Multivariate Gaussian Variational Inference
by Natural Gradient Descent

Timothy D. Barfoot
Institute for Aerospace Studies
University of Toronto
tim.barfoot@utoronto.ca

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Abstract

This short note reviews so-called Natural Gradient Descent (NGD) for multivariate Gaussians. The Fisher Information Matrix (FIM) is derived for several different parameterizations of Gaussians. Careful attention is paid to the symmetric nature of the covariance matrix when calculating derivatives. We show that there are some advantages to choosing a parameterization comprising the mean and inverse covariance matrix and provide a simple NGD update that accounts for the symmetric (and sparse) nature of the inverse covariance matrix.

Keywords Gaussian variational inference · natural gradient descent · Kronecker algebra · Fisher information matrix

1 Mathematical Tools

This first section introduces some less common tools that make it possible to take derivatives of general expressions of symmetric matrices. Readers familiar with these already can jump to the next section.

1.1 Vectorization

There are several identities involving the Kronecker product, \( \otimes \), and \( \text{vec} (\cdot) \) operator (that stacks the columns of a matrix) of which we will make use:

\[
\begin{align*}
\text{vec}(a) & \equiv a \\
\text{vec}(ab^T) & \equiv b \otimes a \\
\text{vec}(ABC) & \equiv (C^T \otimes A) \text{vec}(B) \\
\text{vec}(A^T)\text{vec}(B) & \equiv \text{tr}(AB) \\
(A \otimes B)(C \otimes D) & \equiv (AC) \otimes (BD) \\
(A \otimes B)^{-1} & \equiv A^{-1} \otimes B^{-1} \\
(A \otimes B)^T & \equiv A^T \otimes B^T \\
|A_{N \times N} \otimes B_{M \times M}| & \equiv |A|^M |B|^N \\
\text{rank}(A \otimes B) & \equiv \text{rank}(A) \text{rank}(B) \\
\text{tr}(A \otimes B) & \equiv \text{tr}(A) \text{tr}(B) \\
a^T BCB^T d & \equiv \text{vec}(B)^T (C \otimes da^T) \text{vec}(B)
\end{align*}
\]

We shall also define the \( \text{mat}(\cdot) \) operator to mean the inverse of the \( \text{vec}(\cdot) \) operator; in other words it unstacks the columns back into the original matrix, whose original size is presumably remembered somehow. Thus

\[
\text{mat} (\text{vec} (A)) \equiv A.
\]

It is worth noting that \( \otimes, \text{vec}(\cdot), \) and \( \text{mat}(\cdot) \) are all linear operators.
1.2 Matrix Calculus Using Differentials

To handle taking derivatives of complicated expressions involving matrices, we follow the approach of Magnus and Neudecker (2019, §18). This section discusses (unconstrained) differentials before moving on to how to handle symmetric matrices. Some of the less usual results that we will make use of include

\[
\begin{align*}
\frac{d\text{tr}(X)}{dX} &= \text{tr}(dX) \quad (3a) \\
\frac{d|X|}{dX} &= |X| \text{tr}(X^{-1} dX) \quad (3b) \\
\frac{d\ln|X|}{dX} &= \text{tr}(X^{-1} dX) \quad (3c) \\
X^{-1} &= -X^{-1} dX X^{-1} \quad (3d) \\
\frac{df}{dX} &= \text{tr} \left( \frac{\partial f}{\partial X} dX \right) \quad (3e)
\end{align*}
\]

All of the usual linear operations for differentials apply as well. From the last relationship, we see that if we can manipulate our differential into the form

\[
\frac{df}{dX} = \text{tr} \left( \frac{\partial f}{\partial X} dX \right) \quad (4)
\]

we can read the Jacobian matrix,

\[
A = \frac{\partial f}{\partial X} \quad (5)
\]

directly. Another way to see this is to make use of vectorization. We can rewrite the differential as

\[
\frac{df}{dX} = \text{vec} \left( \frac{\partial f}{\partial X} dX \right) = \text{vec}(A)^T \text{vec}(X) \quad (6)
\]

so that

\[
\frac{\partial f}{\partial \text{vec}(X)^T} = \text{vec}(A) \quad (7)
\]

Then, converting back to a matrix we have

\[
\frac{\partial f}{\partial X} = \text{mat} \left( \frac{\partial f}{\partial \text{vec}(X)^T} \right) = \text{mat}(\text{vec}(A)) = A \quad (8)
\]

These expressions can be used recursively to calculate second differentials as well. The main idea to minimize tedious calculations is to first build all the differentials then use the vectorization tools from the previous section to assemble them into a Jacobian and/or Hessian.

1.3 Parameterizing Symmetric Matrices Without Duplication

In the previous section, we introduced tools to calculate the first and second derivatives of expressions with respect to a matrix. However, if the matrix is symmetric, we need to modify the results because the elements above and below the main diagonal are duplicated. We again follow the approach of Magnus and Neudecker (2019, §18).

We begin by introducing the \( \text{vech}(\cdot) \), operator\(^1\) that stacks up the elements in a matrix, excluding all the elements above the main diagonal. Then, we define the \( \text{duplication matrix} \), \( D \), that allows us to build the full symmetric matrix from its unique parts:

\[
\text{vec}(A) = D \text{vech}(A) \quad \text{(symmetric } A \text{)} \quad (9)
\]

It is useful to consider a simple \( 2 \times 2 \) example:

\[
A = \begin{bmatrix} a & b \\ b & c \end{bmatrix}, \quad \text{vec}(A) = \begin{bmatrix} a \\ b \\ b \\ c \end{bmatrix}, \quad D = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \text{vech}(A) = \begin{bmatrix} a \\ b \\ c \end{bmatrix}. \quad (10)
\]

If we want to convert back to a matrix it is useful to define a corresponding \( \text{matf}(\cdot) \) operator\(^2\) so that

\[
\text{matf}(\text{vech}(A)) = \text{mat}(D \text{vech}(A)) = \text{mat}(\text{vec}(A)) = A \quad \text{(symmetric } A \text{)} \quad (11)
\]

---

\(^1\)Presumably the addition of ‘h’ indicates the lower ‘half’.

\(^2\)The ‘f’ indicates we are converting a half vector back into a ‘full’ symmetric matrix.
The Moore-Penrose pseudoinverse of $D$ will be denoted $D^+$ and is given by

$$D^+ = (D^T D)^{-1} D^T. \quad (12)$$

We can then use $D^+$ to calculate the unique vector from the nonunique vector:

$$\text{vech}(A) = D^+ \text{vec}(A) \quad \text{(symmetric A).} \quad (13)$$

For our $2 \times 2$ example we have

$$D^+ = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 \end{bmatrix}. \quad (14)$$

Useful identities involving $D$ are then

$$D^+ D \equiv 1 \quad (15a)$$

$$D^+ D^T \equiv DD^+ \quad (15b)$$

$$DD^+ \text{vec}(A) \equiv \text{vec}(A) \quad \text{(symmetric A)} \quad (15c)$$

$$DD^+ (A \otimes A) D \equiv (A \otimes A) D \quad \text{(any A)} \quad (15d)$$

which can be found in Magnus and Neudecker (1980). We can also define the $\text{sym}(-)$ operator as

$$\text{sym}(A) = A + A^T - A \circ 1, \quad (16)$$

with $\circ$ the Hadamard (elementwise) product. Then we can relate the $\text{sym}(-)$ operator to the duplication matrix as follows:

$$DD^T \text{vec}(A) = \text{vec} \left( \text{sym}(A) \right), \quad (17)$$

which holds for any $A$.

### 1.4 Differentials for Symmetric Matrices

It is now straightforward to calculate derivatives of functions of symmetric matrices. The key idea is to use the symmetry-aware parameterization from the last section:

$$\text{vec}(A) = D \text{vech}(A). \quad (18)$$

Taking the differential of this we have

$$d\text{vec}(A) = D d\text{vech}(A). \quad (19)$$

We can insert this whenever we have a differential involving a symmetric matrix:

$$df(X) = d\text{vec} \left( X^T \right) \text{vec} \left( \frac{\partial f}{\partial X} \right) = d\text{vech} \left( X^T \right) D^T \text{vec} \left( \frac{\partial f}{\partial X} \right), \quad (20)$$

so that

$$\frac{\partial f(X)}{\partial \text{vech}(X)^T} = D^T \text{vec} \left( \frac{\partial f}{\partial X} \right). \quad (21)$$

What the extra $D^T$ effectively does is add together the unconstrained elements of the derivative corresponding to the same element above and below the diagonal and then maps this to a single parameter in the unique representation.

If we define $\partial$ to indicate a partial derivative with respect to a full symmetric matrix (where we have accounted for the symmetry) we can write

$$\frac{\partial f}{\partial X} = \text{mat} \left( \frac{\partial f(X)}{\partial \text{vech}(X)^T} \right) = \text{mat} \left( D - \frac{\partial f(X)}{\partial \text{vech}(X)^T} \right) = \text{mat} \left( DD^T \text{vec} \left( \frac{\partial f}{\partial X} \right) \right) = \text{mat} \left( \text{vec} \left( \text{sym} \left( \frac{\partial f}{\partial X} \right) \right) \right) = \text{sym} \left( \frac{\partial f}{\partial X} \right), \quad (22)$$

which is now in terms of the $\text{sym}(-)$ operator.
2 Fisher Information Matrix for a Multivariate Gaussian

To carry out NGD, we will have need of the Fisher Information Matrix (FIM) for a multivariate Gaussian. However, there are several useful ways to parameterize a Gaussian, each with its own FIM, so we will show a few. First we will derive the general expression.

2.1 FIM Derivation

A multivariate Gaussian Probability Density Function (PDF) takes the form

\[ q(x) = \mathcal{N}(\mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^N |\Sigma|}} \exp\left(-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu)\right), \tag{23} \]

which has been parameterized using mean, \( \mu \), and covariance, \( \Sigma \).

We will use the Kullback-Leibler (KL) divergence (Kullback and Leibler, 1951) to define the Fisher Information Matrix (FIM) (Fisher, 1922). The KL divergence between two Gaussians, \( q \) and \( q' \), can be expressed as

\[ \text{KL}(q||q') = -\int q(x) \ln \left(\frac{q'(x)}{q(x)}\right) dx = \mathbb{E}_q \left[ \ln q(x) - \ln q'(x) \right]. \tag{24} \]

If we suppose that \( q \) and \( q' \) are infinitesimally close to one another in some parameter space then

\[ \ln q'(x) \approx \ln q(x) + d \ln q(x) + \frac{1}{2} d^2 \ln q(x), \tag{25} \]

and so

\[ \text{KL}(q||q') \approx \mathbb{E}_q \left[ -d \ln q(x) - \frac{1}{2} d^2 \ln q(x) \right], \tag{26} \]

out to second order in the differentials. For Gaussians (and some other distributions) the first term is in fact zero. To see this, we write the negative log-likelihood of \( q(x) \) as

\[ -\ln q(x) = \frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) + \frac{1}{2} \ln |\Sigma| + \text{constant}. \tag{27} \]

The first differential is

\[ -d \ln q(x) = -d \mu^T \Sigma^{-1} (x - \mu) + \frac{1}{2} (x - \mu)^T d\Sigma^{-1} (x - \mu) + \frac{1}{2} \text{tr} \left( \Sigma^{-1} d\Sigma \right) \]

\[ = -d \mu^T \Sigma^{-1} (x - \mu) + \frac{1}{2} \text{tr} \left( (\Sigma^{-1} - \Sigma^{-1} (x - \mu)(x - \mu)^T \Sigma^{-1}) d\Sigma \right), \tag{28} \]

and so

\[ \mathbb{E}_q[-d \ln q(x)] = -d \mu^T \Sigma^{-1} \mathbb{E}[x - \mu] + \frac{1}{2} \text{tr} \left( (\Sigma^{-1} - \Sigma^{-1} (x - \mu)(x - \mu)^T \Sigma^{-1}) \mathbb{E}[x - \mu] \right) \mathbb{E}[x - \mu] = 0. \tag{29} \]

Turning the differentials into partial derivatives, we can rewrite (26) as

\[ \text{KL}(q||q') \approx \mathbb{E}_q \left[ -\frac{1}{2} d^2 \ln q(x) \right] = \frac{1}{2} \delta \theta^T \mathbb{E}_q \left[ -\frac{\partial^2 \ln q(x)}{\partial \theta^2} \right] \delta \theta, \tag{30} \]

for some parameterization, \( \theta \), of a Gaussian. The matrix, \( \mathcal{I}_\theta \), is called the Fisher Information Matrix (FIM) and defines a Riemannian metric tensor for the parameters, \( \theta \). As a preview of what is to come, for cost functions that are similar to KL divergence, we will use the FIM as an approximation of the Hessian to build a Newton-like optimizer. We will next work out the FIM for a few parameterizations of Gaussians.

2.2 Canonical Parameterization - Not Accounting for Symmetry

We begin with the most obvious parameterization, the mean and (vectorized) covariance:

\[ \theta = \begin{bmatrix} \mu \\ \text{vec}(\Sigma) \end{bmatrix}. \tag{31} \]
which we will refer to as the *canonical parameterization*. To calculate the FIM, we need the second differential,

\[
-d^2 \ln q(x) = d \mu^T \Sigma^{-1} d \mu - 2 d \mu^T \Sigma^{-1} (x - \mu) + \frac{1}{2} \text{tr} \left( \Sigma^{-1} (x - \mu)(x - \mu)^T \right).
\]

The expected value of the second differential over \(q(x)\) is

\[
-\mathbb{E}_q \left[ d^2 \ln q(x) \right] = d \mu^T \Sigma^{-1} d \mu + \frac{1}{2} \text{tr} \left( \Sigma^{-1} d \Sigma \Sigma^{-1} d \Sigma \right).
\]

Vectorizing \(\Sigma\) we have the nice result

\[
-\mathbb{E}_q \left[ d^2 \ln q(x) \right] = d \theta^T \left[ \Sigma^{-1} 0 \right] d \gamma.
\]  

The inverse FIM is simply

\[
\mathcal{I}^{-1}_\theta = \left[ \Sigma 0 \right] \begin{bmatrix} 0 & 2 \Sigma^{-1} \otimes \Sigma^{-1} \end{bmatrix}.
\]  

The trouble is that we have not accounted for the symmetric nature of \(\Sigma\).

### 2.3 Canonical Parameterization - Accounting for Symmetry

To account for the symmetric nature of \(\Sigma\), we define the symmetry-aware parameterization as

\[
\gamma = \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix} = \begin{bmatrix} \mu \\ \text{vech}(\Sigma) \end{bmatrix}.
\]  

Then we have

\[
d \mu = d \gamma_1, \quad \text{vec} (d \Sigma) = D d \gamma_2,
\]  

or

\[
d \theta = \begin{bmatrix} 1 \\ 0 \end{bmatrix} d \gamma.
\]  

Substituting this into (34), we have

\[
-\mathbb{E}_q \left[ d^2 \ln q(x) \right] = d \gamma^T \left[ \Sigma^{-1} 0 \right] d \gamma.
\]  

The inverse FIM is given by

\[
\mathcal{I}^{-1}_\gamma = \left[ \Sigma 0 \right] \begin{bmatrix} 0 & 2 \Sigma^{-1} \otimes \Sigma^{-1} \end{bmatrix}.
\]

### 2.4 Hybrid Parameterization - Not Accounting for Symmetry

In many real large-scale problems, the inverse covariance matrix is sparse so that it is much more desirable to work with it directly. We call this the *hybrid* parameterization as the mean is as before while we use the inverse covariance:

\[
\alpha = \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} = \begin{bmatrix} \mu \\ \text{vec}(\Sigma^{-1}) \end{bmatrix}.
\]  

We then have

\[
d \mu = d \alpha_1, \quad \text{vec} (d \Sigma^{-1}) = d \alpha_2.
\]

Expanding the second of these we see

\[
d \alpha_2 = \text{vec} (d \Sigma^{-1}) = \text{vec} (- \Sigma^{-1} d \Sigma \Sigma^{-1}) = - (\Sigma^{-1} \otimes \Sigma^{-1}) \text{vec} (d \Sigma),
\]
and so
\[ \text{vec}(d\Sigma) = -(\Sigma \otimes \Sigma) d\alpha_2. \] (44)

We therefore have
\[ d\theta = \begin{bmatrix} 1 & 0 \\ 0 & -(\Sigma \otimes \Sigma) \end{bmatrix} d\alpha. \] (45)

Substituting this into (34) we have
\[ -\mathbb{E}_q[d^2 \ln q(x)] = d\alpha^T \begin{bmatrix} \Sigma^{-1} & 0 \\ 0 & \frac{1}{2} (\Sigma \otimes \Sigma) \end{bmatrix} d\alpha. \] (46)

The inverse FIM is given by
\[ \mathcal{I}^{-1}_\alpha = \begin{bmatrix} \Sigma & 0 \\ 0 & 2 (\Sigma^{-1} \otimes \Sigma^{-1}) \end{bmatrix}, \] (47)

which follows a similar form to the previous section.

2.5 Hybrid Parameterization - Accounting for Symmetry

If we want to account for symmetry we choose
\[ \beta = \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} \mu \\ \text{vech}(\Sigma^{-1}) \end{bmatrix}. \] (48)

Similarly to how we convert to the symmetry-aware version of the canonical representation, we have
\[ d\beta = \begin{bmatrix} 1 & 0 \\ 0 & D \end{bmatrix} d\alpha. \] (49)

Substituting this into (34) we have
\[ -\mathbb{E}_q[d^2 \ln q(x)] = d\beta^T \begin{bmatrix} \Sigma^{-1} & 0 \\ 0 & 2 D^T (\Sigma \otimes \Sigma) D \end{bmatrix} d\beta. \] (50)

The inverse FIM is given by
\[ \mathcal{I}^{-1}_\beta = \begin{bmatrix} \Sigma & 0 \\ 0 & 2 D^+ (\Sigma^{-1} \otimes \Sigma^{-1}) D^{+T} \end{bmatrix}, \] (51)

which follows a similar form to the previous section.

2.6 Natural (or Inverse Covariance Form) Parameterization - Not Accounting for Symmetry

Somewhat confusingly named\(^3\), the natural parameters for a Gaussian can be defined as
\[ \eta = \begin{bmatrix} \Sigma^{-1} \mu \\ \text{vec}(\Sigma^{-1}) \end{bmatrix}. \] (52)

This is also sometimes called the inverse covariance form of a Gaussian. The derivation for these parameters is somewhat more involved as the FIM is no longer block diagonal, making this choice somewhat unnatural.

We will build off the hybrid parameterization as it already deals with the inverse covariance matrix and so the covariance parameter differentials are the same, \(d\eta_2 = d\alpha_2\). The differential for the mean is
\[ d\eta_1 = d\Sigma^{-1} \mu + \Sigma^{-1} d\mu = \Sigma^{-1} d\alpha_1 + (\mu^T \otimes 1) d\alpha_2, \] (53)

which takes a bit of manipulation. Stacking these we have
\[ d\eta = \begin{bmatrix} \Sigma^{-1} & (\mu^T \otimes 1) \\ 0 & 1 \end{bmatrix} d\alpha, \] (54)

\(^3\)There does not seem to be a connection with natural gradient descent.
which is the reverse relationship from what we want, but we will need this coefficient matrix when computing the inverse FIM. Inverting we have

\[ d\alpha = \begin{bmatrix} \Sigma & -\Sigma (\mu^T \otimes 1) \\ 0 & 1 \end{bmatrix} d\eta. \] (55)

The FIM is then

\[ \mathcal{I}_\eta = \begin{bmatrix} \Sigma & -\Sigma (\mu^T \otimes 1) \\ 0 & 1 \end{bmatrix}^T \mathcal{I}_\alpha \begin{bmatrix} \Sigma & -\Sigma (\mu^T \otimes 1) \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} \Sigma & -\Sigma (\mu^T \otimes 1) \\ - (\mu \otimes 1) \Sigma & \frac{1}{2} (\Sigma \otimes \Sigma) + (\mu \otimes 1) \Sigma (\mu^T \otimes 1) \end{bmatrix}. \] (56)

The inverse FIM is then

\[ \mathcal{I}_\eta^{-1} = \begin{bmatrix} \Sigma^{-1} & \mu^T \otimes 1 \\ 0 & 1 \end{bmatrix} \mathcal{I}_\alpha^{-1} \begin{bmatrix} \Sigma^{-1} & \mu^T \otimes 1 \\ 0 & 1 \end{bmatrix}^T \]

\[ = \begin{bmatrix} \Sigma^{-1} + 2 (\mu \otimes 1) (\Sigma^{-1} \otimes \Sigma^{-1}) (\mu^T \otimes 1) & 2 (\mu^T \otimes 1) (\Sigma^{-1} \otimes \Sigma^{-1}) \\ 2 (\Sigma^{-1} \otimes \Sigma^{-1}) (\mu \otimes 1) & 2 (\Sigma^{-1} \otimes \Sigma^{-1}) \end{bmatrix} \]

\[ = \begin{bmatrix} (1 + 2 \mu^T \Sigma^{-1} \mu) \Sigma^{-1} & 2 (\mu^T \Sigma^{-1} \otimes \Sigma^{-1}) \\ 2 (\Sigma^{-1} \mu \otimes \Sigma^{-1}) & 2 (\Sigma^{-1} \otimes \Sigma^{-1}) \end{bmatrix}, \] (57)

where it is worth noting that all of the expressions can be easily built from \( \eta \). We will not pursue the symmetry-aware version of the natural parameters, but it would be straightforward to do so using the same approach as the other parameterizations.

## 3 Natural Gradient Descent

In this section we will use our FIMs to design efficient methods of optimizing functionals of Gaussians. The idea is to exploit the information geometry of whatever our parameterization is to create a better descent direction than regular gradient descent (Amari, 1998).

### 3.1 NGD Derivation

We begin by assuming that we have a loss functional, \( V(q) \), of a Gaussian, \( q \), that we wish to minimize. We assume it can be expressed as the KL divergence between our approximation and true Bayesian posterior, \( p(x|z) \),

\[ V(q) = - \int q(x) \ln \left( \frac{p(x|z)}{q(x)} \right) \, dx, \] (58)

where \( x \) are the variables to be estimated and \( z \) is some data. If \( p(x|z) \) is actually Gaussian, we can make \( V(q) \) zero by setting \( q(x) = p(x|z) \). Usually, \( p(x|z) \) is not Gaussian due to nonlinearities, but presumably it will be somewhat like a Gaussian in order to approximate it as one.

We will employ a Newton-like optimization scheme to minimize the loss. Suppose that we start with a Gaussian estimate, \( q \), and then make a small change in its parameters to result in \( q' \). The change in the loss functional will be

\[ V(q') - V(q) \approx dV + \frac{1}{2} d^2V, \] (59)

correct to second order in the differentials. In terms of parameters, \( \theta \), this will be

\[ V(q') - V(q) \approx \left( \frac{\partial V}{\partial \theta^T} \right)^T \delta \theta + \frac{1}{2} \delta \theta^T \left( \frac{\partial^2 V}{\partial \theta^T \partial \theta} \right) \delta \theta, \] (60)

where the Hessian can be expensive to compute. We can think of this as a quadratic approximation of our loss functional centred at the current estimate, which is minimized by solving

\[ \left( \frac{\partial^2 V}{\partial \theta^T \partial \theta} \right) \delta \theta = - \left( \frac{\partial V}{\partial \theta^T} \right), \] (61)

for \( \delta \theta \) then updating \( \theta' = \theta + \delta \theta \) and iterating to convergence. The key step in Natural Gradient Descent (NGD) is to approximate the Hessian using the FIM in the update scheme so that

\[ \delta \theta = - \mathcal{I}_\theta^{-1} \frac{\partial V}{\partial \theta^T}, \] (62)
where we can precompute the FIM inverse if we like. We can also simply interpret this as a modification to gradient descent that achieves something more like second-order convergence without any second-order derivatives. We saw earlier that the FIM is exactly the Hessian of the KL divergence between two Gaussians. If \( p(x|z) \) is ’close’ to a Gaussian then \( V(q) \) will be well approximated by the KL divergence between two Gaussians.

Inserting the update back into (60) we have

\[
V(q') - V(q) \approx - \left( \frac{\partial V}{\partial \theta^T} \right)^T \left( \mathcal{I}_\theta^{-1} - \frac{1}{2} \mathcal{I}_\theta^{-1} \left( \frac{\partial^2 V}{\partial \theta \partial \theta^T} \right) \mathcal{I}_\theta^{-1} \right) \left( \frac{\partial V}{\partial \theta^T} \right) \approx - \frac{1}{2} \left( \frac{\partial V}{\partial \theta^T} \right)^T \mathcal{I}_\theta^{-1} \left( \frac{\partial V}{\partial \theta^T} \right) \leq 0, \tag{63}
\]

which shows that (under the approximations we have made) the loss will decrease (except at a minimum where \( \frac{\partial V}{\partial \theta^T} = 0 \)) since the FIM is positive definite.

### 3.2 Canonical Parameterization - Not Accounting for Symmetry

We can deconstruct (62) into the updates for \( \mu \) and \( \Sigma \):

\[
\begin{bmatrix}
\delta \mu \\
\text{vec}(\delta \Sigma)
\end{bmatrix} = - \begin{bmatrix} \Sigma & 0 \\
0 & 2 (\Sigma \otimes \Sigma) \end{bmatrix} \begin{bmatrix} \frac{\partial V}{\partial \mu^T} \\
\text{vec} \left( \frac{\partial V}{\partial \Sigma} \right) \end{bmatrix}. \tag{64}
\]

For the mean we simply have

\[
\delta \mu = - \Sigma \frac{\partial V}{\partial \mu^T}, \tag{65}
\]

or rearranging slightly

\[
\Sigma^{-1} \delta \mu = - \frac{\partial V}{\partial \mu^T}, \tag{66}
\]

which looks familiar from Maximum A Posteriori (MAP) inference. For the covariance parameter we have

\[
\text{vec}(\delta \Sigma) = -2 (\Sigma \otimes \Sigma) \text{vec} \left( \frac{\partial V}{\partial \Sigma} \right), \tag{67}
\]

which can be turned back into a matrix equation by applying \( \text{mat}(\cdot) \) to both sides:

\[
\delta \Sigma = -2 \Sigma \frac{\partial V}{\partial \Sigma} \Sigma. \tag{68}
\]

We will next work through the details, accounting for the symmetric nature of the covariance matrix.

### 3.3 Canonical Parameterization - Accounting for Symmetry

The NGD update is now

\[
\delta \gamma = - \mathcal{I}_\theta^{-1} \frac{\partial V}{\partial \gamma^T}, \tag{69}
\]

which becomes

\[
\begin{bmatrix}
\delta \mu \\
\text{vech}(\delta \Sigma)
\end{bmatrix} = - \begin{bmatrix} \Sigma & 0 \\
0 & 2 \mathbf{D}^T (\Sigma \otimes \Sigma) \mathbf{D}^+ \end{bmatrix} \begin{bmatrix} \frac{\partial V}{\partial \mu^T} \\
\text{vech} \left( \frac{\partial V}{\partial \Sigma} \right) \end{bmatrix}. \tag{70}
\]

The mean update is the same as the previous section. For the covariance update we have

\[
\text{vech}(\delta \Sigma) = -2 \mathbf{D}^+ (\Sigma \otimes \Sigma) \mathbf{D}^+ \text{vech} \left( \frac{\partial V}{\partial \Sigma} \right). \tag{71}
\]

We note that

\[
\text{vech} \left( \frac{\partial V}{\partial \Sigma} \right) = \mathbf{D}^T \text{vec} \left( \frac{\partial V}{\partial \Sigma} \right), \tag{72}\]

and

\[
\text{vech}(\delta \Sigma) = \mathbf{D}^+ \text{vec}(\delta \Sigma). \tag{73}\]

Inserting these last two equations into (71) we have

\[
\mathbf{D}^+ \text{vec}(\delta \Sigma) = -2 \mathbf{D}^+ (\Sigma \otimes \Sigma) \mathbf{D}^+ \mathbf{D}^T \text{vec} \left( \frac{\partial V}{\partial \Sigma} \right). \tag{74}
\]
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Premultiplying both sides by $\bf{D}$ we have

$$\begin{align*}
\bf{D} \text{vec}(\delta \Sigma) &= -2 \bf{D}(\Sigma \otimes \Sigma) \bf{D} \text{vec}\left(\frac{\partial V}{\partial \Sigma}\right),
\end{align*}$$

(75)

then

$$\text{vec}(\delta \Sigma) = -2 (\Sigma \otimes \Sigma) \bf{D} \text{vec}\left(\frac{\partial V}{\partial \Sigma}\right),$$

(76)

and then

$$\text{vec}(\delta \Sigma) = -2 (\Sigma \otimes \Sigma) \text{vec}\left(\frac{\partial V}{\partial \Sigma}\right).$$

(77)

Applying the mat(·) operator to both sides we finally have

$$\delta \Sigma = -2 \Sigma \frac{\partial V}{\partial \Sigma},$$

(78)

which amazingly is exactly the update in (68) that we arrived at when we did not account for the symmetric nature of $\Sigma$.

3.4 Hybrid Parameterization - Not Accounting for Symmetry

The NGD update for our symmetry-blind hybrid parameters, $\alpha$ is

$$\delta \alpha = -I^{-1} \alpha \frac{\partial V}{\partial \alpha^T}. \tag{79}$$

Working through the same logic as the symmetry-blind canonical section we have

$$\Sigma^{-1} \delta \mu = -\frac{\partial V}{\partial \mu^T}, \tag{80a}$$

$$\delta \Sigma^{-1} = -2 \Sigma^{-1} \frac{\partial V}{\partial \Sigma^{-1} \Sigma^{-1}}. \tag{80b}$$

The first equation is the same as (66) while the second equation is not equivalent to (78).

3.5 Hybrid Parameterization - Accounting for Symmetry

The NGD update for our symmetry-aware inverse covariance parameters, $\beta$ is

$$\delta \beta = -I^{-1} \beta \frac{\partial V}{\partial \beta^T}. \tag{81}$$

Working through the same logic as the symmetry-aware canonical section we have

$$\Sigma^{-1} \delta \mu = -\frac{\partial V}{\partial \mu^T}, \tag{82a}$$

$$\delta \Sigma^{-1} = -2 \Sigma^{-1} \frac{\partial V}{\partial \Sigma^{-1} \Sigma^{-1}}. \tag{82b}$$

Again, these are the same updates we arrived at not accounting for symmetry in the previous section.

3.6 Choosing the Hybrid Parameterization

Noticing that for our particular choice of $V$ that (Opper and Archambeau, 2009; Barfoot et al., 2020)

$$\begin{align*}
\frac{\partial V}{\partial \mu^T} &= \Sigma^{-1} \mathbb{E}_q[(x - \mu)\phi(x)], \tag{83a} \\
\frac{\partial^2 V}{\partial \mu^T \partial \mu} &= \Sigma^{-1} \mathbb{E}_q[(x - \mu)(x - \mu)^T \phi(x)] \Sigma^{-1} - \Sigma^{-1} \mathbb{E}_q[\phi(x)], \tag{83b} \\
\frac{\partial V}{\partial \Sigma^{-1}} &= -\frac{1}{2} \mathbb{E}_q[(x - \mu)(x - \mu)^T \phi(x)] + \frac{1}{2} \Sigma \mathbb{E}_q[\phi(x)] + \frac{1}{2} \Sigma, \tag{83c}
\end{align*}$$

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where \( \phi(x) = -\ln p(x, z) \), we have the nice relationship

\[
\frac{\partial V}{\partial \Sigma^{-1}} = \frac{1}{2} \Sigma - \frac{1}{2} \Sigma \frac{\partial^2 V}{\partial \mu^T \partial \mu} \Sigma. \tag{84}
\]

Plugging (84) into our canonical covariance update from (68) we have

\[
\delta \Sigma = -\Sigma^3 + \Sigma^3 \frac{\partial^2 V}{\partial \mu^T \partial \mu} \Sigma^3, \tag{85}
\]

which does not appear to be an improvement.

However, plugging (84) into our hybrid covariance update in (80b) we have

\[
\delta \Sigma^{-1} = -\Sigma^{-1} + \frac{\partial^2 V}{\partial \mu^T \partial \mu}, \tag{86}
\]

which conveniently removes the extra \( \Sigma^{-1} \) matrices. Since \( \delta \Sigma^{-1} \) is the change in the inverse covariance, we can express this update simply as

\[
\Sigma^{-1} \leftarrow \frac{\partial^2 V}{\partial \mu^T \partial \mu}, \tag{87}
\]

which is quite convenient to implement.

We can then express the complete hybrid update neatly as

\[
\Sigma^{-1} \delta \mu = -\frac{\partial V}{\partial \mu^T}, \tag{88a}
\]

\[
\Sigma^{-1} \leftarrow \frac{\partial^2 V}{\partial \mu^T \partial \mu}, \tag{88b}
\]

\[
\mu \leftarrow \mu + \delta \mu, \tag{88c}
\]

where the derivatives of \( V \) will require the current estimate of \( q \) to be evaluated. However, if we cycle through them from top to bottom, we will naturally update both \( \mu \) and \( \Sigma^{-1} \).

### 3.7 Hybrid Update Preserves Sparsity

The hybrid NGD update also has the nice property of preserving the sparsity inherent in the inverse covariance matrix (Barfoot et al., 2020). If we assume that the joint likelihood, \( p(x, z) \), factors then we can express the loss functional as

\[
V(q) = E_q[\ln p(x|z)] + E_q[\ln p(z)] + \frac{1}{2} \ln (|\Sigma^{-1}|) + \text{constant}
\]

\[
= E_q \left[ -\ln \left( \prod_{k=1}^{K} p(x_k, z_k) \right) \right] + \frac{1}{2} \ln (|\Sigma^{-1}|) + \text{constant}
\]

\[
= \sum_{k=1}^{K} E_{q_k} \left[ -\ln \left( \frac{1}{V_k(q_k)} \prod_{k=1}^{K} p(x_k, z_k) \right) \right] + \frac{1}{2} \ln (|\Sigma^{-1}|) + \text{constant}
\]

\[
= V_0 + \sum_{k=1}^{K} V_k(q_k) + \text{constant}, \tag{89}
\]

where

\[
x_k = P_k x \tag{90}
\]

is a subset of the variables associated with the \( k \)th factor and \( P_k \) an appropriate projection matrix. The first derivative of the loss is

\[
\frac{\partial V}{\partial \mu^T} = \frac{\partial V_0}{\partial \mu^T} + \sum_{k=1}^{K} \frac{\partial V_k}{\partial \mu^T} = \sum_{k=1}^{K} P_k^T \frac{\partial V_k}{\partial \mu_k^T}, \tag{91}
\]
where in the last step, the derivative simplifies to being over just \( \mu_k \) since that term only depends on \( q_k \). We have a similar thing for the second derivative:

\[
\Sigma^{-1} = \frac{\partial^2 V}{\partial \mu^T \partial \mu} = \frac{\partial^2 V}{\partial \mu^T \partial \mu} \bigg|_0 + \frac{\partial^2}{\partial \mu^T \partial \mu} \sum_{k=1}^{K} V_k = \sum_{k=1}^{K} \frac{\partial^2 V_k}{\partial \mu^T \partial \mu} = \sum_{k=1}^{K} P_k^T \frac{\partial^2 V_k}{\partial \mu_k^T \partial \mu_k} P_k.
\]  

(92)

From the right-most expression, we see that the inverse covariance will always maintain the same sparsity pattern. From here, Barfoot et al. (2020) show how to use this update scheme to carry out large-scale inference for problems in robotics.

4 Conclusion

We have derived the FIM and NGD updates for a handful of different multivariate Gaussian representations. The take away message is that the hybrid parameterization (comprising mean and inverse covariance) seems to offer advantages over the others and our update in (88) inherently takes care of the symmetric (and sparse) nature of \( \Sigma^{-1} \). Please refer to Barfoot et al. (2020) for an application of this approach to multivariate Gaussian variational inference.

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