A Common Framework for Natural Gradient and Taylor based Optimisation using Manifold Theory

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Abstract

This technical report introduces a mathematical framework to compare and relate standard Taylor approximation based optimisation methods with the method of Natural Gradient, an optimisation approach that is Fisher efficient with probabilistic models. The constructed framework will be shown to also provide a mathematical justification to combine higher order Taylor approximation methods with the method of NG.

1 Introduction

The core premise behind first and second order optimisation methods is Taylor’s theorem. Assuming that the objective function $F(\theta)$ is sufficiently smooth, Taylor’s second order approximation models the local behaviour of the function by the following quadratic function:

\[
F(\theta_k + \Delta \theta) \simeq F(\theta_k) + \Delta \theta^T \nabla F(\theta_k) + \frac{1}{2} \Delta \theta^T H \Delta \theta
\]  

(1)

where $\Delta \theta$ represents any offset within a convex neighbourhood of $\theta_k$ and $H$ is the Hessian of $F$ computed w.r.t $\theta_k$. Instead of optimising the objective function directly, second order methods focus on minimising the above approximate quadratic at each iteration of the optimisation process. The same approach is undertaken by first order methods but such approaches make a further approximation by dropping the quadratic term in Taylor’s formula. This technical report provides a re-derivation of Taylor’s theorem from the perspective of manifold theory. Such a formulation will be shown to provide a consistent framework to compare the above approaches with the method of Natural Gradient [1, 2, 5, 6] for probabilistic discriminative models $P_b(\hat{H}|O)$. The necessary machinery needed to develop this framework relies on the concept of manifold, tangent vectors and directional derivatives from the perspective of Information Geometry. Appendix A contains a glossary of terms referenced in this work and a more in-depth discussion can be found in Amari’s textbook [7].

2 Deriving Taylor’s theorem using manifold theory

A curve on a parameter manifold (Appx. A) $X$ is a continuous map $c : (a, b) \subset \mathbb{R} \rightarrow X$. Let $\mathcal{U}$ be an open convex neighbourhood of the current iterate $\theta_k$. Thus for any point $\theta$ in $\mathcal{U}$, $\exists$ a curve of the form $\theta_k + t(\theta - \theta_k)$ where $t \in [0, 1]$ that is contained in $\mathcal{U}$. 
Let \( c : [0, 1] \rightarrow X \) be a continuous curve such that:

\[
c(t) = \theta_k + t\Delta \theta
\]  

(2)

where \( \Delta \theta \) corresponds to arbitrary offset from \( \theta_k \) such that \( c \) is contained in \( \mathcal{U} \). The derivative of \( c \) at given point \( t_0 \) is then the linear map from the tangent space (Appx. A.3) at \( t_0 \) to the tangent space \( T_{c(t_0)}X \):

\[
d_{c|t_0} \left( \frac{d}{dr} \right) = \left( \frac{\partial}{\partial \theta_1} \frac{\partial}{\partial \theta_2} \cdots \frac{\partial}{\partial \theta_D} \right) \begin{bmatrix} \Delta \theta_1 \\ \Delta \theta_2 \\ \vdots \\ \Delta \theta_D \end{bmatrix} = \sum_i \Delta \theta_i \frac{\partial}{\partial \theta_i} 
\]  

(3)

where \( \frac{d}{dr} \) denotes the basis vector of \( T_{t_0}R \).

Let \( F(\theta) \) be a germ (Appx. A.2) that corresponds to a smooth map from the parameter manifold \( X \) to \( \mathbb{R} \). In the context of optimisation, this corresponds to the smooth objective training criterion. The derivative of \( F(\theta) \) at any given point \( \theta \) is a linear map from the tangent space from \( T_{\theta}X \) to the tangent space \( T_{F(\theta)}\mathbb{R} \):

\[
dF|_\theta \sum_i a_i \frac{\partial}{\partial \theta_i}(\theta) = \left( \frac{d}{dr} \right) \left[ \frac{\partial F}{\partial \theta_1}|\theta \cdot \frac{\partial F}{\partial \theta_2}|\theta \cdot \cdots \frac{\partial F}{\partial \theta_D}|\theta \right] \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_D \end{bmatrix} 
\]  

(4)

Here the vector \( \nabla F(\theta_k) \) is the Jacobian and denotes the particular vector in \( T_{\theta}M \) that yields the greatest \textbf{directional} derivative (Appx. A.4).

Constraining \( F \) on the curve \( c \) is equivalent to applying the composite map \( F \circ c \) from \( \mathbb{R} \rightarrow \mathbb{R} \). The derivative of such a map at given point \( t_0 \) will now correspond to a linear map from a tangent space in \( T_{t_0}\mathbb{R} \) to the tangent space of \( T_{F \circ c(t_0)}\mathbb{R} \). By applying chain rule such a linear map can be shown to correspond to:

\[
d(F \circ c)|_{t_0} \left( \frac{d}{dr} \right) = \left( \frac{d}{dr} \right) [F \circ c]_{t_0} = \left( \frac{d}{dr} \right) \left[ \frac{\partial F}{\partial \theta_1}|_{\theta_k + t_0 \Delta \theta} \cdot \frac{\partial F}{\partial \theta_2}|_{\theta_k + t_0 \Delta \theta} \cdots \frac{\partial F}{\partial \theta_D}|_{\theta_k + t_0 \Delta \theta} \right] \begin{bmatrix} \Delta \theta_1 \\ \Delta \theta_2 \\ \vdots \\ \Delta \theta_D \end{bmatrix} 
\]  

(5)

\[
= \frac{d}{dr} \sum_i \Delta \theta_i \frac{\partial F}{\partial \theta_i}|_{\theta_k + t \Delta \theta} 
\]  

(6)

Using the fact that \( F \circ c \) is differentiable and corresponds to a map from \( \mathbb{R} \rightarrow \mathbb{R} \), by the \textit{fundamental theorem of calculus}:
\[ F(\theta_k + \Delta \theta) = F(\theta_k) + \int_0^1 (F \circ c(t))' \, dt \]

\[ = F(\theta_k) + \int_0^1 \sum_i \Delta \theta_i \frac{\partial F}{\partial \theta_i}(\theta_k + t\Delta \theta) \, dt \]

\[ = F(\theta_k) + \sum_i \Delta \theta_i \int_0^1 \frac{\partial F}{\partial \theta_i}(\theta_k + t\Delta \theta) \, dt \]

(7)

Since individual terms \( \left( \int_0^1 \frac{\partial F}{\partial \theta_i}(\theta_k + t\Delta \theta) \, dt \right) \) themselves are smooth functions defined on the convex neighbourhood of \( \theta_k \), (7) can be expanded even further by recursively applying the fundamental theorem of calculus:

\[ F(\theta_k + \Delta \theta) = F(\theta_k) + \sum_i \frac{\partial F}{\partial \theta_i}(\theta_k) \Delta \theta_i + \sum_i \Delta \theta_i \int_0^1 \left( \sum_j \Delta \theta_j \int_0^1 \frac{\partial^2 F}{\partial \theta_j \partial \theta_i}(\theta_k + t\Delta \theta) \, dt \right) \, dt \]

\[ = F(\theta_k) + \sum_i \frac{\partial F}{\partial \theta_i}(\theta_k) \Delta \theta_i + \sum_i \Delta \theta_i \sum_j \Delta \theta_j \int_0^1 \left( \int_0^1 \frac{\partial^2 F}{\partial \theta_j \partial \theta_i}(\theta_k + t\Delta \theta) \, dt \right) \, dt \]

(8)

As the function \( \frac{\partial^2 F}{\partial \theta_j \partial \theta_i}(\theta) \) is continuous, when \( \Delta \theta \) is sufficiently small, \( \frac{\partial^2 F}{\partial \theta_j \partial \theta_i}(\theta_k + t\Delta \theta) \) can be approximated by \( \left. \frac{\partial^2 F}{\partial \theta_j \partial \theta_i}(\theta_k + t\Delta \theta) \right|_{t=0} \) Under this approximation, the local behaviour of the germ \( F(\theta) \) can be approximated by:

\[ F(\theta_k + \Delta \theta) \simeq F(\theta_k) + \sum_i \frac{\partial F}{\partial \theta_i}(\theta_k) \Delta \theta_i + \sum_i \Delta \theta_i \int_0^1 \left( \sum_j \Delta \theta_j \int_0^1 \frac{\partial^2 F}{\partial \theta_j \partial \theta_i}(\theta_k) \, dt \right) \, dt \]

\[ \simeq F(\theta_k) + \sum_i \frac{\partial F}{\partial \theta_i}(\theta_k) \Delta \theta_i + \frac{1}{2} \sum_i \Delta \theta_i \sum_j \Delta \theta_j \frac{\partial^2 F}{\partial \theta_j \partial \theta_i}(\theta_k) \]

(9)

In vector notation this corresponds to:

\[ F(\theta_k + \Delta \theta) \simeq F(\theta_k) + \Delta \theta^T \nabla F(\theta_k) + \frac{1}{2} \Delta \theta^T H \Delta \theta \]

(10)

with entries \( H_{ji} \) of the Hessian matrix corresponding to \( \frac{\partial^2 F}{\partial \theta_j \partial \theta_i}(\theta_k) \). The above expression corresponds to Taylor’s second order approximation. Re-deriving this expression from the perspective of manifold theory shows how the product \( \Delta \theta^T \nabla F(\theta_k) \) can be interpreted as an inner product between vectors \( \Delta \theta \) and \( \nabla F(\theta_k) \) in \( T_{\theta}X \). This interpretation will become handy in the next section.
3 Formulating Taylor’s quadratic as a minimisation problem in the Tangent space

Instead of minimising the objective function directly, second order methods focus on minimising the quadratic function of (10) at each iteration. The quadratic corresponds to a local model of the behaviour of \( F(\theta) \) within a convex neighbourhood of the current iterate \( \theta_k \). By re-deriving Taylor’s second order approximation from the perspective of manifold theory in the previous section, it was shown how \( \Delta \theta \) corresponds to a particular choice of a tangent vector from \( T_{\theta_k}X \), and \( \nabla F(\theta_k) \) represents the particular vector in \( T_{\theta}X \) that yields the greatest directional derivative under the linear map \( dF_{|\theta} \). Thus, as \( F(\theta_k) \) is a constant, solving the minimisation problem in (10) is equivalent to solving the following minimisation problem in \( T_{\theta_k}X \):

\[
\Delta \hat{\theta} = \arg \min_{\Delta \theta \in T_{\theta_k}X} F(\theta_k) + \langle \Delta \theta, \nabla F(\theta_k) \rangle + \frac{1}{2} \Delta \theta^T H \Delta \theta
\]

where \( \langle \Delta \theta, \nabla F(\theta_k) \rangle \) corresponds to the standard inner product between vectors in \( T_{\theta_k}X \) and \( \Delta \theta^T H \Delta \theta \) corresponds to a linear map \( g : u \in T_{\theta_k}X \rightarrow \mathbb{R} \).

3.1 Relating Gradient Descent with Natural Gradient

Under this framework, first order methods can be seen to solve the following optimisation problem in the tangent space \( T_{\theta_k}X \):

\[
\Delta \theta = \arg \min_{\Delta \theta \in T_{\theta_k}X} F(\theta_k) + \langle \Delta \theta, \nabla F(\theta_k) \rangle
\]

Since \( X \) is a manifold, the inner product endowed on the tangent space \( T_{\theta}X \) at any point \( \theta \) need not be just the identity matrix. The parameter manifold \( X \) can be equipped with any form of a Riemannian metric, a smooth map that assigns to each \( \theta \in X \) an inner product \( I_\theta \) in \( T_{\theta}X \). When the underlying model corresponds to a discriminative probabilistic model \( P_\theta(\mathcal{H}|\mathcal{O}) \), a particular choice of \( I_\theta \) is the Fisher Information matrix [1, 2]:

\[
I_\theta = E_{P_\theta(\mathcal{H}|\mathcal{O})} \left[ (\nabla \log P_\theta(\mathcal{H}|\mathcal{O})) (\nabla \log P_\theta(\mathcal{H}|\mathcal{O}))^T \right]
\]

(13)

Equipping the tangent space \( T_{\theta_k}X \) with the above Riemannian metric allows interpretation of lengths of paths traversed in the parameter space as changes in the KL divergence (Appx. B.1). When \( X \) possesses such a structure, performing first order optimisation within a trust region defined by \( I_\theta \) can be shown to produce the update \( \Delta \theta = I_\theta^{-1} \nabla F(\theta) \) at each iteration [4, 5]. From the perspective of Information Geometry, this corresponds to the direction of steepest descent in the space of \( P_\theta(\mathcal{H}|\mathcal{O}) \). Thus, in this sense, such an update is termed as the direction of Natural Gradient (NG) [1, 2, 5, 6].

Using the fact that \( I_\theta \) is symmetric and positive definite, it is also possible to endow \( X \) with a Riemannian metric of the form \( I_\theta^{-1} \) by the spectral decomposition theorem. With respect to such a metric, solving the minimising problem of (12) in the tangent space \( T_{\theta_k}X \) becomes equivalent to performing NG on the parameter surface. Hence, recasting the optimisation problem to a minimisation problem in \( T_{\theta_k}X \) provides a nice framework to relate Gradient Descent with the method of NG.

In practice, since it is not feasible to compute the expected outer product of the likelihood score exactly, \( I_\theta \) is approximated by its Monte-Carlo estimate \( \hat{I}_\theta \). As such a matrix is only positive semi-definite, it’s inverse is not guaranteed to exist. To address this issue, this work also provides the derivation of an alternative dampened Riemannian metric \( I_\theta^{-1} \) (Appx. C) that is not only guaranteed to be positive definite but has the feature that its image space is the direct sum of the image and the kernel space of the empirical Fisher matrix \( I_\theta^{-1} \). Assigning such a metric has one particular advantage: the very first directions explored by the CG algorithm constitute to directions in the image space of \( I_\theta \) i.e directions considered important by the empirical Fisher are traversed first during the initial stages of a CG run.
4 Summary

To summarise, this report presents a mathematical framework to compare and relate standard Taylor approximation based optimisation methods with the method of Natural Gradient, an optimisation approach that is Fisher efficient with probabilistic models. The constructed framework can be seen to also provide a mathematical justification to combine higher order Taylor approximation methods with the method of NG.

Appendix A Glossary

This section begins with a formal description of the concept of a smooth manifold. Conceptually, a manifold corresponds to any geometric object embedded in $\mathbb{R}^k$ that is locally Euclidean i.e any local patch of the object is topologically equivalent to an open unit ball in a smaller dimensional Euclidean space. In $\mathbb{R}^3$, curves and surfaces are examples of an embedded manifold. When movement is constrained only along these objects, the degrees of freedom with which one can traverse is lower than dimensionality of the embedded 3 dimensional space.

A.1 Formal definition of a manifold

A topological manifold $X$ of dimension $D$ is a second countable Hausdorff topological space that is locally homeomorphic to $\mathbb{R}^D$; that is, for any point $\theta \in X$, there exists an open neighbourhood $U$ of $\theta$ and a homeomorphism $g : U \rightarrow O \subset \mathbb{R}^D$, where $O$ is open in $\mathbb{R}^D$. We call the homeomorphism $g : U \rightarrow O$ a chart, and the neighbourhood $U$ a coordinate neighbourhood of $\theta$.

To clarify the reader, in topology the concept of a homeomorphism is equivalent to a bijective continuous map and the concept of Hausdorff means for any two points $\hat{\theta}, \tilde{\theta} \in X$, it is always possible to find disjoint open neighbourhoods that contain each point.

Let $r_i : \mathbb{R}^D \rightarrow \mathbb{R}$ denote the projection onto the $i$th coordinate. Given a chart $g : U \rightarrow O \subset \mathbb{R}^D$, let $\theta_i : r_i \circ g : U \rightarrow \mathbb{R}$. The functions $\theta_i$ are the local coordinates w.r.t the chart $g$ on $U$. Having established a notion of what it means to be manifold, the next concept that will be introduced is the concept of a tangent vector. To formally define the concept of a tangent vector at any point $\theta \in X$, it is first necessary to formalise the notion of germs associated with a given point in a manifold.

A.2 Germs

Let $X$ be a manifold and $\theta \in X$. Functions $f, g$ defined on open subsets $U, V$ respectively containing $\theta$ are said to have the same germ at $\theta$ if there exists a neighbourhood $W$ of $\theta$ contained in $U \cap V$ such that $f|_W \equiv g|_W$. The notion of germs therefore defines an equivalence relation on the space of functions defined on an open neighbourhood of $\theta$ where $(U, f) \sim (V, g)$ if and only if there exists a neighbourhood $W$ of $\theta$ contained in $U \cap V$ such that $f|_W \equiv g|_W$. Let $C^\infty_\theta$ be the set of all such equivalent function classes. Having defined the concept of class of germs associated with a given point $\theta \in X$, the necessary machinery is now in place to define the concept of a tangent vector associated with the point $\theta \in X$.

A.3 Tangent vector

A tangent vector $v$ at given point $\theta \in X$ is a linear derivation of $C^\infty_\theta$, that is it a special form of a linear map $C^\infty_\theta \rightarrow \mathbb{R}$ that satisfies the property $v(f \cdot g) = f(\theta)v(g) + v(f)g(\theta)$ where $f \cdot g$ denotes the product of functions $f$ and $g \in C^\infty_\theta$. The tangent vectors form a real vector space in the obvious way; this space is denoted by $T_\theta(X)$ and is called the tangent space to $X$ at $\theta$. 

5
The concept of tangent vectors is necessary to do calculus on manifolds. Since manifolds are locally Euclidean, the usual notions of differentiation and integration make sense in any coordinate chart and can be carried over to manifold space. Specifically, a tangent vector as will be shown now is the manifold version of a directional derivative at a point $\theta \in X$.

**Basis for Tangent space** Let $(\theta_1, \theta_2, \cdots, \theta_D)$ denote the standard coordinates of the parameter space $X$. Consider the operator $\frac{\partial}{\partial \theta_i}|_\theta$ defined by $\frac{\partial}{\partial \theta_i}|_\theta(f) = \frac{\partial f}{\partial \theta_i}(\theta)$. Then the set $\left\{\frac{\partial}{\partial \theta_i}|_\theta\right\}_i$ can be shown to be linear derivations of $C^\infty_\theta$ and hence members of $T_\theta(X)$. Furthermore, for $\forall \theta_j$, each operator in this set satisfies

$$\frac{\partial}{\partial \theta_i}|_\theta(\theta_j) = \begin{cases} 1 & i = j \\ 0 & \text{otherwise} \end{cases}$$

It can be shown that, by satisfying the above constraint, the members of $\left\{\frac{\partial}{\partial \theta_i}|_\theta\right\}_i$ correspond to a basis of $T_\theta(X)$. Therefore, w.r.t this basis if $v \in T_\theta(X)$ then $v = \sum_i a_i \frac{\partial}{\partial \theta_i}|_\theta$.

### A.4 Concept of directional derivative

Let $\Phi : X \rightarrow N$ be a vector valued function that corresponds to a smooth map between two manifolds. The directional derivative of $\Phi$ at any point $\theta \in X$ is the linear map

$$d\Phi|_\theta : T_\theta(X) \rightarrow T_{\Phi(\theta)}(N)$$

defined by:

$$d\Phi|_\theta\left(\sum_i a_i \frac{\partial}{\partial \theta_i}|_\theta\right) = \left[ \frac{\partial \Phi_1}{\partial y_1}|_{\Phi(\theta)}; \frac{\partial \Phi_2}{\partial y_2}|_{\Phi(\theta)}; \cdots; \frac{\partial \Phi_D}{\partial y_D}|_{\Phi(\theta)} \right] \left[ a_1 \ a_2 \ \cdots \ a_D \right]$$

where $\left\{\frac{\partial}{\partial y_j}|_{\Phi(\theta)}\right\}_j$ denotes the basis of $T_{\Phi(\theta)}(N)$. Each coordinate of $\frac{\partial}{\partial y_j}|_{\Phi(\theta)}$ corresponds to the directional derivative of $\Phi_j$ w.r.t $\theta$.

### Appendix B

#### B.1 Approximating the KL divergence using the Fisher Information Matrix

Let $X$ denote the parameter manifold. As different realisations of model parameters lead to different probabilistic models $P_\theta(\mathcal{H}|\mathcal{O})$, the manifold is homeomorphic or in other words equivalent to the space of all probability distributions $\mathcal{M}$ that can be captured by the chosen model. The goal of learning is to identify a viable candidate $h(\theta|\mathcal{O}) \in \mathcal{M}$ that avoids rote memorisation and instead generalises to the concepts that can be learned from a given set of examples.

Using the fact that each candidate $h(\theta|\mathcal{O})$ is a valid probability distribution, the derivatives of such densities satisfy the identity:

$$\sum_H \frac{\partial}{\partial \theta_i} h(\theta|\mathcal{O}) = \sum_H \frac{\partial}{\partial \theta_i} P_\theta(\mathcal{H}|\mathcal{O}) = \frac{\partial}{\partial \theta_i} \sum_H P_\theta(\mathcal{H}|\mathcal{O}) = \frac{\partial}{\partial \theta_i} 1 = 0 \quad (15)$$

Since $X$ is homeomorphic to $\mathcal{M}$, adding a small quantity $\Delta \theta$ to the current iterate $\theta$ results in a unique distribution $P_{\theta + \Delta \theta}(\mathcal{H}|\mathcal{O})$. To quantify the degree of separation between this point from the previous point $P_\theta(\mathcal{H}|\mathcal{O})$ in $\mathcal{M}$, a standard divergence measure for probabilistic models is the KL-divergence $KL(P_\theta(\mathcal{H}|\mathcal{O}) || P_{\theta + \Delta \theta}(\mathcal{H}|\mathcal{O}))$. 


The KL-divergence is a functional that maps the space of distributions \( \mathcal{M} \) to \( \mathbb{R} \). Since each distribution itself is a function of \( \theta \), the divergence measure can be interpreted as a smooth function of \( \theta \). This allows the local behaviour of this divergence measure to be approximated within a convex neighbourhood of the current point \( \theta \) by Taylor’s second order approximation:

\[
KL(P_\theta(H|O) \parallel P_{\theta+\Delta \theta}(H|O)) \approx -\frac{1}{2} \Delta \theta^T E_{P_\theta(H|O)} \left[ \nabla^2 \log P_\theta(H|O) \right] \Delta \theta
\]

In (16), the first order term is dropped as it equates to zero by (15). Hence, locally the KL divergence can be approximated by the bilinear form:

\[
KL(P_\theta(H|O) \parallel P_{\theta+\Delta \theta}(H|O)) \approx -\frac{1}{2} \Delta \theta^T I_\theta \Delta \theta
\]

For discriminative models \( P_\theta(H|O) \), the Fisher Information for a random variable \( \theta \) corresponds to the expected outer product of score of the likelihood:

\[
I_\theta = E_{P_\theta(H|O)} \left[ (\nabla \log P_\theta(H|O)) (\nabla \log P_\theta(H|O))^T \right]
\]

In scenarios where (15) holds, \( I_\theta \) can be shown to be equal to the negative of the expectation of the Hessian w.r.t the distribution \( P_\theta(H|O) \). Thus by substituting the expression of \( I_\theta \) into (17), the KL divergence measure is locally equivalent to the inner product:

\[
KL(P_\theta(H|O) \parallel P_{\theta+\Delta \theta}(H|O)) \approx \frac{1}{2} \Delta \theta^T I_\theta \Delta \theta
\]

Let \( \alpha : (a, b) \subset \mathbb{R} \rightarrow X \) be a continuous map on \( X \). Assuming that the curve is regular i.e \( d\alpha \) is injective at every point \( t \in (a, b) \), the arc length of the curve corresponds to:

\[
s(t) = \int_a^b \| \langle d\alpha(t), d\alpha(t) \rangle_{I_\theta} \| dt
\]

If the choice of \( I_\theta \) corresponds to the Fisher Information matrix, length of paths traversed in the parameter manifold can be interpreted as local changes in the KL divergence.

**Appendix C  Adapting the empirical Fisher to a yield a proper Riemannian metric**

To recap, a Riemannian metric on a smooth parameter manifold \( X \) (see Appendix A.1) is a smooth map that assigns to each \( \theta \in X \) an inner product \( I_\theta \) in \( T_\theta X \). As \( I_\theta \) is real and symmetric, by the spectral decomposition theorem [9], there exists a unitary basis of eigenvectors w.r.t the matrix becomes diagonalisable:

\[
I_\theta \equiv V_\theta \Lambda_\theta V_\theta^T
\]

where \( V_\theta \) is a square matrix whose \( i \)-th column corresponds to the \( i \)-th eigenvector of \( I_\theta \), and \( \Lambda_\theta \) is the diagonal matrix whose non-zero entries represent the associated eigenvalues. It should be noted that the entries of these two matrices are functions of \( \theta \). To keep the notation uncluttered, the
dependency on $\theta$ will be dropped for the remainder of this section whenever any of the individual factors in $V_0 \Delta \theta V_0^T$ is mentioned. Since $\hat{I}_\theta$ is only guaranteed to be positive semi-definite, there will exist zero diagonal entries in $\Lambda$ resulting in its rank being $m$ where $m < D$ (the dimensionality of the parameter space). Under such circumstances, $\hat{I}_\theta^{-1}$ will not exist and it will no longer be possible to endow $X$ with Riemannian metric of the form $\hat{I}_\theta^{-1}$. To address this issue, this section derives an alternative metric to $\hat{I}_\theta$ that has the same structure and properties as the damped FI matrix but is guaranteed to be positive definite. From a high level perspective, the construction of the proposed metric is achieved in two stages.

**Step 1:** partition the tangent space $T_\theta X$ into two disjoint subspaces such that one subspace is spanned by eigenvectors of $\hat{I}_\theta$ associated with non-zero eigenvalues. By re-arranging the columns of $V$ such that the eigenvectors associated with the non-zero eigenvalues occupy positions within the first $m$ columns, the image space of $\hat{I}_\theta$ can be then essentially captured by the matrix $V_{\cdot,1:m} \Lambda_{1:m,1:m} V^T_{\cdot,1:m}$.

Let $\phi$ be a map from $X$ to $\mathbb{R}^m$ given by

$$\phi(\theta) = V^T_{\cdot,1:m} \theta$$

(20)

By the *Replacement theorem* [9], such a map can be shown to be maximal i.e the derivative $\mathrm{d}\phi$ is of full rank. Under the *Implicit Function theorem* [10], there exists a chart $h$ (see Appendix A.1) on $X$ and a neighbourhood $V$ of $h(\theta)$ such that $\phi \circ h^{-1}|_V = \pi|_V$ with $\pi : \mathbb{R}^D \to \mathbb{R}^m$ being the projection map. It is easy to see that from the definition of $\phi$ that such a chart does exist and corresponds to $V_{\cdot,1:m}$. Thus, within the open neighbourhood $V$, the derivative of $\phi \circ h^{-1}$ corresponds to the linear map:

$$\mathrm{d} (\phi \circ h^{-1})(v) = [I_{m \times m} \mid 0_{(m+1) \times D}] (v)$$

(21)

With respect to the map $\phi$, the tangent space $T_\theta X$ can thus be expressed the disjoint sum:

$$T_{\phi\circ h^{-1}}X = T_{\phi \circ h^{-1}}(\theta) \mathbb{R}^m \bigoplus \ker (\mathrm{d}(\phi \circ h^{-1}))$$

(22)

where $\ker (\mathrm{d}(\phi \circ h^{-1}))$ denotes the null space$^4$. By the above construction, $T_{\phi \circ h^{-1}}(\theta) \mathbb{R}^m$ can now be identified as a subspace of $T_\theta X$.

**Step 2:** assign the identity matrix scaled by a very small number $\epsilon$ to the tangent subspace captured by the kernel of $\mathrm{d}(\phi \circ h^{-1})$. As the entries in the diagonal of $\Lambda_{1:m,1:m}$ are functions of $\theta$, endowing $T_{\phi \circ h^{-1}}(\theta) \mathbb{R}^m$ with the inner product $\Lambda_{1:m,1:m}$ is equivalent to assigning a Riemannian metric to the associated subspace in $T_\theta X$. Together, the tangent space of $X$ can now be assigned with the following Riemannian metric:

$$\begin{bmatrix} \Lambda_{1:m,1:m} & 0 \\ 0 & \epsilon I_{(D-m) \times (D-m)} \end{bmatrix}$$

Switching back to the original basis coordinates, the proposed metric then takes the particular form:

$$V \begin{bmatrix} \Lambda_{1:m,1:m} & 0 \\ 0 & \epsilon I_{(D-m) \times (D-m)} \end{bmatrix} V^T = \hat{I}_\theta$$

(23)

It can be seen that by construction $\hat{I}_\theta$ corresponds to a positive definite matrix whose image space is the direct sum of the image and the kernel space of the empirical Fisher matrix $\hat{I}_\theta$. Apart from being a proper Riemannian metric, using CG to solve the appropriate linear system $\hat{I}_\theta \Delta \theta = -\nabla F(\theta_k)$, has one particular advantage: the very first directions explored by the CG algorithm constitute to directions in the image space of $\hat{I}_\theta$ [8] i.e directions considered important by the empirical Fisher are traversed first during the initial stages of a CG run.

$^4$ the $\ker$ of a linear map $L : N \to W$ between two vector spaces $N$ and $W$, is the set of all elements $v \in N$ for which $L(v) = 0$
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