4). The improved Bayesian learning rule takes the following form with an additional term shown in red:

\[
\lambda^{ci} \leftarrow \lambda^{ci} - t \tilde{g}^{ci} - \frac{t^2}{2} \Gamma_{ab,ci} \tilde{g}^{ai} \tilde{g}^{bi}
\]

\[\text{Table 1. Table of Indexing Notation}\]

| \( \lambda^{[i]} \) | \( i \)-th block parameter of parameterization \( \lambda \).
| \( \lambda^a \) | \( a \)-th element of block parameter \( \lambda^{[i]} \).
| \( \lambda^a, \lambda^{(a)} \) | \( a \)-th element of parameterization \( \lambda \).
| \( g_a \) | \( a \)-th element of Euclidean gradient \( g \).
| \( \tilde{g}^a \) | \( a \)-th element of Riemannian/natural gradient \( \tilde{g} \).
| \( F_{ab} \) | element of \( F \) with global index \((a, b)\).
| \( F^{ab} \) | element of \( F^{-1} \) with global index \((a, b)\).
| \( \Gamma_{ab} \) | element with global index \((c, a, b)\).
| \( \Gamma_{a,b} \) | element with local index \((a, b)\) in block \( i \).
| \( \Gamma_{a_i,b_i} \) | element with local index \((c, a, b)\) in block \( i \).

where the hidden summations are taken over local index \( a_i \) and \( b_i \) inside block \( i \) in the additional term and \( \Gamma_{a_i,b_i} \), the Christoffel symbol of second kind for the \( i \)-th block at position \((a, b, c)\), is defined as following:

\[
\Gamma_{a_i,b_i} := F^{ci} \Gamma_{di,a_i,b_i}.
\]

Here, \( \Gamma_{d_i,c,a_i,b_i} := \frac{1}{2} \partial_{\lambda^{(c)}} \partial_{\lambda^{(a)}} \partial_{\lambda^{(d)}} A(\lambda) \) is the Christoffel symbol of first kind for block \( \lambda^{[i]} \) at position \((d, a, b)\).

We see that the modification requires computation of the Christoffel symbol which involves third order derivatives of the log-partition function \( A(\lambda)^2 \). We will now discuss a few examples where this computation simplifies and can be carried out with minimal computational increase in the existing Bayesian learning rule. More examples can be found in Appendix G, H, J, K.

### 3.1. Example: Online Newton using Gaussian Approximation

The original learning rule for Gaussian approximations gives the update (5)-(6). This rule is obtained for the natural parameterization of Gaussian. We consider the parameterization \( \mu \) and \( S \), in which the improved learning rule takes the following form (detailed derivation is in Appendix E):

\[
\mu \leftarrow \mu - t S^{-1} E_q \left[ \nabla_\tilde{z} \ell(z) \right]
\]

\[
S \leftarrow (1 - t) S + t E_q \left[ \nabla_\tilde{z}^2 \ell(z) \right] + \frac{t^2}{2} G S^{-1} G,
\]

where \( G := S - E_q \left[ \nabla_\tilde{z}^2 \ell(z) \right] \). The time complexity remains the same thanks to the Cholesky decomposition. The highlighted term in red is the additional term required to ensure that the positive definite constraint is always satisfied. The theorem below proves that this is the case.

**Theorem 1** The updated \( S \) in (9) is positive definite if the initial \( S \) is positive-definite.

\(^2\) We assume \( A(\lambda) \) is (jointly) \( C^n \)-smooth. Note that \( A(\lambda) \) is block-wisely \( C^n \)-smooth due to Johansen (1979).
Proof: We first note that $\mathcal{G}$ is a symmetric matrix. Let $\mathbf{L}$ be the Cholesky of the current $\mathbf{S} = \mathbf{L}^T \mathbf{L}$. Then we can simplify the right hand side of (9) as follows:

$$(1 - t)\mathbf{S} + t \mathbb{E}_q[\nabla^2_\ell(z)] + \frac{t^2}{2} \hat{\mathbf{G}} \mathbf{S}^{-1} \hat{\mathbf{G}}$$

$$= \mathbf{S} - t \hat{\mathbf{G}} + \frac{t^2}{2} \hat{\mathbf{G}} \mathbf{S}^{-1} \hat{\mathbf{G}}$$

$$= \frac{1}{2} \left( 2\mathbf{S} - 2t \hat{\mathbf{G}} + t^2 \hat{\mathbf{G}} \mathbf{S}^{-1} \hat{\mathbf{G}} \right)$$

$$= \frac{1}{2} \left( \mathbf{S} + \left( \mathbf{L} - t \hat{\mathbf{G}} \mathbf{L}^{-T} \right) \left( \mathbf{L}^T - t \mathbf{L}^{-1} \hat{\mathbf{G}} \right) \right)$$

$$= \frac{1}{2} \left( \mathbf{S} + \mathbf{U}^T \mathbf{U} \right),$$

where $\mathbf{U} := \mathbf{L}^T - t \mathbf{L}^{-1} \hat{\mathbf{G}}$. Since the current $\mathbf{S}$ is positive-definite, and $\mathbf{U}^T \mathbf{U}$ is positive semi-definite, we know that the update for $\mathbf{S}$ is positive-definite. $\square$

Similar to Khan & Rue (2019), an online Newton method can be obtained by approximating the expectations at $\mu$, e.g., $\mathbb{E}_q[\nabla_\ell(z)] \approx \nabla_\ell(\mu)$ and $\mathbb{E}_q[\nabla^2_\ell(z)] \approx \nabla^2_\ell(\mu)$. In this case, the algorithm converges to a local minimal of the loss $\ell(z)$. An important point is that, unlike Newton’s method where the preconditioner may not remain positive-definite for nonconvex functions, here $\mathbf{S}$ is always guaranteed to be positive definite.

Even though the update (8)-(9) appears very similar to (5)-(6), there is one difference – the old $\mathbf{S}$ is used as a preconditioner to update $\mu$. However, we expect this to make little difference in practice.

These updates can be used to obtain an improved version of the Variational Online Gauss-Newton (VOGN) algorithm Osawa et al. (2019). It is shown in Figure 1 where the differences in our algorithm are highlighted in red. The algorithm is derived using the reparameterization trick used in a version of the update (8)-(9). A derivation is given in Appendix E2. Our algorithm fixes an implementation issue where these updates can be used to obtain an improved version of the algorithm. The full derivation is given in Appendix F.

$\Gamma_{11}^i = \frac{\partial^2 \psi(\lambda(i))}{\partial \lambda(i)^2} \left( \frac{\Gamma_{ii}^i}{\lambda(i)} - \frac{1}{\lambda(i)^2} \right)$, $\Gamma_{22}^i = -\frac{1}{\lambda(i)^2}$

Our learning rule can be extended to mixture approximations, such as finite mixture of Gaussians (MOG) shown in Appendix J and skew Gaussian approximations given in Appendix K, using the joint FIM as suggested by Lin et al. (2019). By extending the definition of the BNC parameterization to the joint distribution of a mixture, our rule can be easily applied to mixture cases (see Appendix I for details).

4. Derivation of the Improved Rule

First, we introduce the superscript and subscript convention used in Riemannian geometry to derive the rule. The indexing notation is summarized in Table 1. We use the Einstein notation in this section. We denote a Euclidean gradient $g$ using a subscript. A Riemannian gradient $\hat{g}$ is denoted by a superscript. A metric $\sqrt{g}$ is used to characterize distances in a manifold. Given a metric $\mathbf{F}$ such as the FIM, let $F_{ab}$ denote the element of $\mathbf{F}$ at position $(a,b)$ and $F^{ca}$ denote the entry of the inverse of $\mathbf{F}$, $\mathbf{F}^{-1}$, at position $(c,a)$. In other words, $F^{ca}F_{ab} = I^c_b$, where $I^c_b$ is the entry of an identity matrix at position $(c,b)$. A Riemannian gradient is defined as $\hat{g} = F^{cb}g_{bc}$, where $g_{bc}$ is the $b$-th entry of the Euclidean gradient g. When $\mathbf{F}$ is the FIM, a Riemannian gradient becomes a natural gradient.

Now, we discuss Riemannian gradient descent (RGD) and show that the original Bayesian learning rule can be viewed as RGD. Then, we show the improved rule is a new RGD. RGD can be derived from a geodesic, which is a generalization of a straight line to a Riemannian manifold. Given a metric $\sqrt{g}$ is well-defined if it is positive definite everywhere. The geodesic induces an exponential map used in exact RGD.
Handling the Positive-Definite Constraint in the Bayesian Learning Rule

Figure 2. Visualization of posterior approximations on four toy examples. The leftmost figure shows the Gaussian approximation to fit a Bayesian logistic model, where we see that our approximation matches the exact variational Gaussian approximation. Figure 2(b) shows MOG approximation fit to a beta-binomial model for a 2-D problem. The number indicates the number of mixture components used. By increasing the number of components in our approximation, we get better results. Figure 2(c) shows MOG approximation fit to a correlated 2-D Laplace distribution. The number indicates the number of mixture components used. We get smooth approximations of the non-smooth distribution. The last figure shows MOG approximation fit to a double banana distribution. The number indicates the number of mixture components used, where we only show the best 8 MOG approximations. By increasing the number of components in our approximation, we get better results.

a starting point $\lambda \in \Omega$ and a Riemannian direction $-\hat{g}$, a geodesic is an one-parameter differentiable map $L(t)$ so that the ordinary differential equation (ODE) \(^5\) is satisfied.

$$\dot{L}^c(0) = -\hat{g}^c ; \quad L^c(0) = \lambda^c$$ (11)

$$\dot{L}^c(t) = -\Gamma^c_{ab} \dot{L}^a(t) \dot{L}^b(t)$$ (12)

where $\dot{L}^c(t)$ denotes the $c$-th element of $L(t)$, $\dot{L}^c(x) := \frac{dL^c(t)}{dt} \bigg|_{t=x}$, $\ddot{L}^c(x) := \frac{d^2L^c(t)}{dt^2} \bigg|_{t=x}$, and $\Gamma^c_{ab}$, are the Christoffel symbols of second kind defined by

$$\Gamma^c_{ab} := F^{cd} \Gamma_{d,ab} ; \quad \Gamma_{d,ab} := \frac{1}{2} \left[ \partial_a F_{bd} + \partial_b F_{ad} - \partial_d F_{ab} \right]$$

where $\partial_a := \partial_{x^a}$ is for notation simplicity and $\Gamma_{d,ab}$ are the Christoffel symbols of first kind. $\dot{L}$ caracterizes the curvature of a geodesic since a manifold is not flat in general. Since $F$ is not constant, $\Gamma^c_{ab}$ is a function of $t$.

Given a parameterization with $F$ being the FIM, we can compute the Christoffel symbols of first kind using Eq. (14) in Appendix D.1. We will show that a BCN parameterization can simplify the computation of these Christoffel symbols when $F$ is the FIM. In Euclidean cases under the Cartesian coordinate system, $F$ is a constant identity matrix and Eq. (12) vanishes since $\Gamma_{d,ab}$ and $\Gamma^c_{ab}$ are zeros. Therefore, we recover gradient descent in these cases as discussed in Appendix B.

However, it is challenging to exactly solve the geodesic ODE in general. An inexact RGD can be derived by approximating the geodesic.\(^6\) Recall that the original learning rule is a natural gradient descent (NGD) method in the natural parameter space. NGD can be derived by the first-order approximation of the geodesic $L(t)$ at $t = 0$ with metric $F$ being the FIM.

$$\text{NGD} : \quad \lambda \leftarrow L(0) + \hat{L}(0) t = \lambda - \hat{g}$$

Unfortunately, this approximation is only locally well-defined even when the underlying manifold is complete.\(^7\) There usually exists a positive number $b > 0$, so that the NGD update with any step size $t > b$ does not stay in the constraint set $\Omega$. This is the reason why the original Bayesian learning rule could fail. The implication that a small step-size $t$ must be used so that the updated $\lambda \in \Omega$. In stochastic settings, the step-size $t$ should be very small, which may result in slow convergence.

Our learning rule addresses the above issue, which is indeed a new inexact RGD method for useful approximations such as gamma, Gaussian, and MOG. More importantly, the update induced by the rule can use a bigger step-size and often converges faster than NGD in many cases.

Consider cases when $\lambda = \{\lambda^1, \ldots, \lambda^m\}$ has $m$ blocks. We can express a Riemannian gradient as $\hat{g} = \{\hat{g}^1, \ldots, \hat{g}^m\}$. Let’s denote the $a$-th element in block $i$ using a local index $a_i$. Recall that we use the following block summation notation: $\Gamma^{c_{(i)}}_{a_i b_i a_i b_i} : = \sum_{a \in [i]} \sum_{b \in [i]} \sum_{c \in [i]} \Gamma^{c_{(i)}}_{a_i b_i a_i b_i} \hat{g}^a \hat{g}^b$ where $[i]$ denotes block $i$, $(c_{(i)})$ is the corresponding global index of $c_{(i)}$, and $a$ and $b$ are global indexes. Note that $\Gamma^{c_{(i)}}_{a_i b_i a_i b_i} \neq \Gamma^{c_{(i)}}_{a_i b_i a_i b_i}$. This makes our method different from Song et al. (2018) when $\lambda$ has more than one blocks. Song et al. (2018) propose to use a second-order approximation of

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\(^5\)By the knowledge of ODE, the solution is locally unique.

\(^6\)A retraction map can be derived by approximating the geodesic.

\(^7\)The domain of every geodesic is $\mathbb{R}$ in a complete manifold and therefore, the solution of the geodesic ODE is globally unique.
We define a curve \( R(t) \) at \( t = 0 \). However, such approximation does not guarantee the update stays in the constraint set even in univariate Gaussian cases (see Appendix A). Moreover, it is difficult to compute the Christoffel symbols required in Song et al. (2018) since all cross terms between any two blocks are needed in \( \Gamma_{a,b}^{c} \). In our method, we only compute \( \Gamma_{a,b}^{c} = \sum g^{a_{b}} g^{b_{c}} g^{b_{c}} \) for each block \( i \). We can extend the definition of the BC parameterization to a general metric \( F \) shown in Appendix B.1. Using this extension, we have the following lemma for any block \( i \) (see Appendix B.1 for a proof):

**Lemma 1** When \( \lambda \) is a BC parameterization of metric \( F \), we have \( \hat{g}^{a_{i}} = F_{a_{i},b_{i}} g_{b_{i}} \) and \( \Gamma_{a_{i},b_{i}}^{c} = F_{c,d}^{i} \Gamma_{d,a_{i},b_{i}}^{i}. \)

Given a manifold with metric \( F \), consider the solution of an ODE for block \( i \) denoted by \( R_{[i]}(t) \).

\[
\dot{R}_{[i]}(0) = -\hat{g}^{a_{i}} \quad \text{and} \quad R_{[i]}(0) = \lambda^{a_{i}}
\]

\[
\dot{R}_{[i]}(t) = -\Gamma_{a_{i},b_{i}}^{c} \dot{R}_{[i]}(t) \hat{g}^{b_{i}}
\]

where \( R_{[i]}(0), \dot{R}_{[i]}(0), \ddot{R}_{[i]}(t) \) denote the \( c \)-th entry of \( R_{[i]}(0), \dot{R}_{[i]}(0), \ddot{R}_{[i]}(t) \), respectively.

We define a curve \( R(t) := \{ R_{[1]}(t), \ldots, R_{[m]}(t) \} \). By Lemma 1, it is easy to see that a first-order approximation of \( R(t) \) at \( t = 0 \) induces NGD with \( F \) being the FIM under a BC parameterization. Appendix B shows this in details and gives more results.

We propose to use a second-order approximation of \( R(t) \) at \( t = 0 \). Our rule is derived by the approximation of \( R(t) \) as shown below, where \( \lambda \) is a BC parameterization.

Our rule:

\[
\lambda^{a_{i}} = \frac{1}{2} \hat{g}^{a_{i}} \quad \text{and} \quad \lambda^{a_{i}} = -t \hat{g}^{a_{i}} - \frac{1}{2} \Gamma_{a_{i},b_{i}}^{c} \dot{R}_{[i]}(t) \hat{g}^{b_{i}}
\]

where \( \Gamma_{a_{i},b_{i}}^{c} \) is computed at \( t = 0 \) and \( c_{i} \) denotes the \( c \)-th element in the \( i \)-th block. We use a BNC parameterization so that the Christoffel symbols and natural gradients are easy to compute due to Theorem 3 shown in Appendix D.

**Theorem 3** Under a BCN parameterization of exponential family (EF) with the FIM, the natural gradient and the Christoffel symbols of first kind for each block \( i \) can be simplified as

\[
\hat{g}^{a_{i}} = \partial_{m_{a_{i}}} L \quad \text{and} \quad \Gamma_{a_{i},b_{i}}^{c} = \frac{1}{2} \partial_{\lambda^{a_{i}}} \partial_{\lambda^{b_{i}}} \partial_{\lambda^{c_{i}}} A(\lambda)
\]

where \( m_{a_{i}} \) denotes the \( a \)-th element of the block coordinate expectation parameter \( m_{[i]} := \mathbb{E}_{\mathbb{Z}} \phi_{i}(z, \lambda^{[-i]}) \) and \( \lambda^{a_{i}} \) is the \( a \)-th element of \( \lambda^{[i]} \).

A similar theorem for mixtures of EFs is in Appendix I.

Our updates for all six approximations considered in this paper are summarized at Table 2 in Appendix C.

5. Results

5.1. Results on Synthetic Examples

To validate the proposed rule, we visualize posterior approximations obtained by our method in various two-dimensional toy examples, where we use the re-parametrization trick (see (16) in Appendix E for Gaussian approximations and (21) in Appendix J for MOG approximations) to compute gradients. Additional visualization examples such as the banana distribution (Haario et al., 2001) can be found at Figure 5-6 at Appendix L. We then compare our method to existing methods in a higher dimensional example.

We first visualize Gaussian approximations with full covariance structures for the Bayesian Logistic regression example taken from Murphy (2013) \((N = 60, d = 2)\). Figure 2(a) shows posterior Gaussian approximations obtained from various methods. As we can see, approximations obtained from our method matches the exact variational Gaussian approximation shown in blue. For skew-Gaussian approximations (Lin et al., 2019) and mean-field Gaussian approximations, see Figure 6 at Appendix L.

In the second example, we approximate the beta-binomial model for overdispersion considered in Salimans & Knowles (2013) \((N = 20, d = 2)\) by mixture of Gaussians (MOG). The exact posterior is extremely skewed. From Figure 2(b), we see that the approximated posterior approximates the exact posterior better and better as the number of mixture components is increased.

In the third example, we approximate a correlated Laplace distribution \( p(z) = \text{Lap}(z_{1}|0,1)\text{Lap}(z_{2}|z_{1}, 1) \) using MOG, where \( \text{Lap}(z_{2}|z_{1}, 1) = \frac{1}{2} \exp(-|z_{2} - z_{1}|) \). The target distribution is non-smooth. From Figure 2(c), we see that our method gives smooth approximations of the target function.

In the fourth example, we approximate the double banana distribution constructed by Detommaso et al. (2018). The target distribution has two modes and is skewed. As we can see from Figure 2(d), our MOG approximation approximates the target posterior better and better when we increase the number of mixture components. For a complete plot using MOG approximation with all different components, see the rightmost plot of Figure 5 at Appendix L.

Finally, we conduct a comparison study on approximations for a mixture of Student’s T’s distribution \( p(z) = \frac{1}{2} \sum_{k=1}^{C} T(z|\mu_{k}, \Sigma_{k}, \alpha) \) with degrees of freedom \( \alpha = 2 \), where \( z \in \mathbb{R}^d \). We generate each entry of location vector \( \mu_{k} \) uniformly in an interval \((-s, s)\). Each shape matrix \( \Sigma_{k} \) is taken as a form of \( \Sigma_{k} = A_{k}^{T} A_{k} + I_{d} \), where each entry of the \( d \times d \) matrix \( A_{k} \) is independently drawn from a Gaussian distribution with mean 0 and standard deviation 0.1\( d \). We approximate the posterior distribution by MOG with \( K \) components. We consider a case with
$K = 25, C = 10, d = 20, s = 20$. We compare our method to existing gradient-based methods, where the Bayesian learning rule for MOG is proposed by Lin et al. (2019). For simplicity, we fix the mixing weight to be $\frac{1}{K}$ and only update each Gaussian component with the precision $S$, and the mean $\mu$, during training. All methods use the same initialization. We use 10 Monte Carlo (MC) samples to compute the gradients, where gradients are computed using either the re-parametrization trick as shown in (21) in Appendix J (referred to as “-rep”) or the Hessian trick as shown in (22) in Appendix J (referred to as “-hess”). We tune the step size for each method. The leftmost plot of Figure 3 shows the performance of all methods using Gamma approximations to fit a Gamma factor model, where our method clearly outperforms other methods. The rightmost plot shows the performances of methods in a Bayesian MLP network with diagonal Gaussian approximations, where our method performs comparably to VOGN.

5.2. Results on Real Data

Now, we show results on real-world datasets. We consider four models in our experiments. The first model is the Bayesian linear regression, where we can obtain the exact solution. We present results for Gaussian approximations on the “Abalone” dataset ($N = 4177, d = 8$) with 3341 chosen for training. We train the model with mini-batch size 168. In Figure 4(a), we plot the negative training ELBO and the positive-Definite constraint in the Bayesian Learning Rule

$K = 25, C = 10, d = 20, s = 20$. We compare our method to existing gradient-based methods, where the Bayesian learning rule for MOG is proposed by Lin et al. (2019). For simplicity, we fix the mixing weight to be $\frac{1}{K}$ and only update each Gaussian component with the precision $S$, and the mean $\mu$, during training. All methods use the same initialization. We use 10 Monte Carlo (MC) samples to compute the gradients, where gradients are computed using either the re-parametrization trick as shown in (21) in Appendix J (referred to as “-rep”) or the Hessian trick as shown in (22) in Appendix J (referred to as “-hess”). We tune the step size for each method. The leftmost plot of Figure 3 shows the performance of all methods using Gamma approximations to fit a Gamma factor model, where our method clearly outperforms other methods. The rightmost plot shows the performances of methods in a Bayesian MLP network with diagonal Gaussian approximations, where our method performs comparably to VOGN.

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training. We train the model with mini-batch size 17. In Figure 4(b), we plot the test log-loss and compare our method to BBVI and BayesLRule with the re-parametrization trick (referred to as “-rep”). Furthermore, we consider the VOGN method proposed for Gaussian approximations. Note that BayesLRule using the re-parametrization trick does not stay in the constraint set. From the plot, we can see that our method outperforms BayesLRule using the re-parametrization trick since the constraint is violated. Our method performs similarly to VOGN.

Then, we consider the Gamma factor model (Knowles, 2015; Khan & Lin, 2017) using Gamma approximations on the “CyTOF” dataset ($N = 522, 656, d = 40$) with 300,000 chosen for training, where gradients are computed using the implicit re-parametrization trick (Figurnov et al., 2018) (referred to as “-rep”). We train the model with mini-batch size 39. We tune the step size for all methods. In Figure 4(c), we plot the test log-loss and compare our to BayesLRule and BBVI. Note that BayesLRule using the re-parametrization trick does not stay in the constraint set. Our method outperforms BayesLRule and BBVI.

Finally, we consider a Bayesian MLP network with 2 hidden layers, where we use 1000 units for each layer. We train the network with diagonal Gaussian approximations on the “CIFAR-10” dataset ($N = 60, 000, d = 3 \times 32 \times 32$) with 50,000 images for training and 10,000 images for validation. We train the model with mini-batch size 128 and compare our Adam-like update (referred to as “iBayesLRule-adam”) to VOGN. Due to the similarity of both methods, we use the same initialization and the same hyper-parameters in both methods. In Figure 4(d), we plot the validation accuracy. Our method performs similarly to VOGN.

6. Discussion

In this paper, we present an improved Bayesian learning rule to handle the underlying positive-definite constraints of parameterizations.

Our main focus has been on the derivation of simple updates that naturally handle positive-definite constraints. We have presented examples where the updates can be implemented efficiently. We hope to perform extensive experiments in the future to establish the benefits obtained by this new rule.

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A. A counter example for Song et al. (2018)

In this section, we give an example to show that the update suggested by Song et al. (2018) does not stay in the constraint set while our method does.

Let’s consider the following univariate Gaussian distribution under a BC parameterization $\lambda = \{\mu, \sigma\}$, where $\sigma$ denotes the standard deviation. The constraint is $\Omega_1 = \mathbb{R}$ and $\Omega_2 = S_{++}^1$. $\hat{g}^{(1)}$ and $\hat{g}^{(2)}$ are natural gradients for $\mu$ and $\sigma$, respectively.

$$q(z|\lambda) = \exp \left\{ -\frac{1}{2} \left( \frac{z - \mu}{\sigma}\right)^2 - \frac{1}{2} \log(2\pi) - \log(\sigma) \right\}$$

Under this parameterization, the FIM and the Christoffel symbols of second kind are given below, where the Christoffel symbols are computed by using Eq. (14). As we can see, the computation of the Christoffel symbols can be difficult since the parameterization is not a BCN parameterization.

$$F_{ab} = \begin{bmatrix} 1/\sigma^2 & 0 \\ 0 & 1/2\sigma^2 \end{bmatrix}, \quad \Gamma^{1}_{ab} = \begin{bmatrix} 0 & -1/\sigma \\ -1/\sigma & 0 \end{bmatrix}, \quad \Gamma^{2}_{ab} = \begin{bmatrix} 1/2\sigma^2 & 0 \\ 0 & -1/\sigma \end{bmatrix}$$

The update suggested by Song et al. (2018) is

$$\mu \leftarrow \mu - t \hat{g}^{(1)} - t \frac{\Gamma^{1}_{ab} \hat{g}^{(a)} \hat{g}^{(b)}}{\sigma} = \mu - t \hat{g}^{(1)} + \frac{t^2}{2} \left( \frac{2 \hat{g}^{(1)} \hat{g}^{(2)}}{\sigma} \right)$$

$$\sigma \leftarrow \sigma - t \hat{g}^{(2)} - t \frac{\Gamma^{2}_{ab} \hat{g}^{(a)} \hat{g}^{(b)}}{\sigma} = \sigma - t \hat{g}^{(2)} + \frac{t^2}{2} \left( \frac{2 \hat{g}^{(2)} - \hat{g}^{(1)^2}}{2\sigma} \right)$$

Clearly, the updated $\sigma$ does not always satisfy the positivity constraint $S_{++}^1$.

Since every block contains only a scalar, we use global indexes $\lambda^{(i)} = \lambda^{a_i}$, $\hat{g}^{(i)} = \hat{g}^{[i]}$ and $\Gamma_{a_i,b_i,c_i} = \Gamma_{i,ii}$ for notation simplicity. In our update, we can see the update automatically satisfies the constraint as shown below.

$$\mu \leftarrow \frac{\lambda^{(1)}}{\mu} - \frac{t^2}{2} \Gamma^{1}_{11} \hat{g}^{(1)} \hat{g}^{(1)} = \mu - t \hat{g}^{(1)}$$

$$\sigma \leftarrow \frac{\lambda^{(2)}}{\sigma} - \frac{t^2}{2} \Gamma^{2}_{22} \hat{g}^{(2)} \hat{g}^{(2)} = \sigma - t \hat{g}^{(2)} + \frac{t^2}{2} \left( \frac{\hat{g}^{(2)} - \hat{g}^{(1)^2}}{\sigma} \right)$$

Let’s consider another BC parameterization $\lambda = \{\mu, \sigma^2\}$ for the Gaussian distribution, where $\sigma^2$ denotes the variance. Note that we consider the parameterization for univariate Gaussian. For multivariate Gaussian, see Appendix E.3. The underlying constraint is $\Omega = \mathbb{R} \times S_{++}^1$. $\hat{g}^{(1)}$ and $\hat{g}^{(2)}$ are natural gradients for $\mu$ and $\sigma^2$, respectively.

$$q(z|\lambda) = \exp \left\{ -\frac{1}{2} \left( \frac{z - \mu}{\sigma^2}\right)^2 - \frac{1}{2} \log(2\pi) - \frac{1}{2} \log(\sigma^2) \right\}$$

Under this parameterization, the FIM and the Christoffel symbols of second kind are given below, where the Christoffel symbols are computed by using Eq. (14). As we can see, the computation of the Christoffel symbols can be difficult since the parameterization is not a BCN parameterization.

$$F_{ab} = \begin{bmatrix} 1/\sigma^2 & 0 \\ 0 & 1/2\sigma^2 \end{bmatrix}, \quad \Gamma^{1}_{ab} = \begin{bmatrix} 0 & -1/2\sigma \\ -1/2\sigma & 0 \end{bmatrix}, \quad \Gamma^{2}_{ab} = \begin{bmatrix} 1 & 0 \\ 0 & -1/\sigma \end{bmatrix}$$
Handling the Positive-Definite Constraint in the Bayesian Learning Rule

The update suggested by Song et al. (2018) is

\[
\mu \leftarrow \mu - t\dot{g}^{(1)} - \frac{t^2}{2} \Gamma_{11}^{1} \dot{g}^{(1)} \dot{g}^{(1)} = \mu - t\dot{g}^{(1)} + \frac{t^2}{2} \left( \frac{\dot{g}^{(1)} g^{(2)}}{\sigma^2} \right)
\]

\[
\sigma^2 \leftarrow \sigma^2 - t\dot{g}^{(2)} - \frac{t^2}{2} \Gamma_{22}^{2} \dot{g}^{(2)} \dot{g}^{(2)} = \sigma^2 - t\dot{g}^{(2)} + \frac{t^2}{2} \left( \frac{\dot{g}^{(2)} g^{(2)}}{\sigma^2} - (\dot{g}^{(1)})^2 \right)
\]

Obviously, the above updated \( \lambda^{(2)} \) does not always satisfy the positivity constraint.

Similarly since every block contains only a scalar, we use global indexes \( \lambda^{(i)} = \lambda^{a_i} \), \( \dot{g}^{(i)} = \dot{g}^{[i]} \) and \( \Gamma_{a_i,b_i,c_i} = \Gamma_{i,j} \) for notation simplicity. In our update, we can see the update automatically satisfies the constraint as shown below.

\[
\mu \leftarrow \mu - t\dot{g}^{(1)} - \frac{t^2}{2} \Gamma_{11}^{1} \dot{g}^{(1)} \dot{g}^{(1)} = \mu - t\dot{g}^{(1)} + \frac{t^2}{2} \left( \frac{\dot{g}^{(1)} g^{(2)}}{\sigma^2} \right)
\]

\[
\sigma^2 \leftarrow \sigma^2 - t\dot{g}^{(2)} - \frac{t^2}{2} \Gamma_{22}^{2} \dot{g}^{(2)} \dot{g}^{(2)} = \sigma^2 - t\dot{g}^{(2)} + \frac{t^2}{2} \left( \frac{\dot{g}^{(2)} g^{(2)}}{\sigma^2} - (\dot{g}^{(1)})^2 \right)
\]

B. Riemannian Optimization

We first review gradient descent updates and then extend these updates to Riemannian gradient updates, where we derive the update suggested by Song et al. (2018) is

\[
\text{GD: } \lambda \leftarrow \lambda - t\partial_{\lambda} \mathcal{L}(\lambda)
\]

where \( \partial_{\lambda} \mathcal{L}(\lambda) \) denotes a Euclidean gradient and \( t > 0 \) is a scalar step-size. The above update can be viewed as a line \( L(t) \) in the Euclidean space \( \mathbb{R}^d \) as step size \( t \) varies. Given a starting point \( \lambda \) and a Euclidean direction \( -\partial_{\lambda} \mathcal{L}(\lambda) \), the line is an one-parameter differentiable map \( L(t) \) such that the below ordinary differential equation (ODE) is satisfied.

\[
\dot{L}(0) = -\partial_{\lambda} \mathcal{L}(\lambda) ; \quad L(0) = \lambda
\]

where \( \dot{L}(x) := \left. \frac{dL(t)}{dt} \right|_{t=x} \) The unique solution of the ODE is \( L(t) = \lambda - t\partial_{\lambda} \mathcal{L}(\lambda) \), which gives the GD update.

Unfortunately, \( \Omega \) usually is not a Euclidean space but a Riemannian manifold with a metric. A metric is used to characterize distances in a manifold. A common Riemannian metric for statistical manifolds is the FIM.\(^9\)

Now, we generalize gradient descent in a manifold. Here, we use the superscript and subscript convention used in Riemannian geometry. The Einstein notation is used so omit summation symbols in this section. The indexing notation is summarized in Table 1.

We denote a Euclidean gradient \( g \) using a subscript. A Riemannian gradient \( \dot{g} \) is denoted by a superscript. We denote a Riemannian metric using \( F \). Given a metric \( F \), a Riemannian gradient is defined as \( \dot{g} = F^{ca} g_a \), where \( g_a \) is the a-th entry of the Euclidean gradient \( g \).

Now, we discuss the FIM used in statistical manifolds. The FIM is defined as below.

\[
F_{ab} := -\mathbb{E}_{q(z|\lambda)} \left[ \partial_a \partial_b \log q(z|\lambda) \right]
\]

\(^8\)It uses the Cartesian coordinate system.

\(^9\)The FIM indeed is a representation of the Fisher-Rao metric (Fisher, 1922; Rao, 1945) under a parameterization.
where $\partial_x := \partial_{\lambda^x}$ is for notation simplicity. If $F$ is positive-definite for all $\lambda \in \Omega$, a variational family $q(z|\lambda)$ induces a Riemannian manifold denoted by $(\Omega, F)$. The parameterization $\lambda$ gives a coordinate system to represent a distribution in the manifold. In this case, a Riemannian gradient becomes a natural gradient.

Now, we discuss Riemannian gradient descent (RGD). Similar to the GD case, RGD can be derived from a geodesic, which is a generalization of straight line in a Riemannian manifold. Given a starting point $\lambda \in \Omega$ and a Riemannian direction $-\dot{\gamma}$, a geodesic is an one-parameter differentiable map $L(\lambda^t)$ so that the below ODE is satisfied.

$$
\dot{\lambda}^c(0) = -\dot{\gamma}^c ; \quad \dot{\lambda}^c(0) = \lambda^c \\
\ddot{\lambda}^c(t) = -\Gamma^{c}_{ab} \dot{\lambda}^a(t) \dot{\lambda}^b(t)
$$

where $\lambda^c(t)$ denotes the $c$-th element of $L(t)$, $\dot{\lambda}^c(x) := \frac{d\lambda^c(t)}{dt} |_{t=x}$, $\ddot{\lambda}^c(x) := \frac{d^2\lambda^c(t)}{dt^2} |_{t=x}$, and $\Gamma^{c}_{ab}$ are the Christoffel symbols of second kind.

### B.1. Proof of Lemma 1

Let’s consider a parameterization $\lambda := \{\lambda^1, \ldots, \lambda^m\}$ with $m$ blocks for a statistical manifold with metric $F$. We first define a BC parameterization $\lambda$ for a general metric $F$.

**Definition 1 Block Coordinate Parameterization:** A parameterization is block coordinate (BC) if the metric $F$ under this parameterization is block-diagonal according to the block structure of the parameterization.

Recall that we use the following block notation: $\Gamma^{c}_{a_ib_i} := \sum_{a \in [i]} \sum_{b \in [i]} \Gamma^{(c_i)}_{a_ib_i} = \frac{\partial^2 \ln g_{ab}}{\partial x_i \partial x_i}$ where $[i]$ denotes the index set of block $i$, $(c_i)$ is the corresponding global index of $c_i$, and $a$ and $b$ are global indexes.

Now, we prove Lemma 1.

**Proof:** By the definition of a Riemannian gradient $\dot{\gamma}$, we have

$$
\dot{\gamma}^a = \sum_b F^{(a)}_b g^b = \sum_{b \in [i]} F^{(a)}_b g^b + \sum_{b \notin [i]} F^{(a)}_b g^b = \sum_{b \in [i]} F^{(a)}_b g^b = F^{a_i}_{b_i} g^{b_i},
$$

where in the second step, $F^{(a)}_b = 0$ for any $b \notin [i]$ since the parameterization is BC, and we use the definition of the block notation in the last step.

Similarly, we have

$$
\Gamma^{c_i}_{a_i,b_i} = \sum_d F^{(c_i)}_d \Gamma_{d,(a_i)(b_i)} = \sum_{d \in [i]} F^{(c_i)}_d \Gamma_{d,(a_i)(b_i)} + \sum_{d \notin [i]} F^{(c_i)}_d \Gamma_{d,(a_i)(b_i)} = \sum_{d \in [i]} F^{(c_i)}_d \Gamma_{d,(a_i)(b_i)} = F^{c_i, d_i}_{a_i b_i} 
$$

### B.2. NGD is a First-order Approximation of $R(t)$

Now, we assume parameterization $\lambda = \{\lambda^1, \ldots, \lambda^m\}$ is a BC parameterization with $m$ blocks. Recall that we define the curve $R(t)$ as $R(t) := \{R^1(t), \ldots, R^m(t)\}$, where $R^i(t)$ is the solution of following ODE for block $i$.

$$
\dot{R}^{c_i}(0) = -\dot{\gamma}^{c_i} ; \quad R^{c_i}(0) = \lambda^{c_i} \\
\ddot{R}^{c_i}(t) = -\Gamma^{c_i}_{a_i,b_i} \dot{R}^{a_i}(t) \dot{R}^{b_i}(t)
$$

where $R^{c_i}(0)$, $\dot{R}^{c_i}(0)$, and $\ddot{R}^{c_i}(t)$ are the $c$-th entry of $R^{i}(0)$, $\dot{R}^{i}(0)$, and $\ddot{R}^{i}(t)$, respectively.

The first-order approximation of $R(t)$ at $t = 0$ with $F$ being the FIM as shown below is also NGD in this parameterization.

$$
\lambda^{c_i} \leftarrow R^{c_i}(0) + \ddot{R}^{c_i}(0)t \\
= \lambda^{c_i} - t\dot{\gamma}^{c_i}
$$

Since $F$ is the FIM and $\lambda$ is a BC parameterization, by Lemma 1, we know that $\dot{\gamma}^{c_i}$ is indeed the $c$-th entry of natural gradient $\dot{\gamma}^{[i]}$ at block $i$.

---

Such assumption is valid for minimal exponential family.
C. A Summary Table of Approximations Considered in This Work

Table 2. Summary of the Proposed Updates Induced by Our Rule in Various Approximations

| Approximation                  | Parameterization (\(\lambda\)) | Constraints               | Additional Term                     |
|-------------------------------|----------------------------------|---------------------------|-------------------------------------|
| Inverse Gaussian (Appendix H) | \(\lambda^{(1)} = \beta^2\)    | \(\lambda^{(1)} \in S_{++}^1\) | \(\frac{i^2}{2} \left( \frac{3}{\lambda^{(1)}} \right) \left( \hat{g}^{(1)} \right)^2\) |
|                               | \(\lambda^{(2)} = \alpha\)     | \(\lambda^{(2)} \in S_{++}^1\) | \(\frac{i^2}{2} \left( \frac{1}{\lambda^{(2)}} \right) \left( \hat{g}^{(2)} \right)^2\) |
| Gamma (Appendix F)            | \(\lambda^{(1)} = \alpha\)     | \(\lambda^{(1)} \in S_{++}^1\) | \(- \frac{i^2}{2} \left( \frac{\partial_{\lambda^{(1)}} \psi(\lambda^{(1)})}{\lambda^{(1)}} - \frac{1}{\lambda^{(1)}} \right) \left( \hat{g}^{(1)} \right)^2\) |
|                               | \(\lambda^{(2)} = \frac{\beta}{\alpha}\) | \(\lambda^{(2)} \in S_{++}^1\) | \(- \frac{i^2}{2} \left( \frac{1}{\lambda^{(2)}} \right) \left( \hat{g}^{(2)} \right)^2\) |
| Exponential (Appendix G)      | \(\lambda^{(1)} = \lambda\)     | \(\lambda^{(1)} \in S_{++}^1\) | \(- \frac{i^2}{2} \left( \frac{1}{\lambda^{(1)}} \right) \left( \hat{g}^{(1)} \right)^2\) |
| Multivariate Gaussian (Appendix E) | \(\lambda^{(1)} = \mu\)     | \(\lambda^{(1)} \in \mathbb{R}^d\) | \(0\) |
|                               | \(\lambda^{(2)} = \Sigma^{-1}\) | \(\lambda^{(2)} \in S_{++}^{d \times d}\) | \(\frac{i^2}{2} \hat{g}^{(2)} \left( \hat{\lambda}^{(2)} \right)^{-1} \hat{g}^{(2)}\) |
| Mixture of Gaussians (Appendix J) | \(\lambda^{(1)} \in \mathbb{R}^d\) | \(\lambda^{(1)} \in \mathbb{R}^d\) | \(0\) |
|                               | \(\lambda^{(2)} \in S_{++}^{d \times d}\) | \(\lambda^{(2)} \in S_{++}^{d \times d}\) | \(\frac{i^2}{2} \hat{g}^{(2)} \left( \hat{\lambda}^{(2)} \right)^{-1} \hat{g}^{(2)}\) |
|                               | \(\lambda^{(1)} \in S_{++}^{K-1}\) | \(\lambda^{(1)} \in S_{++}^{K-1}\) | \(0^{11}\) |
| Skew Gaussian (Appendix K)    | \(\lambda^{(1)} = \mu\) \(\alpha\) | \(\lambda^{(1)} \in \mathbb{R}^d\) | \(0\) |
|                               | \(\lambda^{(2)} = \Sigma^{-1}\) | \(\lambda^{(2)} \in S_{++}^{d \times d}\) | \(\frac{i^2}{2} \hat{g}^{(2)} \left( \hat{\lambda}^{(2)} \right)^{-1} \hat{g}^{(2)}\) |

D. Exponential Family (EF) Approximation

D.1. Christoffel Symbols

We first show how to simplify the Christoffel symbols of first kind. The FIM and the corresponding Christoffel symbols of first kind are defined as follows.

\[
F_{ab} := -\mathbb{E}_{q(z|\lambda)} \left[ \partial_a \partial_b \log q(z|\lambda) \right]
\]

\[
\Gamma_{d,ab} := \frac{1}{2} \left[ \partial_a F_{bd} + \partial_b F_{ad} - \partial_d F_{ab} \right]
\]

where we denote \(\partial_a = \partial_{\lambda^a}\) for notation simplicity.

Since \(\partial_a F_{bd} = -\mathbb{E}_{q(z|\lambda)} \left[ \partial_b \partial_a \log q(z|\lambda) \partial_d \log q(z|\lambda) \right] - \mathbb{E}_{q(z|\lambda)} \left[ \partial_a \partial_b \partial_d \log q(z|\lambda) \right]\), the Christoffel symbols of first kind induced by the FIM can be computed as follows.

\[
\Gamma_{d,ab} = \frac{1}{2} \left[ \mathbb{E}_{q(z|\lambda)} \left[ \partial_a \partial_b \log q(z|\lambda) \partial_d \log q(z|\lambda) \right] - \mathbb{E}_{q(z|\lambda)} \left[ \partial_b \partial_d \log q(z|\lambda) \partial_a \log q(z|\lambda) \right] \right.
\]

\[
- \mathbb{E}_{q(z|\lambda)} \left[ \partial_a \partial_d \log q(z|\lambda) \partial_b \log q(z|\lambda) \right] - \mathbb{E}_{q(z|\lambda)} \left[ \partial_d \partial_b \partial_a \log q(z|\lambda) \right] \right]
\]

Note that Eq 14 is also applied to a general distribution beyond exponential family distribution. However, the Christoffel symbols are not easy to compute in general. The Christoffel symbols could be easy to compute for an exponential family distribution under some parameterization. Theorem 3 is an example.

\(^{11}\)We do not compute the additional term since \(\lambda_w \in \mathbb{R}^{K-1}\).
D.2. Proof of Theorem 3

In this case, \( q(z|\lambda) \) is an EF distribution. Since \( \lambda \) is a BCN parameterization, given that \( \lambda^{[−i]} \) is known, \( q(z|\lambda) \) is an one-parameter EF distribution as

\[
q(z|\lambda) = h_i(z, \lambda^{[−i]}) \exp \left[ \langle \phi_i(z, \lambda^{[−i]}), \lambda^{[i]} \rangle - A(\lambda) \right]
\]

Therefore, we have the following identities given \( \lambda^{[−i]} \) is known.

\[
\begin{align*}
\partial_{a_i} \partial_{b_i} \log q(z|\lambda) &= -\partial_{a_i} \partial_{b_i} A(\lambda) \\
E_{q(z|\lambda)} [\partial_{a_i} \log q(z|\lambda)] &= 0
\end{align*}
\]

where \( \partial_{a_i} = \partial_{\lambda^{a_i}} \) for notation simplicity.

Using the above identities, we have

\[
E_{q(z|\lambda)} [\partial_{a_i} \partial_{b_i} \log q(z|\lambda) \partial_{d_i} \log q(z|\lambda)] = -\partial_{a_i} \partial_{b_i} A(\lambda) \underbrace{E_{q(z|\lambda)} [\partial_{d_i} \log q(z|\lambda)]}_{0} = 0
\]

Therefore, by Eq. (14), \( \Gamma_{d_i, a_i, b_i} \) can be computed as follows

\[
\Gamma_{d_i, a_i, b_i} = -\frac{1}{2} E_{q(z|\lambda)} [\partial_{a_i} \partial_{b_i} \partial_{d_i} \log q(z|\lambda)] = \frac{1}{2} \partial_{a_i} \partial_{b_i} \partial_{d_i} A(\lambda)
\]

Let \( m_{[i]} = E_{q(z|\lambda)} [\phi_i(z)] \) denote the block coordinate expectation (BCE) parameter. We have

\[
0 = E_{q(z|\lambda)} [\partial_{a_i} \log q(z|\lambda)] = m_{a_i} - \partial_{a_i} A(\lambda)
\]

where \( m_{a_i} \) denotes the \( a \)-th element of \( m_{[i]} \).

Therefore, we know that \( m_{a_i} = \partial_{a_i} A(\lambda) \).

Recall that the \( i \)-th block of \( F \) denoted by \( F^{[i]} \), can be computed as

\[
F_{a_i b_i} = -E_{q(z|\lambda)} [\partial_{b_i} \partial_{a_i} \log q(z|\lambda)] \\
= \partial_{b_i} \partial_{a_i} A(\lambda) \\
= \partial_{b_i} [\partial_{a_i} A(\lambda)] \\
= \partial_{\lambda^{b_i}} m_{a_i}
\]

where \( \partial_{b_i} = \partial_{\lambda^{b_i}} \) is for notation simplicity.

Recall that \( \lambda \) is a BC parameterization with \( n \) blocks and \( F \) is block diagonal as shown below.

\[
F = \begin{bmatrix}
F^{[1]} & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & F^{[n]}
\end{bmatrix}
\]

Note that \( F^{ab} \) denotes the element of \( F^{-1} \) with global index \( (a, b) \) and \( F^{a_i b_i} \) denotes the element of \( \left(F^{[i]}\right)^{-1} \) with local index \( (a, b) \) in block \( i \).

If \( F^{[i]} \) is positive definite everywhere, we have

\[
F^{a_i b_i} = \partial_{m_{a_i}} \lambda^{b_i}
\]

Note that \( F^{[i]} \) is positive definite if \( q(z|\lambda^{[i]}, \lambda^{[−i]}) \) is an one-parameter minimal EF distribution given \( \lambda^{[−i]} \) is known.

By Lemma 1, Riemannian gradient \( \hat{g}^{a_i} \) can be computed as

\[
\hat{g}^{a_i} = F^{a_i b_i} g_{b_i} = \left[ \partial_{m_{a_i}} \lambda^{b_i} \right] \left[ \partial_{\lambda^{b_i}} L \right] = \partial_{m_{a_i}} L
\]

where \( g_{b_i} = \partial_{\lambda^{b_i}} L \) is a Euclidean gradient.
E. Example: Gaussian Approximation

We consider the following parameterization \( \Lambda = \{ \mu, S \} \), where \( \mu \) is the mean and \( S \) is the precision. The open-set constraint is \( \Omega_1 = \mathbb{R}^d \) and \( \Omega_2 = S_{++}^{d \times d} \). Under this parameterization, the distribution can be expressed as below.

\[
q(z|\lambda) = \exp \left( -\frac{1}{2} z^T Sz + z^T S \mu - A(\lambda) \right)
\]

where \( A(\lambda) = \frac{1}{2} [\mu^T S \mu - \log |S/(2\pi)|] \)

**Lemma 2** The Fisher information matrix under this parameterization is block diagonal with two blocks

\[
F = \begin{bmatrix}
F_{\mu} & 0 \\
0 & F_S
\end{bmatrix},
\]

where \( F_{\mu} = \frac{\partial^2}{\partial \mu \partial \mu^T} \log q(z|\mu, S) \) and \( F_S = \frac{\partial^2}{\partial S \partial \mu^T} \log q(z|\mu, S) \).

Therefore, \( \lambda = \{ \mu, S \} \) is a BC parameterization.

**Proof:** We denote the \( i \)-th element of \( \mu \) using \( \mu^i \). Similarly, we denote the element of \( S \) at position \((j, k)\) using \( S_{jk} \). We prove this statement by showing cross terms in the Fisher information matrix denoted by \( F_{\mu S} \) are all zeros. To show \( F_{\mu S} = 0 \), it is equivalent to show \( -\mathbb{E}_{q(\lambda)} \left[ \partial_{S_{jk}} \partial_{\mu^i} \log q(z|\lambda) \right] = 0 \) each \( \mu^i \) and \( S_{jk} \).

Notice that \( \mathbb{E}_{q(\lambda)} \left[ z_{\mu^i} \right] = \mu \). We can obtain the above expression since

\[
\mathbb{E}_{q(\lambda)} \left[ \partial_{S_{jk}} \partial_{\mu^i} \log q(z|\lambda) \right] = \mathbb{E}_{q(\lambda)} \left[ \partial_{S_{jk}} (z^T Se_i - e_i^T S \mu) \right]
\]

\[
= \mathbb{E}_{q(\lambda)} \left[ (z^T I_{jk} e_i - e_i^T I_{jk} \mu) \right]
\]

\[
= e_i^T I_{jk} \mathbb{E}_{q(\lambda)} \left[ z - \mu \right] \]

\[
= 0
\]

where \( e_i \) denotes an one-hot vector where all entries are zeros except the \( i \)-th entry with value 1, and \( I_{jk} \) denotes an one-hot matrix where all entries are zeros except the entry at position \((j, k)\) with value 1.

The above expression also implies that \( \mathbb{E}_{q(\lambda)} \left[ \partial_{S_{jk}} \partial_{\mu^i} \log q(z|\lambda) \right] = 0 \). \( \square \)

Now, we show that \( \lambda = \{ \mu, \Sigma \} \) is also a BC parameterization. Note that

\[
- \mathbb{E}_{q(\lambda)} \left[ \partial_{\Sigma_{jk}} \partial_{\mu^i} \log q(z|\lambda) \right]
\]

\[
= - \mathbb{E}_{q(\lambda)} \left[ \text{Tr} \left( (\partial^{2}_{\Sigma_{jk}} S) \partial_{S} \partial_{\mu^i} \log q(z|\lambda) \right) \right]
\]

\[
= - \text{Tr} \left( (\partial^{2}_{\Sigma_{jk}} S) \mathbb{E}_{q(\lambda)} \left[ \partial_{S} \partial_{\mu^i} \log q(z|\lambda) \right] \right) = 0,
\]

Since \( F_{\mu \Sigma} = -\mathbb{E}_{q(\lambda)} \left[ \partial_{\Sigma_{jk}} \partial_{\mu^i} \log q(z|\lambda) \right] \) and \( -\mathbb{E}_{q(\lambda)} \left[ \partial_{\Sigma_{jk}} \partial_{\mu^i} \log q(z|\lambda) \right] = 0 \) from above expression for any \( i, j, \) and \( k \), we have \( F_{\mu \Sigma} = 0 \). Therefore, \( \lambda = \{ \mu, \Sigma \} \) is also a BC parameterization since the cross terms of FIM under this new parameterization denoted by \( F_{\mu \Sigma} \) are zeros.

We denote the Christoffel symbols of first kind and second kind for \( \mu \) as \( \Gamma_{a_1,b_1,c_1} \) and \( \Gamma^{a_1}_{b_1,c_1} \), respectively.

**Lemma 3** All entries of \( \Gamma^{a_1}_{b_1,c_1} \) are zeros.

**Proof:** We will prove this by showing that all entries of \( \Gamma_{a_1,b_1,c_1} \) are zeros. For notation simplicity, we use \( \Gamma_{a,b,c} \) to denote \( \Gamma_{a_1,b_1,c_1} \) in the following proof. Let \( \mu^a \) denote the \( a \)-th element of \( \mu \). The following expression holds for any valid \( a, b, \) and \( c \).

\[
\Gamma_{a,b,c} = \frac{1}{2} \mathbb{E}_{q(\lambda)} \left[ \partial_{\mu^a} \partial_{\mu^b} \partial_{\mu^c} A(\lambda) \right] = 0
\]
We can obtain the above expression since
\[
E_{q(z|\lambda)} \left[ \partial_{\mu}^{b} \partial_{\mu} \partial_{\mu}^{a} A(\lambda) \right] = E_{q(z|\lambda)} \left[ \partial_{\mu}^{b} \partial_{\mu} \left( e_{a}^{T} S \mu \right) \right] \\
= E_{q(z|\lambda)} \left[ \partial_{\mu}^{b} \left( e_{a}^{T} S \mu \right) \right] \\
= 0
\]
where in the last step we use the fact that \( S, e_{a}, \) and \( e_{c} \) do not depend on \( \mu \).

Similarly, we denote the Christoffel symbols of second kind for \( \text{vec}(S) \) as \( \Gamma^{a_{2}}_{b_{2}c_{2}} \). It is not efficient to directly compute the Christoffel symbol \( \Gamma^{c_{2}}_{a_{2}b_{2}} \) since \( S \) is now a matrix. Recall that \( R^{[2]}(t) \) is the solution of the following ODE for block \( \text{vec}(S) \):
\[
\dot{R}^{a_{2}}(0) = -\dot{g}^{a_{2}}; \quad R^{a_{2}}(0) = S^{a_{2}} \\
\dot{R}^{a_{2}}(t) = -\Gamma^{a_{2}}_{b_{2}c_{2}} \dot{R}^{b_{2}}(t) \dot{R}^{c_{2}}(t),
\]
where \( R^{a_{2}}(t) \) denotes the \( a \)-th element of \( R^{[2]}(t) \) and \( S^{a_{2}} \) denotes the \( a \)-th entry of \( \text{vec}(S) \).

**Lemma 4** The additional term for \( S \) is \( \text{Mat}(\Gamma^{a_{2}}_{b_{2}c_{2}} \dot{g}^{b_{2}} \dot{g}^{c_{2}}) = -\dot{g}^{[2]} S^{-1} \dot{g}^{[2]} \) where \( \dot{g}^{a_{2}} \) denotes the \( a \)-th element of \( \text{vec}(\dot{g}^{[2]}) \).

**Proof:** Given that \( \mu \) is known, \( R^{[2]}(t) \) has the following closed-form expression (Pennec et al., 2006; Fletcher & Joshi, 2004; Minh & Murino, 2017).
\[
\text{Mat}(R^{[2]}(t)) = U \text{Exp}(t U^{-1} \dot{g}^{[2]} U^{-1}) U
\]
where \( U = S^{\frac{1}{2}} \) denotes the matrix square root and \( \text{Exp}(X) := I + \sum_{n=1}^{\infty} \frac{X^n}{n!} \) denotes the matrix exponential function.\(^{12}\)

The additional term for \( S \) can be obtained as follows.
\[
-\text{Mat}(\Gamma^{a_{2}}_{b_{2}c_{2}} \dot{g}^{b_{2}} \dot{g}^{c_{2}}) = \text{Mat}(\dot{R}^{[2]}(0)) \\
= \text{Mat}(\nabla_{t}^{2} R^{[2]}(t) \big|_{t=0}) \\
= \nabla_{t}^{2} \text{Mat}(R^{[2]}(t)) \big|_{t=0} \\
= \nabla_{t}^{2} \left( \text{Exp}(U^{-1} t \dot{g}^{[2]} U^{-1}) \right) \big|_{t=0} \\
= U \nabla_{t}^{2} \left( \text{Exp}(U^{-1} t \dot{g}^{[2]} U^{-1}) \right) \big|_{t=0} \cdot U \\
= U (U^{-1} \dot{g}^{[2]} U^{-1})(U^{-1} \dot{g}^{[2]} U^{-1}) U \\
= U (U^{-1} \dot{g}^{[2]} U^{-1}) S^{-1} \dot{g}^{[2]} U^{-1} U \\
= \dot{g}^{[2]} S^{-1} \dot{g}^{[2]}
\]
where we use the following expression to move from step 5 to step 6.
\[
\nabla_{t}^{2} \text{Exp}(t X) \big|_{t=0} = \nabla_{t}^{2} \left( I + \sum_{n=1}^{\infty} \frac{(t X)^n}{n!} \right) \big|_{t=0} \\
= X^2
\]

Finally, by Lemma 3 and 4, the update for Gaussians induced by the proposed rule is
\[
\mu^{c} \leftarrow \mu^{c} - t \dot{g}^{c_{1}} - \frac{t \times t}{2} \Gamma^{c_{1}}_{a_{1}b_{1}} \dot{g}^{a_{1}} \dot{g}^{b_{1}} \\
s^{c} \leftarrow s^{c} - t \dot{g}^{c_{2}} - \frac{t \times t}{2} \Gamma^{c_{2}}_{a_{2}b_{2}} \dot{g}^{a_{2}} \dot{g}^{b_{2}}
\]

\(^{12}\) The function is well-defined since the matrix series is absolutely convergent element-wisely.
where \( s^c \) is the \( c \)-th element of \( \text{vec}(S) \).

Therefore, we have

\[
\mathbf{\mu} \leftarrow \mathbf{\mu} - t \mathbf{\hat{g}}^{[1]} \\
\mathbf{S} \leftarrow \text{Mat}(s^c) \mathbf{S} \text{Mat}(s^c) - t \mathbf{g}^{[2]} + \frac{t \times t}{2} \mathbf{g}^{[2]} \mathbf{S}^{-1} \mathbf{g}^{[2]} - \text{Mat}(t^c) \mathbf{g}^{[2]} \mathbf{S}^{-1} \mathbf{g}^{[2]} \mathbf{g}^{[2]}.
\]

### E.1. Natural Gradients and the Reparameterization Trick

Since \( \lambda = \{ \mu, S \} \) is a BCN parameterization of an exponential family distribution, gradients w.r.t. BC expectation parameters are natural gradients for BC natural parameters as shown in Theorem 3.

Given that \( S \) is known, the BC expectation parameter is \( \mathbf{m}_{[1]} = \mathbb{E}_{q(z)} [\mathbf{S} \mathbf{z}] = \mathbf{S} \mathbf{\mu} \). In this case, we know that \( \partial_\mu \mathcal{L} = \mathbf{S} \partial_{m_{[1]}} \mathcal{L} \).

Therefore, the natural gradient w.r.t. \( \mu \) is \( \mathbf{\hat{g}}^{[1]} = \partial_{m_{[1]}} \mathcal{L} = \mathbf{S}^{-1} \partial_\mu \mathcal{L} = \Sigma \partial_\mu \mathcal{L} \).

Likewise, given that \( \mu \) is known, the BC expectation parameter is \( \mathbf{m}_{[2]} = \mathbb{E}_{q(z)} \left[ -\frac{1}{2} \mathbf{z} \mathbf{z}^T + \mathbf{\mu} \mathbf{z}^T \right] = \frac{1}{2} (\mathbf{\mu} \mathbf{\mu}^T - \mathbf{S}^{-1}) \).

Therefore, the natural gradient w.r.t. \( S \) is \( \mathbf{\hat{g}}^{[2]} = \partial_{m_{[2]}} \mathcal{L} = -2 \partial_S \mathcal{L} = -2 \partial_{\Sigma} \mathcal{L} \).

Recall that \( \mathcal{L}(\lambda) = \mathbb{E}_{q(z|\lambda)} [\ell(D, \mathbf{z}) - \log p(\mathbf{z}) + \log q(\mathbf{z}|\lambda)] \), by the Gaussian identities (Opper & Archambeau, 2009; Särkkä, 2013), we have

\[
\begin{align*}
\partial_\mu \mathcal{L}(\lambda) &= \partial_\mu \left[ \mathbb{E}_{q(z|\lambda)} [\ell(D, \mathbf{z}) - \log p(\mathbf{z})] - \frac{1}{2} \log |2\pi \Sigma| \right] \\
&= \partial_\mu \mathbb{E}_{q(z|\lambda)} [\ell(D, \mathbf{z}) - \log p(\mathbf{z})] \\
&= \mathbb{E}_{q(z|\lambda)} [\nabla_\mu \ell(D, \mathbf{z}) - \log p(\mathbf{z})] \\
&= \mathbb{E}_{q(z|\lambda)} \left[ \nabla_\mu \ell(D, \mathbf{z}) - \log p(\mathbf{z}) \right] - \frac{1}{2} \Sigma^{-1} \Sigma^{-1} \\
&= \frac{1}{2} \mathbb{E}_{q(z|\lambda)} \left[ \Sigma^{-1} (\mathbf{z} - \mathbf{\mu}) \nabla_\mu \ell(D, \mathbf{z}) - \log p(\mathbf{z}) \right] - \frac{1}{2} \Sigma^{-1} \Sigma^{-1} \\
&= \frac{1}{2} \mathbb{E}_{q(z|\lambda)} \left[ \Sigma^{-1} (\mathbf{z} - \mathbf{\mu}) \nabla_\mu \left[ \ell(D, \mathbf{z}) - \log p(\mathbf{z}) \right] \right] - \frac{1}{2} \Sigma^{-1} \Sigma^{-1}
\end{align*}
\]

where (15) is also known as the reparameterization trick for the mean, (16) is also known as the reparameterization trick for the covariance, and we call (17) the Hessian trick.

Using Monte Carlo approximation, we have

\[
\mathbf{z} \sim q(\mathbf{z}|\lambda) = \mathcal{N}(\mathbf{z}|\mu, \Sigma) \\
\partial_\mu \mathcal{L} \approx \nabla_\mu [\ell(D, \mathbf{z}) - \log p(\mathbf{z})] \\
\partial_\Sigma \mathcal{L} \approx \frac{1}{4} \left( \mathbf{S} + \mathbf{S}^T \right) - \frac{1}{2} \Sigma^{-1} \\
\partial_\Sigma \mathcal{L} \approx \frac{1}{2} \left[ \nabla_\Sigma^2 [\ell(D, \mathbf{z}) - \log p(\mathbf{z})] \right] - \frac{1}{2} \Sigma^{-1}
\]

where \( \mathbf{S} := \Sigma^{-1} (\mathbf{z} - \mathbf{\mu}) \nabla_\mu^T [\ell(D, \mathbf{z}) - \log p(\mathbf{z})] \)

### E.2. Adam-like Update

We consider to solve the following problem

\[
\min_{\mu, s} \mathcal{L}(\mu, s) = \mathbb{E}_{q(z|\mu, s)} \left[ \sum_{i=1}^N \ell_i(\mathbf{z}) \right] - \log \mathcal{N}(\mathbf{z}|\mathbf{0}, \lambda^{-1} \mathbf{I}) + \log q(\mathbf{z}|\mu, s)
\]

where \( q(\mathbf{z}|\mu, s) = \mathcal{N}(\mathbf{z}|\mu, s) \), and \( s = \sigma^{-2} \).
Note that

\[ \partial_\mu \mathcal{L}(\mu, s) := \sum_{i=1}^{N} \partial_\mu \mathbb{E}_{q(z|\mu, s)} [\ell_i(z)] + \lambda \mu \]

\[ \partial_{\sigma^2} \mathcal{L}(\mu, s) := \sum_{i=1}^{N} \partial_{\sigma^2} \mathbb{E}_{q(z|\mu, s)} [\ell_i(z)] + \frac{1}{2} \lambda - \frac{1}{2} s \]

where \( \partial_\mu \mathbb{E}_{q(z|\mu, s)} [\ell_i(z)] \) and \( \partial_{\sigma^2} \mathbb{E}_{q(z|\mu, s)} [\ell_i(z)] \) can be computed by the reparameterization trick with MC approximations as follows.

\[ z \sim \mathcal{N}(z|\mu, s) \]

\[ \partial_\mu \mathbb{E}_{q(z|\mu, s)} [\ell_i(z)] = \mathbb{E}_{q(z|\mu, s)} [\nabla_z \ell_i(z)] \approx \nabla_z \ell_i(z) \]

\[ \partial_{\sigma^2} \mathbb{E}_{q(z|\mu, s)} [\ell_i(z)] = \frac{1}{2} \mathbb{E}_{q(z|\mu, s)} [s \odot (z - \mu) \odot \nabla_z \ell_i(z)] \approx \frac{1}{2} [s \odot (z - \mu) \odot \nabla_z \ell_i(z)] \]

The natural gradients can be computed as follows.

\[ \hat{g}^{[1]}_k = \sigma^2 \left( \partial_\mu \mathcal{L}(\mu, s) \big|_{\mu=\mu_k, s=s_k} \right) \]

\[ \hat{g}^{[2]}_k = -2 \partial_{\sigma^2} \mathcal{L}(\mu, s) \big|_{\mu=\mu_k, s=s_k} \]

The update induced by our rule with exponential step-sizes and the natural momentum (Khan et al., 2018) shown in blue is given as follows.

\[ \mu_{k+1} = \mu_k - t_1 \hat{g}^{[1]}_k + t_2 \sigma^2 \odot \sigma^{-2} \cdot \odot (\mu_k - \mu_{k-1}) \]

\[ \sigma^2_{k+1} = \sigma^2 - t_3 \hat{g}^{[2]}_k + t_4 \odot \sigma^2 \odot \hat{g}^{[2]}_k \]

where \( t_1 = t(1 - r_1) \frac{1 - r_2}{1 - r_1} \), \( t_2 = r_1 \frac{1 - r_2}{1 - r_1} \frac{1 - r_k}{1 - r_2} \), and \( t_3 = (1 - r_2) \).

Therefore, the update becomes

\[ \mu_{k+1} = \mu_k - t(1 - r_1) \frac{1 - r_2}{1 - r_1} \hat{s}_k - 1 \odot \hat{s}_k + r_1 \frac{1 - r_2}{1 - r_1} \frac{1 - r_k}{1 - r_2} \hat{s}_k - 1 \odot \hat{s}_k - 1 \odot (\mu_k - \mu_{k-1}) \]

\[ \hat{s}_{k+1} = \hat{s}_k + (1 - r_2) \hat{h}_k + \frac{(1 - r_2)^2}{2} \hat{h}_k \odot \hat{s}_k - 1 \odot \hat{h}_k \]

\[ s_{k+1} = \hat{s}_{k+1} \]

where \( g_k := \frac{1}{N} \sum_{i=1}^{N} \partial_\mu \mathbb{E}_{q(z|\mu, s)} [\ell_i(z)] \big|_{\mu=\mu_k, s=s_k} + \lambda \mu_k \) and \( h_k := \frac{2}{N} \sum_{i=1}^{N} \partial_{\sigma^2} \mathbb{E}_{q(z|\mu, s)} [\ell_i(z)] \big|_{\mu=\mu_k, s=s_k} + \frac{\lambda}{N} - \hat{s}_k \).
Let’s define $m_k := \frac{1-r_k}{t(1-r_k^2)} \hat{s}_{k-1} \odot (\mu_{k-1} - \mu_k)$. We can further simplify the above update as shown below.

$$
\mu_{k+1} = \mu_k - t(1-r_1) \frac{1-r_k}{1-r_1^2} \hat{s}_{k-1} \odot g_k + tr(1-r_1^2) \frac{1-r_k}{1-r_1^2} \hat{s}_{k-1} \odot (\mu_k - \mu_{k-1})
$$

$$
= \mu_k - t \frac{1-r_k}{1-r_1^2} \hat{s}_{k-1} \odot [(1-r_1)g_k + r_1 m_k]
$$

$$
m_{k+1} = \frac{1-r_k}{t(1-r_1^2)} \hat{s}_{k} \odot (\mu_k - \mu_{k+1})
$$

$$
= \frac{1-r_k}{t(1-r_1^2)} \frac{1-r_k}{1-r_1^2} [(1-r_1)g_k + r_1 m_k]
$$

$$
= (1-r_1)g_k + r_1 m_k
$$

$$
\hat{s}_{k+1} = \hat{s}_k + (1-r_2)h_k + \frac{(1-r_2)^2}{2} h_k \odot \hat{s}_{k}^{-1} \odot h_k
$$

$$
= \frac{1}{\lambda} [\hat{s}_k + (\hat{s}_k - (1-r_2)h_k) \odot \hat{s}_k^{-1} \odot (\hat{s}_k + (1-r_2)h_k)]
$$

$$
s_{k+1} = N\hat{s}_{k+1}
$$

where $z \sim q(z|\mu_k, s_k)$, $g_k \approx \nabla_z \ell(z) + \frac{1}{N} \mu_k$, and $h_k \approx [(N\hat{s}_k) \odot (z - \mu)] \odot \nabla_z \ell(z) + \frac{1}{N} \mu - \hat{s}_k$.

### E.3. Tran et al. (2019) is a special case of our update

In the Gaussian case, Tran et al. (2019) gives the following update

$$
\mu \leftarrow \mu - t \Sigma (\partial_\mu \mathcal{L})
$$

$$
= \Sigma \leftarrow \Sigma - t \hat{g}^{[2]} + \frac{t \times t}{2} \hat{g}^{[2]} \Sigma^{-1} \hat{g}^{[2]}
$$

where $\hat{g}^{[2]} = 2 \Sigma (\partial_2 \mathcal{L}) \Sigma$.

However, Tran et al. (2019) do not justify the use of the retraction map, which is just a retraction map developed for positive definite matrices. In this section, we show how to derive this update from our rule.

Now, we show that our rule can recover the above update using the parameterization $\lambda = \{\mu, \Sigma\}$. Recall that this parameterization is a BC parameterization. Given that $\Sigma$ is known, $\mu$ is the natural parameter and the expectation parameter is $m^{[1]}_i = E_{q(z)} [\Sigma^{-1} z] = \Sigma^{-1} \mu$ as shown in Appendix E.1. Therefore, the natural gradient w.r.t. $\mu$ is $\hat{g}^{[1]} = \partial_{m^{[1]}} \mathcal{L} = \Sigma \partial_\mu \mathcal{L}$.

Now, we show that the natural gradients w.r.t. $\Sigma$ is

$$
\hat{g}^{[2]} = 2 \Sigma (\partial_2 \mathcal{L}) \Sigma
$$

A proof using matrix calculus is provided below. See Barfoot (2020) for another proof using matrix calculus. By matrix calculus, we have

$$
- \mathbb{E}_{q(z)} \left[ \partial_{\Sigma^{[1]}} \partial_\Sigma \left[ \log q(z|\mu, \Sigma) \right] \right]
$$

$$
= \mathbb{E}_{q(z)} \left[ \partial_{\Sigma^{[1]}} \partial_\Sigma \left[ \frac{1}{2} (z - \mu)^T \Sigma^{-1} (z - \mu) + \frac{1}{2} \log |\Sigma|/(2\pi) \right] \right]
$$

$$
= \frac{1}{2} \mathbb{E}_{q(z)} \left[ \partial_{\Sigma^{[1]}} \left[ -\Sigma^{-1} (z - \mu)^T \Sigma^{-1} (z - \mu) \right] + \Sigma^{-1} \right]
$$

$$
= \frac{1}{2} \mathbb{E}_{q(z)} \left[ -\partial_{\Sigma^{[1]}} \left[ \Sigma^{-1} \right] (z - \mu)^T \Sigma^{-1} (z - \mu) \right] + \frac{1}{2} \partial_{\Sigma^{[1]}} \left[ \Sigma^{-1} \right]
$$

$$
= - \frac{1}{2} \partial_{\Sigma^{[1]}} \left[ \Sigma^{-1} \right] \mathbb{E}_{q(z)} \left[ (z - \mu)^T (z - \mu)^T \right] \Sigma^{-1} - \frac{1}{2} \Sigma^{-1} \mathbb{E}_{q(z)} \left[ (z - \mu)^T (z - \mu)^T \right] \partial_{\Sigma^{[1]}} \left[ \Sigma^{-1} \right] + \frac{1}{2} \partial_{\Sigma^{[1]}} \left[ \Sigma^{-1} \right]
$$

$$
= \frac{1}{2} \left[ -\partial_{\Sigma^{[1]}} \left[ \Sigma^{-1} \right] I - I \partial_{\Sigma^{[1]}} \left[ \Sigma^{-1} \right] + \partial_{\Sigma^{[1]}} \left[ \Sigma^{-1} \right] \right]
$$

$$
= - \frac{1}{2} \partial_{\Sigma^{[1]}} \left[ \Sigma^{-1} \right] \Sigma
$$
We denote the Christoffel symbols of second kind for \( \Sigma \) where we use the identity

\[
\mathbf{F}^{-1} = -2\partial_{\text{vec}(\Sigma^{-1})} [\text{vec}(\Sigma^{-1})]
\]

by the above expression. Note that \( \mathbf{F}^{-1} = -2\partial_{\text{vec}(\Sigma^{-1})} [\text{vec}(\Sigma)] \).

Note that \( \hat{g}^{[2]} \) is the natural gradient for \( \Sigma \). Since \( \lambda = \{ \mu, \Sigma \} \) is a BC parameterization, by Lemma 1, the natural gradient w.r.t. \( \text{vec}(\Sigma) \) is

\[
\text{vec}(\hat{g}^{[2]}) := \mathbf{F}^{-1} \text{vec}(\partial_{\Sigma} \mathcal{L}) = -2\partial_{\text{vec}(\Sigma^{-1})} [\text{vec}(\Sigma)] \text{vec}(\partial_{\Sigma} \mathcal{L}) = -2\partial_{\text{vec}(\Sigma^{-1})} [\text{vec}(\Sigma)] \partial_{\text{vec}(\Sigma)} \mathcal{L} = -2\partial_{\text{vec}(\Sigma^{-1})} \mathcal{L} = -2\text{vec}(\partial_{\Sigma^{-1}} \mathcal{L})
\]

where we obtain the fourth step using the chain rule.

Therefore, we have \( \hat{g}^{[2]} = -2\partial_{\Sigma^{-1}} \mathcal{L} \). By matrix calculus, we have

\[
\partial_{\Sigma^{-1}} \mathcal{L} = -\Sigma (\partial_{\Sigma} \mathcal{L}) \Sigma \]

Finally, we have

\[
\hat{g}^{[2]} = 2\Sigma (\partial_{\Sigma} \mathcal{L}) \Sigma
\]

Now, we show that the additional term for \( \mu \) is 0 under parameterization \( \lambda = \{ \mu, \Sigma \} \). Since \( \lambda \) is a BC parameterization, by Lemma 3, all entries of \( \Gamma^a_{b_1 c_1} \) for \( \mu \) are zeros. Therefore, the additional term for \( \mu \) is 0.

We denote the Christoffel symbols of second kind for \( \text{vec}(\Sigma) \) as \( \Gamma^a_{b_2 c_2} \). Now, we show that the additional term for \( \Sigma \) is \( -\hat{g}^{[2]} \Sigma^{-1} \hat{g}^{[2]} \).

Recall that the natural gradient for \( S = \Sigma^{-1} \) is \( G = -2\partial_{\Sigma} \mathcal{L} \). Under parameterization \( \lambda = \{ \mu, S \}, \hat{R}^{[2]}(t) \) has the following closed-form expression.

\[
\text{Mat}(\hat{R}^{[2]}(t)) = U \text{Exp}(t U^{-1} G U^{-1}) U
\]

where \( U = S^{\frac{1}{2}} \) and \( \text{Exp}(X) := I + \sum_{n=1}^{\infty} \frac{X^n}{n!} \).

Note that \( \Sigma = S^{-1} \). Therefore, under parameterization \( \lambda = \{ \mu, \Sigma \}, \) we have

\[
\text{Mat}(\hat{R}^{[2]}(t)) = \left[ \text{Mat}(\hat{R}^{[2]}(t)) \right]^{-1} = \left( U \text{Exp}(t U^{-1} G U^{-1}) U \right)^{-1} = U^{-1} \text{Exp}(-t U^{-1} G U^{-1}) U^{-1} = \Sigma^{1/2} \text{Exp}(-t \Sigma^{1/2} G \Sigma^{1/2}) \Sigma^{1/2} = \Sigma^{1/2} \text{Exp}(t \Sigma^{1/2} (2\partial_{\Sigma} \mathcal{L}) \Sigma^{1/2}) \Sigma^{1/2} = \Sigma^{1/2} \text{Exp}(t \Sigma^{1/2} [2\Sigma (\partial_{\Sigma} \mathcal{L}) \Sigma^{-1/2}] \Sigma^{1/2} \hat{g}^{[2]} = \Sigma^{1/2} \text{Exp}(t \Sigma^{-1/2} \hat{g}^{[2]} \Sigma^{-1/2} \hat{g}^{[2]} = \Sigma^{1/2} \text{Exp}(t \Sigma^{-1/2} \hat{g}^{[2]} \Sigma^{-1/2} \hat{g}^{[2]}),
\]

where we use the identity \( (\text{Exp}(t U^{-1} G U^{-1}))^{-1} = \text{Exp}(-t U^{-1} G U^{-1}) \).

Note that a geodesic is invariant under parameterization. Alternatively, we can obtain the above equation by using the fact that \( R^{[2]}(t) \) is a geodesic of Gaussian distribution with a constant mean.

Using a similar proof as shown in Lemma 4, the additional term for \( \Sigma \) is

\[
\text{Mat}(\Gamma^a_{b_2 c_2} \hat{g}^{[2]} \hat{g}^{[2]} = -\hat{g}^{[2]} \Sigma^{-1} \hat{g}^{[2]}
\]

where \( \Gamma^a_{b_2 c_2} \) is the Christoffel symbol for \( \text{vec}(\Sigma) \) and \( \hat{g}^{[2]} \) denotes the \( a \)-th element of \( \text{vec}(\hat{g}^{[2]}) \).
F. Example: Gamma Approximation

We consider the gamma distribution under the parameterization $\lambda = \{\lambda^{[1]}, \lambda^{[2]}\}$, where $\lambda^{[1]} = \alpha$ and $\lambda^{[2]} = \beta$. Since every block contains only a scalar, we use global indexes as $\lambda^{(i)} = \lambda^{a_i}$ and $\Gamma_{a_i,b_i,c_i} = \Gamma_{i,ii}$ for notation simplicity. The open-set constraint is $\Omega_1 = S_1^{++}$ and $\Omega_2 = S_2^{++}$. Under this parameterization, we can express the distribution as below.

$$q(z|\lambda) = z^{-1} \exp \left( \lambda^{(1)} \log z - z \lambda^{(1)} \lambda^{(2)} - A(\lambda) \right)$$

where $A(\lambda) = \log \Gamma_\alpha(\lambda^{(1)}) - \lambda^{(1)} \left( \log \lambda^{(1)} + \log \lambda^{(2)} \right)$ and $\Gamma_\cdot(\cdot)$ is the gamma function.

Lemma 5  The Fisher information matrix is diagonal under this parameterization. It implies that this parameterization is a BC parameterization.

Proof: Notice that $\mathbb{E}_{q(z|\lambda)} [z] = \frac{1}{\lambda^{(1)}}$. The Fisher information matrix is diagonal as shown below.

$$F(\lambda) = -\mathbb{E}_{q(z|\lambda)} \left[ \partial_2^2 \log q(z|\lambda) \right] = \mathbb{E}_{q(z|\lambda)} \left[ \partial_2^2 A(\lambda) \right] = \left[ \partial_\lambda(\psi) \frac{\lambda^{(1)}}{\lambda^{(2)}}, 0 \right]$$

where $\psi(\cdot)$ denotes the digamma function. □

Lemma 6  $\lambda$ is a BCN parameterization.

Proof: By Lemma 5, we know that $\lambda$ is a BC parameterization. Now, we show that $\lambda = \{\lambda^{(1)}, \lambda^{(2)}\}$ is a BCN parameterization. Clearly, each $\lambda^{(i)} \in S_{i}^{++}$ has all degrees of freedom.

The gamma distribution which can be written as following exponential form:

$$q(z|\lambda^{[1]}, \lambda^{[2]}) = z^{-1} \exp \left( \lambda^{(1)} \log z - z \lambda^{(1)} \lambda^{(2)} - A(\lambda) \right)$$

Considering two blocks with $\lambda^{(1)}$ and $\lambda^{(2)}$ respectively, we can express this distribution in the following two ways where the first equation is for the $\lambda^{(1)}$ block while the second equation is for the $\lambda^{(2)}$ block:

$$q(z|\lambda^{[1]}, \lambda^{[2]}) = z^{-1} \exp \left( \log z - z \lambda^{(2)} \lambda^{(1)} - A(\lambda) \right)$$

Therefore, by the definition of BCN, we know that $\lambda$ is a BCN parameterization. □
Using this BCN parameterization, the Christoffel symbols can be readily computed as below.

\[ \Gamma_{1,11} = \frac{1}{2} \partial_{\lambda^{(1)}}^3 A(\lambda) = \frac{1}{2} \partial_{\lambda^{(1)}}^2 \psi(\lambda^{(1)}) + \frac{1}{(\lambda^{(1)})^2} \]

\[ \Gamma_{2,22} = \frac{1}{2} \partial_{\lambda^{(2)}}^3 A(\lambda) = -\frac{\lambda^{(1)}}{(\lambda^{(2)})^3} \]

\[ \Gamma^1_{11} = \frac{\Gamma_{1,11}}{F_{11}} = \frac{\partial_{\lambda^{(1)}}^2 \psi(\lambda^{(1)}) + \frac{1}{(\lambda^{(1)})^2}}{2 \left( \partial_{\lambda^{(1)}} \psi(\lambda^{(1)}) - \frac{1}{\lambda^{(1)}} \right)} \]

\[ \Gamma^2_{22} = \frac{\Gamma_{2,22}}{F_{22}} = -\frac{1}{\lambda^{(2)}} \]

F.1. Proof of Theorem 2

We first prove the following lemma.

**Lemma 7** \( \Gamma_{1,11} < -\frac{1}{\lambda^{(1)}} \).

**Proof:** By Eq 1.4 at Batir (2005) and the last inequality at page 13 of Koumandos (2008), we have the following inequalities when \( \lambda^{(1)} > 0 \).

\[ \partial_{\lambda^{(1)}} \psi(\lambda^{(1)}) - \frac{1}{\lambda^{(1)}} > \frac{1}{2 (\lambda^{(1)})^2} > 0 \] Batir (2005) (18)

\[ \partial_{\lambda^{(1)}}^2 \psi(\lambda^{(1)}) < \frac{1}{(\lambda^{(1)})^2} - \frac{2 \partial_{\lambda^{(1)}} \psi(\lambda^{(1)})}{\lambda^{(1)}} \] Koumandos (2008) (19)

By (19), we have

\[ \partial_{\lambda^{(1)}}^2 \psi(\lambda^{(1)}) + \frac{1}{\lambda^{(1)}} > \frac{2}{(\lambda^{(1)})^2} - \frac{2 \partial_{\lambda^{(1)}} \psi(\lambda^{(1)})}{\lambda^{(1)}} = \frac{2}{\lambda^{(1)}} \left( \frac{1}{\lambda^{(1)}} - \partial_{\lambda^{(1)}} \psi(\lambda^{(1)}) \right) \]

Since \( \partial_{\lambda^{(1)}} \psi(\lambda^{(1)}) - \frac{1}{\lambda^{(1)}} > 0 \), we have

\[ 2 \Gamma^1_{11} = \frac{\partial_{\lambda^{(1)}}^2 \psi(\lambda^{(1)}) + \frac{1}{(\lambda^{(1)})^2}}{\partial_{\lambda^{(1)}} \psi(\lambda^{(1)}) - \frac{1}{\lambda^{(1)}}} < -\frac{2}{\lambda^{(1)}} \]

which shows \( \Gamma^1_{11} < -\frac{1}{\lambda^{(1)}} \).

□

Now, we give a proof for Theorem 2.

**Proof:** The proposed update for \( \lambda^{(1)} \) with step-size \( \tau \) is given below.

\[
\lambda^{(1)} \leftarrow \lambda^{(1)} - \tau \hat{g}^{(1)} - \frac{\tau^2}{2} \left( \Gamma^1_{11} \right) \left( \hat{g}^{(1)} \right)^2 \\
> \lambda^{(1)} - \tau \hat{g}^{(1)} - \frac{\tau^2}{2} \left( \frac{1}{\lambda^{(1)}} \right) \left( g^{(1)} \right)^2 \\
= \frac{1}{2\lambda^{(1)}} \left[ \frac{1}{2\lambda^{(1)}} - \frac{1}{\lambda^{(1)}} \right] \left( \lambda^{(1)} \right)^2 - \frac{\left( \lambda^{(1)} - \tau \hat{g}^{(1)} \right)^2}{2\lambda^{(1)}} \\
= \frac{1}{2\lambda^{(1)}} \left( \lambda^{(1)} \right)^2 + \left( \lambda^{(1)} - \tau \hat{g}^{(1)} \right)^2 \\
\geq 0
\]
Handling the Positive-Definite Constraint in the Bayesian Learning Rule

where in the second step we use the inequality $\Gamma_{11}^{11} < -\frac{1}{\lambda^{1\prime}}$ shown by Lemma 7.

Similarly, we can show the update for $\lambda^{(2)}$ also satisfies the constraint.

$$
\lambda^{(2)} \leftarrow \lambda^{(2)} - t\hat{g}^{(2)} + \frac{t^2}{2} \left( \frac{1}{\lambda^{(2)}} \right) \left( \hat{g}^{(2)} \right)^2
$$

$$
= \frac{1}{2\lambda^{(2)} > 0} \left[ \left( \lambda^{(2)} \right)^2 + \left( \lambda^{(2)} - t\hat{g}^{(2)} \right)^2 \right]_{>0}^{\geq 0}
$$

It is obvious to see that the proposed update satisfies the underlying constraint.

□

F.2. Natural Gradients

Recall that $\hat{g}$ are the natural-gradients, which can be computed as shown below.

$$
\hat{g}^{(1)} = \frac{\partial \lambda^{(1)}}{\partial \lambda^{(1)}} \frac{L}{\lambda^{(1)}} \psi (\lambda^{(1)}) - \frac{1}{\lambda^{(1)}} \hat{g}^{(2)} = \left( \frac{\lambda^{(2)}}{\lambda^{(1)}} \right)^2 \frac{\partial \lambda^{(2)}}{\partial \lambda^{(1)}} L
$$

Recall that $\lambda^{(1)} = \alpha$ and $\lambda^{(2)} = \frac{\beta}{\alpha}$. Using the chain rule, we know that

$$
\partial \lambda^{(1)} L = \partial_\alpha L + \frac{\beta}{\alpha} \partial_\beta L, \quad \partial \lambda^{(2)} L = \alpha \partial_\beta L
$$

$\partial_\alpha L$ and $\partial_\beta L$ can be computed by the implicit reparameterization trick (Figurnov et al., 2018).

G. Example: Exponential Approximation

In this case, there is only one block with a scalar. We denote $\lambda^{[1]} = \lambda^{(1)}$ and $\Gamma_{[a_1,b_1,c_1]} = \Gamma_{11}$ for notation simplicity. We consider an exponential distribution under the natural parameterization $\lambda = \lambda^{(1)}$ with the open-set constraint $\Omega = S_{+\cdot}^1$:

$$
q(z|\lambda) = \exp \left( -\lambda^{(1)} z - A(\lambda) \right)
$$

where $A(\lambda) = -\log \lambda^{(1)}$. The FIM is a scalar $F_{11} = \frac{1}{(\lambda^{(1)})^2}$. It is obvious that $\lambda$ is a BCN parameterization. The Christoffel symbols can be readily computed as below.

$$
\Gamma_{11}^{11} = \frac{1}{2} \partial_\lambda^3 A(\lambda) = -\frac{1}{(\lambda^{(1)})^3}
$$

$$
\Gamma_{11} = \frac{\Gamma_{11}^{11}}{F_{11}} = -\frac{1}{\lambda^{(1)}}
$$

The proposed natural-gradient update with step-size $t$ is

$$
\lambda^{(1)} = \lambda^{(1)} - t\hat{g}^{(1)} + \frac{t^2}{2} \left( \frac{1}{\lambda^{(1)}} \right) \left( \hat{g}^{(1)} \right)^2
$$

where $\hat{g}^{(1)}$ is the natural-gradient. Note that $\hat{g}^{(1)}$ is the natural-gradient, which can be computed as shown below.

$$
\hat{g}^{(1)} = \left( \lambda^{(1)} \right)^2 \partial \lambda^{(1)} L.
$$

where $\partial \lambda^{(1)} L$ can be computed by the implicit reparameterization trick as $\partial \lambda^{(1)} L = \partial \lambda \partial_z \partial_z L$.

Lemma 8 The proposed update satisfies the underlying constraint.
Proof: The proposed natural-gradient update with step-size $t$ is given below.

$$\lambda^{(1)} \leftarrow \lambda^{(1)} - t \hat{g}^{(1)} + \frac{t^2}{2} \left( \frac{1}{\lambda^{(1)}} \right) \left( \hat{g}^{(1)} \right)^2$$

$$= \frac{1}{2\lambda^{(1)}} \left[ 2 \left( \lambda^{(1)} \right)^2 - 2t \hat{g}^{(1)} \lambda^{(1)} + \left( t \hat{g}^{(1)} \right)^2 \right]$$

$$= \frac{1}{2\lambda^{(1)}} \left[ \left( \lambda^{(1)} \right)^2 + \left( \lambda^{(1)} - t \hat{g}^{(1)} \right)^2 \right]$$

It is obvious to see that the proposed update satisfies the underlying constraint. □

G.1. Implicit reparameterization gradient

Now, we discuss how to compute the gradients w.r.t. $\lambda$ using the implicit reparameterization trick. To use the implicit reparameterization trick, we have to compute the following term.

$$\partial_\lambda z = \frac{-\partial_\lambda Q(z|\lambda)}{q(z|\lambda)}$$

$$= \frac{-\partial_\lambda (1 - \exp(-\lambda z))}{\lambda \exp(-\lambda z)}$$

$$= \frac{z \exp(-\lambda z)}{-\lambda \exp(-\lambda z)}$$

$$= \frac{z}{\lambda}$$

where $Q(z|\lambda)$ is the C.D.F. of $q(z|\lambda)$.

H. Example: Inverse Gaussian Approximation

We consider the following distribution.

$$q(z|\alpha, \beta) = \sqrt{\frac{1}{2\pi z^3}} \exp \left( -\frac{z\alpha\beta^2}{2} - \frac{\alpha}{2z} + \log \alpha + \alpha\beta \right)$$

We consider a BCN parameterization $\lambda = \{\lambda^{(1)}, \lambda^{(2)}\}$, where $\lambda^{(1)} = \beta^2$ and $\lambda^{(2)} = \alpha$ and the open-set constraint is $\Omega_1 = S_{++}^1$ and $\Omega_2 = S_{++}^2$. Since every block contains only a scalar, we denote $\lambda^{(i)} = \lambda[i]$ and $\Gamma_{a,b,c} = \Gamma_{i,ii}$ for notation simplicity. Under this parameterization, we can re-express the distribution as

$$q(z|\lambda) = \sqrt{\frac{1}{2\pi z^3}} \exp \left( -\frac{z}{2} \lambda^{(1)} \lambda^{(2)} - \frac{\lambda^{(2)}}{2z} - A(\lambda) \right)$$

where $A(\lambda) = -\frac{\log \lambda^{(2)}}{2} - \lambda^{(2)} \sqrt{\lambda^{(1)}}$.

Lemma 9 The FIM is (block) diagonal under this parameterization.

Proof: Notice that $E_{q(z|\lambda)}[z] = \frac{1}{\sqrt{\lambda^{(1)}}}$ The FIM is (block) diagonal as shown below.

$$F(\lambda) = -E_{q(z|\lambda)} \left[ \partial^2_\lambda \log q(z|\lambda) \right]$$

$$= -E_{q(z|\lambda)} \left[ \begin{array}{c}
\frac{1}{2} - \frac{\partial^2_{\lambda^{(1)}} A(\lambda)}{\sqrt{\lambda^{(1)}}} \\
\frac{1}{2} \left( -z + \frac{1}{\sqrt{\lambda^{(1)}}} \right) - \frac{\partial^2_{\lambda^{(2)}} A(\lambda)}{\lambda^{(2)}} \\
\end{array} \right]$$

$$= E_{q(z|\lambda)} \left[ \begin{array}{cc}
\partial^2_{\lambda^{(1)}} A(\lambda) & 0 \\
0 & \partial^2_{\lambda^{(2)}} A(\lambda) \\
\end{array} \right]$$

$$= \begin{bmatrix}
\frac{1}{4} (\lambda^{(1)})^{-3/2} & 0 \\
0 & \frac{1}{2} (\lambda^{(2)})^{-2}
\end{bmatrix}$$
It is easy to show that $\lambda$ is a BCN parameterization since $\lambda$ satisfies Assumption 1 to 3. Due to the BCN parameterization, the Christoffel symbols can be readily computed as below.

\[
\begin{align*}
\Gamma_{1,11} &= \frac{1}{2} \partial_{\lambda(1)}^3 A(\lambda) = -\frac{3}{16} (\lambda^{(1)})^{-5/2} \lambda^{(2)}, \\
\Gamma_{2,22} &= \frac{1}{2} \partial_{\lambda(2)}^2 A(\lambda) = -\frac{1}{2} (\lambda^{(2)})^{-3}, \\
\Gamma_{11}^1 &= \frac{\Gamma_{1,11}}{F_{11}} = -\frac{3}{4\lambda^{(1)}}, \\
\Gamma_{22}^2 &= \frac{\Gamma_{2,22}}{F_{22}} = -\frac{1}{\lambda^{(2)}}.
\end{align*}
\]

The proposed natural-gradient update with step-size $t$ is

\[
\begin{align*}
\lambda^{(1)} &\leftarrow \lambda^{(1)} - t\hat{g}^{(1)} + \frac{t^2}{2} \left( -\frac{3}{4\lambda^{(1)}} \right) \left( \hat{g}^{(1)} \right)^2, \\
\lambda^{(2)} &\leftarrow \lambda^{(2)} - t\hat{g}^{(2)} + \frac{t^2}{2} \left( \frac{1}{\lambda^{(2)}} \right) \left( \hat{g}^{(2)} \right)^2.
\end{align*}
\]

**Lemma 10** The update above satisfies the underlying constraint.

**Proof:** The proposed natural-gradient update with step-size $t$ is given below.

\[
\begin{align*}
\lambda^{(1)} &\leftarrow \lambda^{(1)} - t\hat{g}^{(1)} + \frac{t^2}{2} \left( -\frac{3}{4\lambda^{(1)}} \right) \left( \hat{g}^{(1)} \right)^2 \\
&= \frac{1}{4\lambda^{(1)}} \left[ 4 \left( \lambda^{(1)} \right)^2 - 4t\hat{g}^{(1)} \lambda^{(1)} + \frac{3}{2} \left( t\hat{g}^{(1)} \right)^2 \right] \\
&= \frac{1}{4\lambda^{(1)}} \left[ \left( 2\lambda^{(1)} \right)^2 - t\hat{g}^{(1)} \lambda^{(1)} \right] \left( \hat{g}^{(1)} \right)^2 \\
\lambda^{(2)} &\leftarrow \lambda^{(2)} - t\hat{g}^{(2)} + \frac{t^2}{2} \left( \frac{1}{\lambda^{(2)}} \right) \left( \hat{g}^{(2)} \right)^2 \\
&= \frac{1}{2\lambda^{(2)}} \left[ 2 \left( \lambda^{(2)} \right)^2 - 2t\hat{g}^{(2)} \lambda^{(2)} \right] \left( \hat{g}^{(2)} \right)^2 \\
&= \frac{1}{2\lambda^{(2)}} \left[ \left( \lambda^{(2)} \right)^2 + \left( \lambda^{(2)} - t\hat{g}^{(2)} \right)^2 \right].
\end{align*}
\]

It is obvious to see that the proposed update satisfies the underlying constraint. □

Recall that $\hat{g}$ are the natural-gradients, which can be computed as shown below.

\[
\hat{g}^{(1)} = \frac{4}{\lambda^{(2)}} \left( \lambda^{(1)} \right)^{3/2} \partial_{\lambda^{(1)}} L, \quad \hat{g}^{(2)} = 2 \left( \lambda^{(2)} \right)^2 \partial_{\lambda^{(2)}} L.
\]

Using the chain rule, we know that

\[
\begin{align*}
\partial_{\lambda^{(1)}} L &= \frac{1}{2\beta} \partial_{\beta} L, \\
\partial_{\lambda^{(2)}} L &= \partial_{\alpha} L
\end{align*}
\]

$\partial_{\alpha} L$ and $\partial_{\beta} L$ can be computed by the implicit reparameterization trick (Salimans & Knowles, 2013; Figurnov et al., 2018) as $\partial_{\eta} L = [\partial_{\eta} \theta] [\nabla_{\theta} L]$, where $\eta = \{\alpha, \beta\}$. 

H.1. Implicit reparameterization gradient

Now, we discuss how to compute the gradients w.r.t. $\alpha$ and $\beta$ using the implicit reparameterization trick. To use the implicit reparameterization trick, we have to compute the following term.

$$
\partial_w z = -\frac{\partial_q Q(z|\eta)}{q(z|\eta)} = \frac{\partial_q [\Phi(\sqrt{\frac{z}{2}} (z\beta - 1)) + \exp(2\alpha \beta) \Phi(-\sqrt{\frac{z}{2}} (z\beta + 1))]}{\sqrt{\frac{1}{2\pi z^3}} \exp \left( -\frac{z\alpha^2}{2} - \frac{\alpha}{2z} + \log \frac{\alpha}{2} + \alpha \beta \right)}
$$

where $\eta = \{\alpha, \beta\}$, $Q(z|\eta)$ is the C.D.F. of the inverse Gaussian distribution, and $\Phi(x) = \int_{-\infty}^{x} N(t|0, 1) dt$ is the C.D.F. of the standard Gaussian distribution. We use the following fact to simplify the above expression.

$$
\delta(z, \alpha, \beta) := \frac{\exp(2\alpha \beta) \Phi(-\sqrt{\frac{z}{2}} (z\beta + 1))}{N(\sqrt{\frac{z}{2}} (z\beta - 1)|0, 1)} = \frac{\Phi(-\sqrt{\frac{z}{2}} (z\beta + 1))}{N(-\sqrt{\frac{z}{2}} (z\beta + 1)|0, 1)}
$$

where $\delta(z, \alpha, \beta)$ is known as the Mills ratio of Gaussian distribution. Using this fact, we can get the simplified expressions as follows.

$$
\partial_\alpha z = \frac{z}{\alpha} - 2 \beta z^{3/2} \alpha^{-1/2} \delta(z, \alpha, \beta)
$$
$$
\partial_\beta z = -2 z^{3/2} \alpha^{1/2} \delta(z, \alpha, \beta)
$$

where it is numerical stable to compute $\log(\delta(z, \alpha, \beta))$ since the logarithm of Gaussian cumulative distribution function can be computed by using existing libraries, such as the scipy.special.log_ndtr() function.

In fact, we have closed-form expressions of gradients of the entropy term as shown below.

$$
\mathbb{E}_{q(z|\eta)} [-\log q(z|\eta)] = \frac{1}{2} [\log \alpha - 3 \log \beta + \exp(2\alpha \beta) E_1(2\alpha \beta)] + 1 + \log(2\pi)
$$
$$
\partial_\alpha \mathbb{E}_{q(z|\eta)} [-\log q(z|\eta)] = \frac{1}{\alpha} - 3 \beta \exp(2\alpha \beta) E_1(2\alpha \beta)
$$
$$
\partial_\beta \mathbb{E}_{q(z|\eta)} [-\log q(z|\eta)] = -3 \alpha \exp(2\alpha \beta) E_1(2\alpha \beta)
$$

where $E_1(x) := \int_{x}^{\infty} \frac{e^{-t}}{t} dt$ is the exponential integral. It is not numerical stable to compute the product $\exp(x) E_1(x)$ when $x > 100$. In this case, we can use the asymptotic expansion (see Eq 3 at Tseng & Lee (1998)) for the exponential integral to approximate the product as shown below.

$$
\exp(x) E_1(x) \approx \frac{1}{x} \left[ 1 + \sum_{n=1}^{N} \frac{(-1)^n n!}{x^n} \right] \text{ when } x > 100,
$$

where $N$ is an integer such as $N \leq x < N + 1$.

I. Mixture of Exponential Family Distributions

Let’s consider the following mixture of exponential family distributions $q(z) = \int q(z, w) dw$. The joint distribution $q(z, w|\lambda) = q(w|\lambda_w) q(z|w, \lambda_z)$ is called the conditional exponential family (CEF) by Lin et al. (2019).

$$
q(w|\lambda_w) := h_w(w) \exp \left( \{\phi_w(w), \lambda_w\} - A_w(\lambda_w) \right)
$$
$$
q(z|w, \lambda_z) := h_z(w, z) \exp \left( \{\phi_z(w, z), \lambda_z\} - A_z(w, \lambda_z) \right)
$$

where $\lambda = \{\lambda_z, \lambda_w\}$.

We will use the joint Fisher information matrix suggested by Lin et al. (2019) as the metric $F$ to derive our improved learning rule for mixture approximations.
I.1. The Joint Fisher Information Matrix and Christoffel Symbols

Lin et al. (2019) propose to use the FIM of the joint distribution \( q(w, z | \lambda) \), where they refer this FIM as the joint FIM. The joint FIM and the corresponding Christoffel symbols of first kind are defined as follows.

\[
F_{ab} := -\mathbb{E}_{q(w,z|\lambda)} [\partial_a \partial_b \log q(w, z | \lambda)] \\
\Gamma_{d,ab} := \frac{1}{2} [\partial_b F_{db} + \partial_b F_{ab} - \partial_d F_{ab}]
\]

where we denote \( \partial_a = \partial_{\lambda^a} \) for notation simplicity.

Like the exponential family cases as shown in Eq. (14), the Christoffel symbols of first kind can be computed as

\[
\Gamma_{d,ab} = \frac{1}{2} \left[ \mathbb{E}_{q(w,z|\lambda)} [\partial_a \partial_b \log q(w, z | \lambda) \partial_d \log q(w, z | \lambda)] - \mathbb{E}_{q(w,z|\lambda)} [\partial_d \partial_a \log q(w, z | \lambda)] \left[ \partial_b \log q(w, z | \lambda) \right] - \mathbb{E}_{q(w,z|\lambda)} [\partial_d \partial_b \log q(w, z | \lambda)] \right]
\]

(20)

I.2. The BCN Parameterization

Now, we show that how to simplify the computation of the Christoffel symbols by extending the BCN parameterization for this kind of mixtures.

To this end, we first assume that \( \lambda \) can be partitioned with \((m + n)\) blocks to satisfy Assumption 1 in the main text.

\[
\lambda = \left\{ \lambda_s^{[1]}, \ldots, \lambda_s^{[m]} \right\} \cup \left\{ \lambda_w^{[m+1]}, \ldots, \lambda_w^{[m+n]} \right\}
\]

Then, we extend the definition of BC parameterization to conditional exponential family, which is similar to Assumption 2 in the main text and a concrete example of Definition 1 in Appendix B.1.

**Assumption 2 [Block Coordinate Parameterization]**: A parameterization is block coordinate (BC) if the joint FIM under this parameterization is block-diagonal according to the block structure of the parameterization.

As shown in Lin et al. (2019), for any parameterization \( \lambda = \{\lambda_s, \lambda_w\} \), the joint FIM has the following two blocks: \( F_z \) for block \( \lambda_s \) and \( F_w \) for block \( \lambda_w \).

\[
F = \begin{bmatrix} F_z & 0 \\ 0 & F_w \end{bmatrix}
\]

Assumption 2 implies that \( F_w \) and \( F_z \) are both block-diagonal according to the block structure of \( \lambda_w \) and \( \lambda_s \), respectively. The block diagonal structure is given below if \( \lambda = \{\lambda_s^{[1]}, \ldots, \lambda_s^{[m]} \cup \lambda_w^{[m+1]}, \ldots, \lambda_w^{[m+n]}\} \) is a BC parameterization.

\[
F = \begin{bmatrix}
\begin{bmatrix} F_z^1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & F_z^m \end{bmatrix} & 0 \\
0 & \begin{bmatrix} F_w^{m+1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & F_w^{m+n} \end{bmatrix}
\end{bmatrix}
\]

**Assumption 3 [Block Natural Parameterization for Conditional Exponential-Family]**: For a conditional exponential-family distribution \( q(w, z | \lambda) = q(w | \lambda_w) q(z | w, \lambda_s) \),

- \( \lambda_w \) is a BCN parameterization of the exponential family distribution \( q(w | \lambda_w) \).
\( \lambda_z \) is a parameterization of \( q(z|w, \lambda_z) \), where there exist function \( \phi_z \) and \( h_z \), for each block \( \lambda_z[i] \) such that conditioning on \( w \), \( q(z|w, \lambda_z) \) can be re-expressed as a minimal conditional exponential family distribution (see Lin et al. (2019) for the definition of the minimality) given that the rest of blocks \( \lambda_z[-i] \) are known.

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

We say \( \lambda = \{\lambda_z, \lambda_w\} \) is a BCN parameterization for the mixture if it satisfies Assumption 1 to 3.

Mixture approximations studied in Lin et al. (2019) have a BCN parameterization. For concrete examples, see Appendix J and K.

**I.3. Our Learning Rule for Mixture Approximations**

Now, we are ready to discuss the learning rule for mixture approximations. Under a BC parameterization \( \lambda = \{\lambda_z, \lambda_w\} \), our learning rule remains the same as shown below.

\[
\lambda^c_i \leftarrow \lambda^{c_i} - t \ddot{g}^{c_i} - \frac{t^2}{2} \Gamma^{c_i}_{a,b_i} \ddot{g}^a_i \ddot{g}^b_i
\]

where \( i \) can be either a block of \( \lambda_w \) or \( \lambda_z \).

First, note that the sub-block matrix \( F_{w} \) of the joint FIM is indeed the FIM of \( q(w|\lambda_w) \). Furthermore, \( q(w|\lambda_w) \) is an exponential family distribution. If \( \lambda = \{\lambda_z, \lambda_w\} \) is a BCN parameterization, it is easy to see that the computation of the Christoffel symbols for \( \lambda_w \) is exactly the same as the exponential family cases as discussed in Appendix D.

Furthermore, we can simplify the Christoffel symbols for \( \lambda_z \) due to the following Theorem.

**Theorem 4** If \( \lambda \) is a BCN parameterization of a conditional exponential family (CEF) with the joint FIM, natural gradient and the Christoffel symbols of first kind for block \( \lambda_z[i] \) can be simplified as

\[
\ddot{g}^{c_i} = \partial_{m_{a_i}} \mathcal{L} ; \quad \Gamma^{c_i}_{a,b_i} = \frac{1}{2} \mathbb{E}_{q(w|\lambda_w)} \left[ \partial_{\lambda_z[a_i]} \partial_{\lambda_z[b_i]} \partial_{\lambda_z[c_i]} A_z(w, \lambda_z) \right]
\]

where \( m_{a_i} \) denotes the \( a \)-th element of the block coordinate expectation parameter \( m[i] \) as \( m[i] = \mathbb{E}_{q(w,z|\lambda)} \left[ \phi_z(z, w, \lambda_z[-i]) \right] \) and \( \lambda_z^{c_i} \) is the \( a \)-th element of \( \lambda_z[i] \).

**I.4. Proof of Theorem 4**

We assume \( \lambda_z = \{\lambda_z[1], \ldots, \lambda_z[m]\} \) is partitioned with \( m \) blocks.

Since \( \lambda \) is a BCN parameterization, conditioning on \( w \) and given \( \lambda_z[-i] \) and \( \lambda_w \) are known, we can re-express \( q(z|w, \lambda_z) \) as

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

where \( q(z|w, \lambda_z) \) is also an one-parameter EF distribution conditioning on \( \lambda_z[-i] \) and \( w \). Similarly, we have the following results.

\[
\mathbb{E}_{q(z|w, \lambda_z)} \left[ \partial_{a_i} \log q(z|w, \lambda_z) \right] = 0
\]

where \( \partial_{a_i} = \partial_{\lambda_z^{c_i}} \) is for notation simplicity. Using the above identities, we have

\[
\mathbb{E}_{q(z|w, \lambda_z)} \left[ \partial_{a_i} \log q(z|w, \lambda_z) \partial_{b_i} \log q(z|w, \lambda_z) \right] = \mathbb{E}_{q(z,w|\lambda_z)} \left[ \partial_{a_i} \partial_{b_i} \log q(z|w, \lambda_z) \partial_{d_i} \log q(z|w, \lambda_z) \right]
\]

\[
= \mathbb{E}_{q(z,w|\lambda_z)} \left[ \partial_{a_i} \log q(z|w, \lambda_z) \partial_{d_i} \log q(z|w, \lambda_z) \right]
\]

\[
= -\mathbb{E}_{q(z,w|\lambda_z)} \left[ \partial_{a_i} \partial_{b_i} A_z(w, \lambda_z) \mathbb{E}_{q(z|w, \lambda_z)} \left[ \partial_{d_i} \log q(z|w, \lambda_z) \right] \right]
\]

\[
= 0
\]
Therefore, by Eq. (20), we can simplify the Christoffel symbols for $\lambda_z^{[i]}$ as follows.

$$
\Gamma_{d_i,a_i,b_i} = - \frac{1}{2} \mathbb{E}_{q(z,w|\lambda)} \left[ \partial_{a_i} \partial_{b_i} \partial_{d_i} \log q(z,w|\lambda) \right]
$$

$$
= - \frac{1}{2} \mathbb{E}_{q(w|\lambda_z)} \left[ \partial_{a_i} \partial_{b_i} \partial_{d_i} \log q(z,w,\lambda_z) \right]
$$

$$
= \frac{1}{2} \mathbb{E}_{q(w|\lambda_z)} \left[ \partial_{a_i} \partial_{b_i} A_z(\lambda_z, w) \right]
$$

where we use $d_i$ to denote the $d$-th entry of block $\lambda_z^{[i]}$.

Likewise, let $m_{[i]} = \mathbb{E}_{q(z,w|\lambda)} \left[ \dot{\phi}_{z_i}(z,w,\lambda_z^{[-i]}) \right]$ denote the block coordinate expectation parameter. We have

$$
0 = \mathbb{E}_{q(w|\lambda_z)} \left[ \partial_{a_i} \partial_{z_i} \log q(z,w,\lambda_z) \right] = m_{a_i} - \mathbb{E}_{q(w|\lambda_z)} \left[ \partial_{a_i} A_z(\lambda, w) \right]
$$

where $m_{a_i}$ denotes the $a$-th element of $m_{[i]}$.

Therefore, we know that $m_{a_i} = \mathbb{E}_{q(w|\lambda_z)} \left[ \partial_{a_i} A_z(\lambda, w) \right]$.

Recall that the sub-block of joint FIM for $\lambda_z^{[i]}$ denoted by $F_z^{[i]}$ can be computed as

$$
F_{a_i,b_i} = - \mathbb{E}_{q(z,w|\lambda)} \left[ \partial_{b_i} \partial_{a_i} \log q(z,w|\lambda) \right]
$$

$$
= - \mathbb{E}_{q(z,w|\lambda)} \left[ \partial_{b_i} \partial_{a_i} \log q(z,w,\lambda_z) \right]
$$

$$
= - \mathbb{E}_{q(z,w|\lambda)} \left[ - \partial_{b_i} \partial_{a_i} A_z(\lambda_z, w) \right]
$$

$$
= \mathbb{E}_{q(z,w|\lambda)} \left[ \partial_{b_i} \partial_{a_i} A_z(\lambda_z, w) \right]
$$

$$
= \partial_{b_i} m_{a_i}
$$

where we use the fact that $\lambda_w$ does not depend on $\lambda_z^{[i]}$ and $\partial_{b_i} = \partial_{\lambda_z^{[i]}}$ to move from the fourth step to the fifth step.

Recall that when $\lambda$ is a BC parameterization, the joint FIM $F$ is block-diagonal as shown below.

$$
F = \begin{bmatrix}
F_z & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \vdots \\
0 & \cdots & F_z^{[m]} & 0 \\
0 & \cdots & 0 & F_w^{[m+1]} \cdots 0 \\
\vdots & \ddots & \vdots & \vdots \\
0 & \cdots & 0 & \cdots F_w^{[m+n]} \\
\end{bmatrix}
$$

If $F_z^{[i]}$ is positive definite everywhere, we have

$$
F_{a_i,b_i} = \partial_{m_{a_i}} \lambda_z^{[i]}
$$

The above assumption is true if given that $\lambda_z^{[-i]}$ and $\lambda_w$ are known, $q(w,z|\lambda)$ is an one-parameter minimal CEF distribution (Lin et al., 2019).

The above result implies that we can compute natural gradients as follows.

$$
\hat{g}_{a_i} = F_{a_i,b_i} g_{b_i} = \left[ \partial_{m_{a_i}} \lambda_z^{[i]} \right] \left[ \partial_{\lambda_z^{[i]}} \mathcal{L} \right] = \partial_{m_{a_i}} \mathcal{L}
$$

where $g_{b_i} = \partial_{\lambda_z^{[i]}} \mathcal{L}$. 

J. Example: Finite Mixture of Gaussians Approximation

We consider a K-mixture of Gaussians under this parameterization \( \mathbf{\lambda} = \{ \mathbf{\mu}_c, \mathbf{S}_c \}_{c=1}^K, \mathbf{\lambda}_w \)  

\[
q(\mathbf{z}, \mathbf{\pi}, \{ \mathbf{\mu}_c, \mathbf{S}_c \}_{c=1}^K) = \sum_{c=1}^K \pi_c \mathcal{N}(\mathbf{z} | \mathbf{\mu}_c, \mathbf{S}_c)
\]

where \( \pi_c \) is the mixing weight so that \( \sum_{c=1}^K \pi_c = 1 \). \( \mathbf{S}_c = \mathbf{\Sigma}_c^{-1}, \mathbf{\lambda}_w = \{ \log(\pi_c / \pi_K) \}_{c=1}^{K-1} \) and \( \pi_K = 1 - \sum_{c=1}^{K-1} \pi_c \). The constraints are \( \mathbf{\lambda}_w \in \mathbb{R}^{K-1}, \mathbf{\mu}_c \in \mathbb{R}^d, \) and \( \mathbf{S}_c \in \mathbb{S}_{++}^{d \times d} \).

Under this parameterization, the joint distribution can be expressed as below.

\[
q(\mathbf{z}, \mathbf{w} | \mathbf{\lambda}) = q(\mathbf{w} | \mathbf{\lambda}_w)q(\mathbf{z} | \mathbf{w}, \{ \mathbf{\mu}_c, \mathbf{S}_c \}_{c=1}^K)
\]

\[
q(\mathbf{w} | \mathbf{\lambda}_w) = \exp(\sum_{c=1}^{K-1} \mathbb{1}(w = c) \lambda_{wc} - A_w(\mathbf{\lambda}_w))
\]

\[
q(\mathbf{z} | \mathbf{w}, \{ \mathbf{\mu}_c, \mathbf{S}_c \}_{c=1}^K) = \exp\left( \sum_{c=1}^K \mathbb{I}(w = c) \left[ -\frac{1}{2} \mathbf{z}^T \mathbf{S}_c \mathbf{z} + \mathbf{z}^T \mathbf{S}_c \mathbf{\mu}_c - A_z(\{ \mathbf{\mu}_c, \mathbf{S}_c \}_{c=1}^K, w) \right] \right)
\]

where \( B(\mathbf{\mu}_c, \mathbf{S}_c) = \frac{1}{2} [\mathbf{\mu}_c^T \mathbf{S}_c \mathbf{\mu}_c - \log |\mathbf{S}_c|/(2\pi)] \), \( A_z(\{ \mathbf{\mu}_c, \mathbf{S}_c \}_{c=1}^K, w) = \sum_{c=1}^K \mathbb{I}(w = c) B(\mathbf{\mu}_c, \mathbf{S}_c), \lambda_{wc} = \log(\frac{\pi_c}{\pi_K}), A_w(\mathbf{\lambda}_w) = \log(1 + \sum_{c=1}^{K-1} \exp(\lambda_{wc})) \).

**Lemma 11** The joint FIM is block diagonal under this parameterization.

\[
F = \begin{bmatrix}
F_{\mu_1} & 0 & \cdots & 0 & 0 \\
0 & F_{\mu_2} & \cdots & 0 & 0 \\
\vdots & \ddots & \ddots & \vdots & \vdots \\
0 & \cdots & F_{\mu_K} & 0 & 0 \\
0 & \cdots & 0 & F_{S_K} & 0
\end{bmatrix}
\]

Therefore, this parameterization is a BC parameterization.

**Proof:** We will prove this lemma by showing that all cross terms are zeros.

Case 1: First, we will show that cross terms (shown in red) between \( \mathbf{\lambda}_w \) and \( \mathbf{\lambda}_z := \{ \mathbf{\mu}_c, \mathbf{S}_c \}_{c=1}^K \) are zeros.

Let’s denote \( \lambda_{w}^i \) be an element of \( \mathbf{\lambda}_w \) and \( \lambda_{z}^i \) be an element of \( \mathbf{\lambda}_z \). By the definition, each cross term in this case is defined as follows.

\[
- \mathbb{E}_{q(\mathbf{z}, \mathbf{w} | \mathbf{\lambda})} \left[ \partial_{\lambda_{w}^i} \partial_{\lambda_{z}^j} \log q(\mathbf{z}, \mathbf{w} | \mathbf{\lambda}) \right] = - \mathbb{E}_{q(\mathbf{z}, \mathbf{w} | \mathbf{\lambda})} \left[ \partial_{\lambda_{w}^i} \partial_{\lambda_{z}^j} \left( \log q(\mathbf{w} | \mathbf{\lambda}_w) + \log q(\mathbf{z} | \mathbf{\lambda}_z) \right) \right] = 0
\]

Case 2: Next, we will show that cross terms between (shown in blue) any two Gaussian components are zeros.

Let’s denote \( \lambda_{a}^i \) be an element of \( \{ \mathbf{\mu}_a, \mathbf{S}_a \} \) and \( \lambda_{b}^i \) be an element of \( \{ \mathbf{\mu}_b, \mathbf{S}_b \} \), where \( a \neq b \).
By the definition, each cross term in this case is defined as belows.

\[- E_{q(z,w|\lambda)} \left[ \partial_{\lambda_a}^i \partial_{S_u}^j \log q(z, w|\lambda) \right] = - E_{q(z,w|\lambda)} \left[ \partial_{\lambda_a}^i \partial_{S_u}^j \left( \log q(z|w, \{\mu_c, S_c\}_{c=1}^K) \right) \right] = - E_{q(z,w|\lambda)} \left[ I(w = b) \partial_{\lambda_a}^i \left( \partial_{\lambda_a}^j \left( -\frac{1}{2} z^T S_a z + z^T S_a \mu_a - B(\mu_a, S_a) \right) \right) \right] = 0 \]

It is obvious that the above expression is 0 since \( \partial_{\lambda_a}^i u(z, \mu_b, \Sigma_b) = 0 \) when \( a \neq b \).

Case 3: Finally, we will show that for each component \( a \), cross terms (shown in green) between \( \mu_a \) and \( S_a \) are zeros.

Let’s denote \( \mu_a^i \) be the \( i \)-th element of \( \mu_a \) and \( S_a^{jk} \) be the element of \( S_a \) at position \((j, k)\). Furthermore, \( e_j \) denotes an one-hot vector where all entries are zeros except the \( i \)-th entry with value 1, and \( I_{jk} \) denotes an one-hot matrix where all entries are zeros except the entry at position \((j, k)\) with value 1. By the definition, the cross term is defined as belows.

\[- E_{q(z,w|\lambda)} \left[ \partial_{\mu_a^i} \partial_{S_a^{jk}} \log q(z, w|\lambda) \right] = - E_{q(z,w|\lambda)} \left[ \partial_{\mu_a^i} \partial_{S_a^{jk}} \left( \log q(z|w, \{\mu_c, S_c\}_{c=1}^K) \right) \right] = - E_{q(z,w|\lambda)} \left[ I(w = a) \left( \partial_{\mu_a^i} \partial_{S_a^{jk}} \left( I(w = a) -\frac{1}{2} e_i^T S_a z + e_i^T S_a \mu_a - B(\mu_a, S_a) \right) \right) \right] = \pi_a e_i^T I_{jk} \mu_a = 0 \]

where we use the following fact in the last step.

\[ E_{q(z,w|\lambda)} \left[ I(w = a) z \right] = \pi_a \mu_a \]
\[ E_{q(z,w|\lambda)} \left[ I(w = a) \right] = \pi_a \]

\[ \square \]

**Lemma 12** The parameterization \( \lambda = \{ \{\mu_c, S_c\}_{c=1}^K, \lambda_w \} \) is a BCN parameterization.

**Proof:** Clearly, this parameterization satisfies Assumption 1 described in the main text. By Lemma 11, we know that this parameterization is a BC parameterization. Now, we will show that this parameterization also satisfies Assumption 3 in Appendix 1.2.

First note that \( \lambda_w \) has only one block and it is the natural parameterization of exponential family distribution \( q(w|\lambda_w) \), which implies that \( \lambda_w \) is a BCN parameterization for \( q(w|\lambda_w) \).

Note that given the rest blocks are known and conditioning on \( w \), \( q(z|w, \lambda_z) \) can be re-expressed as follows in terms of block \( \mu_k \).

\[ q(z|w, \lambda_z) = \exp \left( \sum_{c=1}^K I(w = c) \left( -\frac{1}{2} z^T S_c z + z^T S_c \mu_c \right) - A_z(\{\mu_c, S_c\}_{c=1}^K, w) \right) \]
\[ = \exp \left( \sum_{c \neq k} [I(w = c) \left( -\frac{1}{2} z^T S_c z + z^T S_c \mu_c \right) + I(w = k) \left( -\frac{1}{2} z^T S_k z \right)] \right) \exp \left( \left. \frac{1}{2} \right| \phi_{x_k} \left( w, \lambda_{-k1} \right) \right) \]
\[ = h_{x_k}(w, \lambda_{-k1}) \]
Similarly, for block $S_k$, $q(z|w, \lambda_z)$ can be re-expressed as follows

$$q(z|w, \lambda_z) = \exp \left( \sum_{c \neq k} \left[ \tilde{I}(w = c) \left( -\frac{1}{2} z^T S_c z + z^T S_c \mu_c \right) \right] \right) \exp \left( \left\{ \tilde{I}(w = k) \left[ -\frac{1}{2} z z^T + \mu_k z^T \right], S_k \right\} - \Lambda_z \left( \{ \mu_c, S_c \}_{c=1}^K, w \right) \right)$$

Since this parameterization satisfies Assumption 1 to 3, this parameterization is a BCN parameterization.

We denote the Christoffel symbols of first kind and second kind for $\mu_k$ as $\Gamma_{a_k,b_k,c_k}$ and $\Gamma^{\alpha_k}_{b_k,c_k}$, respectively.

**Lemma 13** For each component $k$, all entries of $\Gamma^{\alpha_k}_{b_k,c_k}$ for $\mu_k$ are zeros.

**Proof:** The proof is very similar to the proof of Lemma 3. We will prove this by showing that all entries of $\Gamma_{a_k,b_k,c_k}$ are zeros. For notation simplicity, we use $\Gamma_{a,b,c}$ to denote $\Gamma_{a_k,b_k,c_k}$. Let $\mu_k^a$ denote the $a$-th element of $\mu_k$.

The following expression holds for any valid $a$, $b$, and $c$.

$$\Gamma_{a,b,c} = \frac{1}{2} E_{q(z,w|\lambda)} \left[ \partial_{\mu_k^a} \partial_{\mu_k^b} \partial_{\mu_k^c} A_z(\{ \mu_j, S_j \}_{j=1}^K, w) \right]$$

where in the last step we use the fact that $S_k$, $e_a$, and $e_c$ do not depend on $\mu_k$. 

Similarly, we denote the Christoffel symbols second kind for vec($S_k$) as $\Gamma^{\alpha_k}_{b_k,c_k}$.

**Lemma 14** For each component $k$, the additional term for $S_k$ is $-\tilde{g}_k S_k^{-1} \tilde{g}_k^T$.

**Proof:** Recall that, in the Gaussian case $N(\mu, \tilde{S})$, the additional term for $S$ is $\text{Mat}(\Gamma_{b_k,c_k}^{a_k}) = \tilde{g}_k^T \tilde{S}^{-1} \tilde{g}_k$, where $\Gamma_{b_k,c_k}^{a_k}$ denotes the Christoffel symbols of second kind for vec($S$).

To prove the statement, we will show that the Christoffel symbols of second kind for vec($S_k$) is exactly the same as the Gaussian case, when $\tilde{S} = S_k$. In other words, when $\tilde{S} = S_k$, we will show $\Gamma_{b_k,c_k}^{a_k} = \Gamma_{b_k,c_k}^{a_k}$.

We denote the Christoffel symbols of second kind for vec($S_k$) using $\Gamma^{a_k}_{b_k,c_k}$. By definition, the Christoffel symbols of second kind for vec($S_k$) is defined as follows since $\lambda$ is a BC parameterization.

$$\Gamma^{a_k}_{b_k,c_k} = F^{a_k}_{b_k,c_k} \Gamma^{a_k}_{b_k,c_k}$$

We will first show that $\Gamma_{d_k,b_k,c_k} = \pi_k \Gamma_{d_k,b_k,c_k}$.

In the Gaussian case, by definition, we have

$$\Gamma_{d_k,b_k,c_k} = \frac{1}{2} E_{q(z,w|\lambda)} \left[ \partial_{S_{d_k}} \partial_{S_{b_k}} \partial_{S_{c_k}} A(\mu, S) \right] = \frac{1}{4} \partial \tilde{S}_{d_k} \partial \tilde{S}_{b_k} \partial \tilde{S}_{c_k} \left( \log |S| \right)$$

where $A(\mu, S) = \frac{1}{2} [\mu^T \tilde{S} \mu - \log |\tilde{S}/(2\pi)|]$ is the log partition function of the Gaussian distribution and $\tilde{S}^d$ denotes the $d$-th element of vec($S$) in the Gaussian case.
Handling the Positive-Definite Constraint in the Bayesian Learning Rule

Therefore, we have the following result in the MOG case when $S_k = \bar{S}$.

\[
\Gamma_{dk_2,dk_2} = \frac{1}{2} \mathbb{E}_{q(z,w|\lambda)} \left[ \partial_{S_k} \partial_{S_k} \partial_A z \left( \{ \mu_j, S_j \}_{j=1}^K, w \right) \right] \\
= \frac{1}{2} \mathbb{E}_{q(z,w|\lambda)} \left[ (w = k) \partial_{S_k} \partial_{S_k} \partial_B B(\mu_k, S_k) \right] \\
= \frac{1}{2} \mathbb{E}_{q(z,w|\lambda)} \left[ (w = k) \partial_{S_k} \partial_{S_k} \partial_{S_k} ^{c} \left( -\frac{1}{2} \log |S_k|/(2\pi) \right) \right] \\
= -\pi_k \frac{1}{4} \partial_{S_k} \partial_{S_k} \partial_{S_k} ^{c} (\log |S_k|) \\
= \pi_k \bar{\Gamma}_{d_2,b_2c_2}
\]

where $S_k^a$ denotes the $a$-th element of $\text{vec}(S_k)$ and $\mathbb{E}_{q(z,w|\lambda)} [ (w = k) ] = \pi_k$.

Let $F_{a_2d_2}$ denote the element at position $(a, d)$ of the sub-block matrix of the joint FIM for block $\text{vec}(S_k)$ in the MOG case. Similarly, when $S_k = \bar{S}$, we can show that $F_{a_2d_2} = \pi_k \bar{F}_{a_2d_2}$, where $F_{a_2d_2}$ denotes the element at position $(a, d)$ of the sub-block matrix of the FIM for block $\text{vec}(S)$ in the Gaussian case.

Therefore, $F_{a_2d_2} = \pi_k^{-1} \bar{F}_{a_2d_2}$ when $\bar{S} = S_k$.

Finally, when $\bar{S} = S_k$, we obtain the desired result since

\[
\Gamma_{a_2b_2c_2}^{a_2b_2c_2} = F_{a_2d_2} \Gamma_{d_2,b_2c_2} \\
= (\pi_k^{-1} \bar{F}_{a_2d_2}) (\pi_k \bar{\Gamma}_{d_2,b_2c_2}) \\
= \bar{F}_{a_2d_2} \bar{\Gamma}_{d_2,b_2c_2} \\
= \bar{\Gamma}_{b_2c_2}
\]

where $\bar{\Gamma}_{b_2c_2}$ denotes the Christoffel symbols of second kind for $\text{vec}(\bar{S})$ in the Gaussian case.

\[\square\]

J.1. Natural Gradients

Recall that $\mathcal{L}(\lambda) = \mathbb{E}_{q(z|\lambda)}[\ell(D, z) - \log p(z) + \log q(z|\lambda)]$, where $q(z|\lambda) = \int q(z, w|\lambda)dw$.

Note that $\lambda_w$ is the natural parameter of exponential family distribution $q(w|\lambda_w)$, we can obtain the natural gradient by computing the gradient w.r.t. the mean parameter as shown by Lin et al. (2019).

\[
\hat{g}_w = \partial_{\mu} \mathcal{L},
\]

where $\partial_{\pi_c} \mathcal{L}$ denotes the $c$-th element of $\partial_{\pi} \mathcal{L}$, $\pi_c := \mathbb{E}_{q(w)} \left[ I(w = c) \right]$ and the gradient $\partial_{\pi_c} \mathcal{L}$ can be computed as below as suggested by Lin et al. (2019).

\[
\partial_{\pi_c} \mathcal{L} = \mathbb{E}_{q(z)} \left[ (\delta_c - \delta_k) b(z) \right]
\]

where $b(z) := \ell(D, z) - \log p(z) + \log q(z|\lambda)$, and $\delta_c := N(z|\mu_c, S_c) / \sum_{k=1}^K \pi_k N(z|\mu_k, S_k)$.

Recall that $\lambda_w$ is unconstrained in this case, there is no need to compute the addition term for $\lambda_w$.

Now, we discuss how to compute the natural gradients $\{ \hat{g}_{[1]}^c, \hat{g}_{[2]}^c \}_{c=1}^K$. Since $\{ \mu_c, S_c \}_{c=1}^K$ are BCN parameters, we can obtain the natural gradients by computing gradients w.r.t. its BC expectation parameter due to Theorem 4.

Given the rest of blocks are known, the BC expectation parameter for block $\mu_k$ is

\[
\mathbb{E}_{q(w|z)} \left[ I(w = k) \right] (S_k z)
\]

In this case, we know that $\partial_{\mu_k} \mathcal{L} = \pi_k S_k \partial_{\mu_k} \mathcal{L}$. Therefore, the natural gradient w.r.t. $\mu_k$ is $\hat{g}_{[1]}^k = \partial_{\mu_k} \mathcal{L} = \pi_k^{-1} S_k^{-1} \partial_{\mu_k} \mathcal{L} = \pi_k^{-1} \Sigma_k \partial_{\mu_k} \mathcal{L}$, where the gradient $\partial_{\mu_k} \mathcal{L}$ can be computed as below as suggested by Lin et al. (2019).

\[
\partial_{\mu_k} \mathcal{L} = \mathbb{E}_{q(z)} \left[ \pi_k \delta_k \nabla z b(z) \right]
\]
Likewise, given the rest of blocks are known, the BC expectation parameter for block $S_k$ is

$$m_{k, z} = E_{q(w, z)} \left[ \mathbb{E}(w = k) \left( -\frac{1}{2}zz^T + \mu_k z^T \right) \right]$$

$$= \frac{\pi_k}{2} (\mu_k \mu_k^T - S_k^{-1})$$

Therefore, the natural gradient w.r.t. $S_k$ is $\hat{g}_k^{[2]} = \partial_{m_{k, z}} \mathcal{L} = -\frac{1}{\pi_k} \partial_{S_k} \mathcal{L} = -\frac{1}{\pi_k} \partial_{S_k} f$, where the gradient $\partial_{S_k} f$ can be computed as below as suggested by Lin et al. (2019).

$$\partial_{S_k} \mathcal{L} = \frac{1}{2} \mathbb{E}_{q(z)} \left[ \pi_k \delta_k \nabla_z^2 b(z) \right]$$

Alternatively, we can use the re-parametrization trick to compute the gradient as below.

$$\partial_{S_k} \mathcal{L} = \frac{1}{2} \mathbb{E}_{q(z)} \left[ \pi_k \delta_k (z - \mu_k) \nabla_z^2 b(z) \right]$$

By Lemma 13 and 14, the proposed update induced by our rule is

$$\log(p_c / \pi_K) \leftarrow \log(p_c / \pi_K) - t \mathbb{E}_{q(z)} [(\delta_c - \delta_K) b(z)]$$

$$\mu_c \leftarrow \mu_c - t S_c^{-1} \mathbb{E}_{q(z)} [\delta_c \nabla_z b(z)]$$

$$S_c \leftarrow S_c - t G_c + \frac{j^2}{2} G_c (S_c)^{-1} G_c$$

where we do not compute the additional term for $\lambda_w$ since $\lambda_w$ is unconstrained, $\delta_c := \mathcal{N}(z | \mu_c, S_c) / \sum_{k=1}^K \pi_k \mathcal{N}(z | \mu_k, S_k)$, $b(z) := \ell(D, z) - \log p(z) + \log q(z | \lambda)$ and $G_c$ can be computed as below.

Note that $b(z)$ can be the logarithm of an unnormalized target function. Lin et al. (2019) suggest to use the Hessian trick to compute $G_c$ as shown in (22). We can also use the re-parametrization trick to compute $G_c$ as shown in (21).

$$G_c = -\mathbb{E}_{q(z)} [\delta_c S_c (z - \mu_c) \nabla_z^2 b(z)]$$

$$= -\mathbb{E}_{q(z)} [\delta_c \nabla_z^2 b(z)]$$

We use the MC approximation to compute $\hat{G}_c$ as below.

$$z \sim q(z)$$

$$\hat{G}_c \approx \hat{S}_c + \hat{S}_c^T$$

referred to as “-rep”

$$\hat{G}_c \approx -\delta_c \nabla_z^2 b(z)$$

referred to as “-hess”

where $\hat{S}_c := \delta_c S_c (z - \mu_c) \nabla_z^2 b(z)$

**K. Example: Skew Gaussian Approximation**

We consider the skew Gaussian approximation proposed by Lin et al. (2019). The joint distribution is given below.

$q(z, w | \alpha, \mu, \Sigma) = q(z | w, \alpha, \mu, \Sigma) \mathcal{N}(w | 0, 1)$

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

$$= \exp \left\{ \mathbb{E} \left( -\frac{1}{2} \Sigma^{-1} zz^T + |w| \alpha_T \Sigma^{-1} z + \mu_T \Sigma^{-1} z - \frac{1}{2} (|w| \alpha_T \Sigma^{-1} + \mu_T \Sigma^{-1}) + \mathbb{E} \left( \log |2 \pi \Sigma| \right) \right) \right\}$$

We consider the parameterization $\lambda = \{ [\mu \alpha], S \}$, where $S = \Sigma^{-1}$, $\lambda^{[1]} = [\mu \alpha]$, and $\lambda^{[2]} = S$. The open-set constraint is $\lambda \in \mathbb{R}^{2d \times d} \times \mathbb{R}^{d \times d}$. Under this parameterization, the distribution $q(z | w)$ can be re-expressed as below.

$$q(z | w, \lambda) = \exp \left\{ \mathbb{E} \left( -\frac{1}{2} S z z^T + z^T S (Q(w))^T \lambda^{[1]} - A_z(\lambda, w) \right) \right\}$$

where $Q(w) := \left[ \begin{array}{c|c} I_d & \frac{1}{2} \mu \alpha^T \end{array} \right]$ is a $2d$-by-$d$ matrix and $A_z(\lambda, w) = \frac{1}{2} \left[ \begin{array}{c} \mu_T \alpha^T \end{array} \right] (Q(w))^T \left[ \begin{array}{c} \mu \\ \alpha \end{array} \right] - \mathbb{E} \left( |S| / (2 \pi) \right)$.
Lemma 15 The joint FIM is block diagonal with two blocks under this parameterization.

\[ \mathbf{F} = \begin{bmatrix} \mathbf{F}^{[1]} & 0 \\ 0 & \mathbf{F}^{[2]} \end{bmatrix} \]

Therefore, this parameterization is a BC parameterization.

Proof: We will prove this lemma by showing that all cross terms shown in red are zeros.

Let’s denote \( \lambda^{a_1} \) be the \( a \)-th element of \( \lambda^{[1]} \) and \( S^{bc} \) be the element of \( S \) at position \((b, c)\). Furthermore, \( e_a \) denotes an one-hot vector where all entries are zeros except the \( a \)-th entry with value 1, and \( I_{bc} \) denotes an one-hot matrix where all entries are zeros except the entry at position \((b, c)\) with value 1.

By definition, the cross term is defined as follows:

\[- \mathbb{E}_{q(z|w, \lambda)} [\partial_{w^1} \partial_{S^{bc}} \log q(z|w)] = - \mathbb{E}_{q(z|w, \lambda)} \left[ z^T I_{bc} (Q(w))^T e_a - \left( \lambda^{[1]} \right)^T Q(w) I_{bc} (Q(w))^T e_a \right] = - \mathbb{E}_{q(w)} \left[ \mathbb{E}_{q(z|w, \lambda)} \left[ z^T I_{bc} (Q(w))^T e_a - \left( \lambda^{[1]} \right)^T Q(w) I_{bc} (Q(w))^T e_a \right] \right] = - \mathbb{E}_{q(w)} \left[ \left( \lambda^{[1]} \right)^T Q(w) I_{bc} (Q(w))^T e_a - \left( \lambda^{[1]} \right)^T Q(w) I_{bc} (Q(w))^T e_a \right] = 0 \]

where we use the following expression in the last step.

\[ \mathbb{E}_{q(z|w, \lambda)} [z] = |w| \alpha + \mu = (Q(w))^T \lambda^{[1]} \]

\[ \square \]

Note that another parameterization \( \{\mu, \alpha, S\} \) is not a BC parameterization since the joint FIM is not block-diagonal under this parameterization.

Lemma 16 Parameterization \( \lambda \) is a BCN parameterization.

Proof: Clearly, this parameterization satisfies Assumption 1 described in the main text. By Lemma 15, we know that this parameterization is a BC parameterization. Now, we will show that this parameterization also satisfies Assumption 3 in Appendix 1.2.

Note that given the rest blocks are known and conditioning on \( w \), \( q(z|w, \lambda) \) can be re-expressed as follows in terms of block \( \lambda^{[1]} \).

\[ q(z|w, \lambda) = \exp \left\{ \text{Tr} \left( - \frac{1}{2} S z z^T \right) + z^T S (Q(w))^T \lambda^{[1]} - A_z(\lambda, w) \right\} \]

\[ = \exp \left\{ \text{Tr} \left( - \frac{1}{2} S z z^T \right) \right\} \exp \left[ (Q(w) S z, \lambda^{[1]}) - A_z(\lambda, w) \right] \]

Similarly, for block S, \( q(z|w, \lambda) \) can be re-expressed as follows

\[ q(z|w, \lambda) = \underbrace{\exp \left\{ - \frac{1}{2} z z^T + z \left( \lambda^{[1]} \right)^T Q(w) S \right\} - A_z(\lambda, w)}_{h_2(w, z, \lambda^{-1})} \]

Since this parameterization satisfies Assumption 1 to 3, this parameterization is a BCN parameterization.

We denote the Christoffel symbols of first kind and second kind for \( \lambda^{[1]} \) as \( \Gamma_{a_1, b_1 c_1}^{a_1} \) and \( \Gamma_{b_1 c_1}^{a_1} \) respectively.

Lemma 17 All entries of \( \Gamma_{a_1, b_1 c_1}^{a_1} \) for \( \lambda^{[1]} \) are zeros.
Handling the Positive-Definite Constraint in the Bayesian Learning Rule

Proof: We will prove this by showing that all entries of $\Gamma_{b_1c_1}^{a_1}$ are zeros. Let $\lambda^{a_1}$ denote the $a$-th element of $\lambda^{[1]}$.

The following expression holds for any valid $a$, $b$, and $c$.

$$\Gamma_{a_1,b_1c_1} = \frac{1}{2} \mathbb{E}_{q(z,w|\lambda)} \left[ \partial_{\lambda^{a_1}} \partial_{\lambda^{c_1}} \partial_{\lambda^{b_1}} A_z(\lambda, w) \right]$$

$$= \frac{1}{2} \mathbb{E}_{q(z,w|\lambda)} \left[ \partial_{\lambda^{a_1}} \partial_{\lambda^{c_1}} \left( (e_a)^T Q(w) S (Q(w))^T \lambda^{[1]} \right) \right]$$

$$= \frac{1}{2} \mathbb{E}_{q(z,w|\lambda)} \left[ \partial_{\lambda^{a_1}} \left( (e_a)^T Q(w) S (Q(w))^T e_c \right) \right] = 0$$

where in the last step we use the fact that $S$, $Q(w)$, $e_a$, and $e_c$ do not depend on $\lambda^{[1]}$.

\[\square\]

We denote the Christoffel symbols of second kind for $\vec{\Gamma}$ as $\vec{\Gamma}_{b_2c_2}^{a_2}$.

Lemma 18 The additional term for $S$ is $-\hat{g}^{[2]} S^{-1} \hat{g}^{[2]}$

Proof: Recall that, in the Gaussian case $\mathcal{N}(\mu, \hat{S})$, the additional term for $S$ is $\text{Mat}(\vec{\Gamma}_{b_2c_2} S^{b_2c_2}) = \hat{g}^{[2]} S^{-1} \hat{g}^{[2]}$, where $\vec{\Gamma}_{b_2c_2}$ denotes the Christoffel symbols of second kind for $\vec{\Gamma}$.

To prove the statement, we will show that the Christoffel symbols of second kind for $\vec{\Gamma}$ is exactly the same as the Gaussian case, when $\hat{S} = S$.

We denote the Christoffel symbols of second kind for $\vec{\Gamma}$ as $\vec{\Gamma}_{b_2c_2}^{a_2}$. By definition, the Christoffel symbols of second kind for $\vec{\Gamma}$ is defined as follows.

$$\vec{\Gamma}_{b_2c_2}^{a_2} = F_{a_2d_2} \vec{\Gamma}_{d_2,b_2c_2}$$

We will show that $\vec{\Gamma}_{a_2,b_2c_2} = \vec{\Gamma}_{a_2,b_2c_2}$.

In the Gaussian case, we have

$$\vec{\Gamma}_{d_2,b_2c_2} = -\frac{1}{4} \partial_{S^a} \partial_{S^c} \partial_{S^d} \left( \log |S| \right)$$

where $A(\mu, \hat{S}) = \frac{1}{2} \left[ \mu^T \hat{S} \mu - \log |\hat{S}|/(2\pi) \right]$ is the log partition function of the Gaussian distribution and $\hat{S}^{a}$ is the $a$-th element of $\vec{S}$ in the Gaussian case.

Therefore, we have the following result when $\hat{S} = S$.

$$\vec{\Gamma}_{d_2,b_2c_2} = \frac{1}{2} \mathbb{E}_{q(z,w|\lambda)} \left[ \partial_{S^a} \partial_{S^c} \partial_{S^d} A_z(\lambda, w) \right]$$

$$= -\frac{1}{4} \partial_{S^a} \partial_{S^c} \partial_{S^d} \log |S|$$

$$= \vec{\Gamma}_{d_2,b_2c_2}$$

where $S^a$ denotes the $a$-th element of $\vec{S}$.

Let $F_{a_2d_2}$ denote the element at position $(a, d)$ of the sub-block matrix of the joint FIM for $\vec{\Gamma}$. Similarly, we can show that $F_{a_2d_2} = \hat{F}_{a_2d_2}$, where $\hat{F}_{a_2d_2}$ denotes the element at position $(a, d)$ of the FIM for $\vec{S}$ in the Gaussian case. Therefore, $F_{a_2d_2} = \hat{F}_{a_2d_2}$.

Finally, when $\hat{S} = S$, we obtain the desired result since

$$\vec{\Gamma}_{b_2c_2}^{a_2} = F_{a_2d_2} \vec{\Gamma}_{d_2,b_2c_2}$$

$$= \hat{F}_{a_2d_2} \vec{\Gamma}_{d_2,b_2c_2}$$

$$= \vec{\Gamma}_{b_2c_2}^{a_2}$$

where $\vec{\Gamma}_{b_2c_2}^{a_2}$ denotes the Christoffel symbols of second kind for $\vec{\Gamma}$ in the Gaussian case.

\[\square\]
Using these lemmas, the proposed update induced by our rule is

\[
\begin{bmatrix}
\mu \\
\alpha
\end{bmatrix} \leftarrow \begin{bmatrix}
\mu \\
\alpha
\end{bmatrix} - t \hat{g}^{[1]}
\]

\[
S \leftarrow S - t \hat{g}^{[2]} + \frac{t^2}{2} \hat{g}^{[2]} S^{-1} \hat{g}^{[2]}
\]

where \( \hat{g}^{[1]} \) and \( \hat{g}^{[2]} \) are natural gradients.

Similarly, it can be shown that the above update satisfies the underlying constraints.

**K.1. Natural Gradients**

Now, we discuss how to compute the natural gradients. Since the parameterization is a BCN parameterization, gradients w.r.t. BC expectation parameters are natural gradients for BCN parameters due to Theorem 4.

Recall that \( \lambda^{[1]} = \begin{bmatrix} \mu \\ \alpha \end{bmatrix} \). Let \( m^{[1]} = \begin{bmatrix} m_\mu \\ m_\alpha \end{bmatrix} \) denote the BC expectation parameter for \( \lambda^{[1]} \). Given \( S \) is known, the BC expectation parameter is

\[
\begin{bmatrix}
m_\mu \\
m_\alpha
\end{bmatrix} = \mathbb{E}_{q(w,z)} [Q(w)Sz]
\]

\[
= \mathbb{E}_{q(w)} \left[ Q(w)S (Q(w))^T \lambda^{[1]} \right]
\]

\[
= \mathbb{E}_{q(w)} \left[ \begin{bmatrix} I_d \\ |w| I_d \end{bmatrix} S [I_d \ |w| I_d] \lambda^{[1]} \right]
\]

\[
= \mathbb{E}_{q(w)} \left[ \begin{bmatrix} S \\ |w| S \\
|w|S \\ w^2 S \end{bmatrix} \begin{bmatrix} \mu \\ \alpha \end{bmatrix} \right]
\]

\[
= \begin{bmatrix} S \\
|w| S \\
|w|S \\
S \mu + cS \alpha \\
S \mu + S \alpha
\end{bmatrix}
\]

where \( c = \mathbb{E}_{q(w)} [|w|] = \sqrt{\frac{2}{\pi}} \).

Since \( S = \Sigma^{-1} \), we have the following expressions.

\[
\mu = \frac{1}{1 - c^2} \Sigma (m_\mu - cm_\alpha)
\]

\[
\alpha = \frac{1}{1 - c^2} \Sigma (m_\alpha - cm_\mu)
\]

By the chain rule, we have

\[
\partial_{m_\mu} L = \Sigma \left( \frac{1}{1 - c^2} \partial_{m_\mu} L - \frac{c}{1 - c^2} \partial_{m_\alpha} L \right)
\]

\[
\partial_{m_\alpha} L = \Sigma \left( \frac{1}{1 - c^2} \partial_{m_\alpha} L - \frac{c}{1 - c^2} \partial_{m_\mu} L \right)
\]

Therefore, the natural gradient w.r.t. \( \lambda^{[1]} = \begin{bmatrix} \mu \\ \alpha \end{bmatrix} \) is

\[
\hat{g}^{[1]} = \begin{bmatrix} \partial_{m_\mu} L \\ \partial_{m_\alpha} L \end{bmatrix}
\]

where the gradient \( \partial_{m_\mu} L \) and \( \partial_{m_\alpha} L \) can be computed as suggested by Lin et al. (2019).
Likewise, the BC expectation parameter for block $S$ is

\[
\mathbf{m}_{[2]} = \mathbb{E}_{q(w,z)} \left[ -\frac{1}{2} \mathbf{z} \mathbf{z}^T + \mathbf{z} \left( \lambda^{[1]} \right)^T \mathbf{Q}(w) \right] \\
= -\frac{1}{2} \mathbf{S}^{-1} + \mathbb{E}_{q(w)} \left[ \frac{1}{2} (\mathbf{Q}(w))^T \lambda^{[1]} (\lambda^{[1]})^T \mathbf{Q}(w) \right]
\]

Since $\lambda^{[1]}$ is known, $\mathbb{E}_{q(w)} \left[ \frac{1}{2} (\mathbf{Q}(w))^T \lambda^{[1]} (\lambda^{[1]})^T \mathbf{Q}(w) \right]$ does not depend on $S$. Therefore, the natural gradient w.r.t. $S$ is $\hat{\mathbf{g}}_{[2]} = \partial_{\mathbf{m}_{[2]}} \mathcal{L} = -2 \partial_{\mathbf{S}^{-1}} \mathcal{L} = -2 \partial_{\mathbf{S}} \mathcal{L}$, where the gradient $\partial \mathcal{L}$ can be computed as suggested by Lin et al. (2019).

L. More Results

Figure 5. The leftmost plot is MOG approximations for the banana distribution mentioned at Section 5.1, where the number indicates the number of components used in the approximations. The rightmost plot is a complete version of MOG approximations for the double banana distribution (the rightmost plot in Figure 2), where the number indicates the number of components used in the approximations.

Figure 6. The leftmost plot is mean-field Gaussian approximations for the toy Bayesian logistic regression example considered at Section 5.1. The rightmost plot is a skew-Gaussian approximation with full covariance structure for the same example.
Figure 7. This is a complete version of the leftmost figure in Figure 2. The figure shows MOG approximation (with $K = 25$) to fit an MOG model with 10 components in a 20 dimensional problem.
Handling the Positive-Definite Constraint in the Bayesian Learning Rule

Figure 8. This is the first 60 marginal distributions obtained from a MOG approximation with $K = 60$ for a 300-dimensional mixture of Student’s T distribution with 20 components. The problem is mentioned at Section 5.1, where the approximation is obtained by our method, which iterates 50,000 iterations.
Figure 9. This is the second 60 marginal distributions obtained from a MOG approximation with $K = 60$ for a 300-dimensional mixture of Student’s T distribution with 20 components. The problem is mentioned at Section 5.1, where the approximation is obtained by our method, which iterates 50,000 iterations.
Figure 10. This is the third 60 marginal distributions obtained from a MOG approximation with $K = 60$ for a 300-dimensional mixture of Student’s T distribution with 20 components. The problem is mentioned at Section 5.1, where the approximation is obtained by our method, which iterates 50,000 iterations.
Figure 11. This is the fourth 60 marginal distributions obtained from a MOG approximation with $K = 60$ for a 300-dimensional mixture of Student’s T distribution with 20 components. The problem is mentioned at Section 5.1, where the approximation is obtained by our method, which iterates 50,000 iterations.
Figure 12. This is the last 60 marginal distributions obtained from a MOG approximation with $K = 60$ for a 300-dimensional mixture of Student’s T distribution with 20 components. The problem is mentioned at Section 5.1, where the approximation is obtained by our method, which iterates 50,000 iterations.