

# New insights and perspectives on the natural gradient method

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**Editor:**

## Abstract

Natural gradient descent is an optimization method traditionally motivated from the perspective of information geometry, and works well for many applications as an alternative to stochastic gradient descent. In this paper we critically analyze this method and its properties, and show how it can be viewed as a type of approximate 2nd-order optimization method, where the Fisher information matrix can be viewed as an approximation of the Hessian. This perspective turns out to have significant implications for how to design a practical and robust version of the method. Additionally, we make the following contributions to the understanding of natural gradient and 2nd-order methods: a thorough analysis of the convergence speed of stochastic natural gradient descent (and more general stochastic 2nd-order methods) as applied to convex quadratics, a critical examination of the oft-used “empirical” approximation of the Fisher matrix, and an analysis of the (approximate) parameterization invariance property possessed by natural gradient methods, which we show still holds for certain choices of the curvature matrix other than the Fisher, but notably not the Hessian.

**Keywords:** natural gradient methods, 2nd-order optimization, neural networks, convergence rate, parameterization invariance

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## 1. Introduction and overview

The natural gradient descent approach, pioneered by Amari and collaborators (e.g. Amari, 1998), is a popular alternative to traditional gradient descent methods which has received a lot of attention over the past several decades, motivating many new and related approaches. It has been successfully applied to a variety of problems such as blind source separation (Amari and Cichocki, 1998), reinforcement learning (Peters and Schaal, 2008), and neural network training (e.g. Park et al., 2000; Martens and Grosse, 2015; Desjardins et al., 2015).

Natural gradient descent is generally applicable to the optimization of probabilistic models<sup>1</sup>, and involves the use of the so-called “natural gradient” in place of the standard gradient, which is defined as the gradient times the inverse of the model’s Fisher information matrix (see **Section 5**). In many applications, natural gradient descent seems to require far fewer total iterations than gradient descent, making it a potentially attractive alternative method. Unfortunately, for models with very many parameters such as large neural networks, computing the natural gradient is impractical due to the extreme size of the Fisher information matrix (“the Fisher”). This problem can be addressed through the use of one of various approximations to the Fisher (e.g. Le Roux et al., 2008; Ollivier, 2015; Grosse and Salakhudinov, 2015; Martens and Grosse, 2015) that are designed to be easier to compute, store and invert than the exact Fisher.

Natural gradient descent is classically motivated as a way of implementing steepest descent in the space of realizable distributions<sup>2</sup> instead of the space of parameters, where distance in the distribution space is measured with a special “Riemannian metric” (Amari and Nagaoka, 2007). This metric depends only on the properties of the distributions themselves and not their parameters, and in particular is defined so that it approximates the square root of the KL divergence within small neighborhoods. Under this interpretation (discussed in detail in **Section 6**), natural gradient descent is invariant to any smooth and invertible reparameterization of the model, putting it in stark contrast to gradient descent, whose performance is highly parameterization dependent.

In practice however, natural gradient descent still operates within the default parameter space, and works by computing directions in the space of distributions and then translating them back to the default space before taking a discrete step. Because of this, the above discussed interpretation breaks down unless the step-size becomes arbitrarily small, and as discussed in **Section 10**, this breakdown has important implications for designing a natural gradient method that can work well in practice. Another problem with this interpretation is that it doesn’t provide any obvious reason why a step of natural gradient descent should make more progress optimizing the objective than a step of standard gradient descent (assuming well chosen step-sizes for both).

Given a large step-size one also loses the parameterization invariance property of the natural gradient method, although it will still hold *approximately* under certain conditions which are described in **Section 13**.

In **Section 10** we argue for an alternative view of natural gradient descent: as an approximate 2nd-order method which utilizes the Fisher as an approximation to the Hessian, so that the natural gradient approximates a 2nd-order step computed using the Hessian. As

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1. This includes neural networks, which can be cast as conditional models.

2. Those distributions which correspond to some setting of the model’s parameters.

discussed in **Section 7**, 2nd-order methods work by forming a local quadratic approximation to the objective around the current iterate and produce the next iterate by optimizing this approximation within some restricted region where the approximation is thought to be accurate. According to this view, natural gradient descent makes more progress per step than gradient descent because it implicitly uses a local quadratic model/approximation of the objective function which is more accurate and less conservative than the one implicitly used by gradient descent.

In support of this view is the fact that the Fisher can be cast as an approximation of the Hessian in at least two different ways (provided the objective has the form discussed in **Section 4**). First, as discussed in **Section 5**, it corresponds to the expected Hessian of the loss under the model’s distribution over predicted outputs instead of the usual empirical one used to compute the exact Hessian. And second, as we establish in **Section 9**, it is very often equivalent to the so-called “Generalized Gauss-Newton matrix” (GGN) (defined in **Section 8**), which is a well established and rigorously justified approximation of the Hessian that has been used in practical 2nd-order optimizations such as those of Martens (2010) and Vinyals and Povey (2012).

Viewing natural gradient descent as an approximate 2nd-order method is also prescriptive, since it suggests the use of various damping/regularization techniques often used in the optimization literature for dealing with the problem of quadratic model trust. Indeed, such techniques have been successfully applied in 2nd-order methods such as that of Martens (2010) and Martens and Grosse (2015), where they proved crucial in achieving good and robust performance in practice.

The Fisher, which is used in computing the natural gradient direction, is defined as the covariance of the gradient of the model’s log likelihood function with respect to cases sampled from its distribution. Because it is often simpler to implement and somewhat more economical, a commonly used approximation of the Fisher, which we discuss in **Section 11**, is to use cases sampled from the training set instead. Known as the “empirical Fisher”, this matrix differs from the usual Fisher in subtle but very important ways, which as shown in **Section 11.1**, make it considerably less useful as an approximation to the Fisher and as a curvature matrix within 2nd-order optimization methods. Using the empirical Fisher also breaks some of the theory regarding natural gradient descent, although it nonetheless preserves the (approximate) parameterization invariance enjoyed by the method (as shown in **Section 13**). Despite these objections, the empirical Fisher has been used in many works such as Le Roux et al. (2008) and the recent spate of methods based on diagonal approximations of this matrix (which we review and critically examine in **Section 11.2**).

A well-known and often quoted result about stochastic natural gradient descent is that it is asymptotically “Fisher efficient” Amari (1998). Roughly speaking, this means that it provides an asymptotically unbiased estimate of the parameters with the lowest possible variance among all unbiased estimators (given the same amount of data), thus achieving the best possible expected objective function value. Unfortunately, as discussed in **Section 12.1**, this result comes with several important caveats which severely limit its applicability. Moreover even when it is applicable it only provides an *asymptotically* accurate characterization of the method which may not accurately describe its behavior given a realistic number of iterations.

To address these issues we build on the work of Murata (1998) in **Section 12.2** and **Section 12.3** to develop a more powerful convergence theory for approximate stochastic 2nd-order methods (including natural gradient descent) as applied to convex quadratic objectives. Our results provide a more precise expression for the convergence speed of such methods than existing results do, and properly account for the effect of the starting point. And as we discuss in **Section 12.2.1** and **Section 12.3.1** they imply various interesting consequences about the relative performance of various 1st and 2nd-order stochastic optimization methods.

Perhaps the most interesting conclusion of this analysis is that with parameter averaging applied, stochastic gradient descent with a constant step-size/learning-rate achieves the same *asymptotic* convergence speed as natural gradient descent (and is thus also “Fisher efficient”), although 2nd-order methods (such as the latter) can enjoy a more favorable dependence on the starting point, which means that they can make much more progress given a limited iteration budget.

Unfortunately these results fail to fully explain why 2nd-order optimization with the GGN/Fisher works so much better than classical 2nd-order schemes such as Newton’s method. And so in **Section 15** we propose several important open questions in this direction that we leave for future research.

Table of notation

Notation	Description
$[v]_i$	$i$ -th entry of a vector $v$
$[A]_{i,j}$	$(i, j)$ -th entry a matrix $A$
$\nabla\gamma$	gradient of a scalar function $\gamma$
$J_\gamma$	Jacobian of a vector-valued function $\gamma$
$H_\gamma$	Hessian of a scalar function $\gamma$ (typically taken with respect to $\theta$ unless otherwise specified)
$\theta$	vector of parameters
$W_i$	weight matrix at layer $i$
$s_i$	unit inputs at layer $i$
$a_i$	unit activities at layer $i$
$\ell$	number of layers
$m$	dimension of the network's output $f(x, \theta)$
$m_i$	number of units in $i$ -th layer of the network
$f(x, \theta)$	function mapping the neural network's inputs to its output
$L(y, z)$	loss function
$h$	objective function
$S$	training set
$k$	current iteration
$n$	dimension of $\theta$
$M(\delta)$	local quadratic approximation of $h$ at $\theta$
$\lambda$	strength constant for penalty-based damping
$\lambda_j(A)$	$j$ -th largest eigenvalue a symmetric matrix $A$
$G$	generalized Gauss-Newton matrix (GGN)
$P_{x,y}(\theta)$	model's distribution
$Q_{x,y}(\theta)$	data distribution
$\hat{Q}_{x,y}(\theta)$	training/empirical distribution
$R_{y z}$	predictive distribution used at network's output (so $P_{y x}(\theta) = R_{y f(x,\theta)}$ )
$p, q, r$	density functions associated with above $P$ , $Q$ , and $R$ (resp.)
$F$	Fisher information matrix (typically associated with $P_{x,y}$ )
$F_D$	Fisher information matrix associated with parameterized distribution $D$

Table 1: A table listing some of the notation used throughout this document.

## 2. Neural Networks

Feed-forward neural networks are structured very similarly to classical circuits. They typically consist of a sequence of  $\ell$  “layers” of units, where each unit in a given layer receive inputs from the units in the previous layer, and computes an affine function of these, followed by a scalar non-linear function called an “activation function”. The input vector to the network, denoted by  $x$ , is given by the units of the first layer, which is called the “input layer” (and is not counted towards the total  $\ell$ ). The output vector of the network, denoted by  $f(x, \theta) \in \mathbb{R}^{m_\ell} = \mathbb{R}^m$ , is given by the units of the network’s last layer (called the “output layer”). The other layers are referred to as the network’s “hidden layers”.

Formally, given input  $x \in \mathbb{R}^{m_0}$ , and parameters  $\theta \in \mathbb{R}^n$  which determine weight matrices  $W_1 \in \mathbb{R}^{m_1 \times m_0}, W_2 \in \mathbb{R}^{m_2 \times m_1}, \dots, W_\ell \in \mathbb{R}^{m_\ell \times m_{\ell-1}}$  and biases  $b_1 \in \mathbb{R}^{m_1}, b_2 \in \mathbb{R}^{m_2}, \dots, b_\ell \in \mathbb{R}^{m_\ell}$ , the network computes its output  $f(x, \theta) = a_\ell$  according to

$$\begin{aligned} s_i &= W_i a_{i-1} + b_i \\ a_i &= \phi_i(s_i), \end{aligned}$$

where  $a_0 = x$ . Here,  $a_i$  is the vector of values (“activities”) of the network’s  $i$ -th layer, and  $\phi_i(\cdot)$  is the vector-valued non-linear function computed at layer  $i$ , and is often given by some simple monotonic activation function applied coordinate-wise.

Note that most of the results discussed in this document will apply to the more general setting where  $f(x, \theta)$  is an arbitrary differentiable function (in both  $x$  and  $\theta$ ).

## 3. Supervised learning framework

The goal of optimization/learning is to find some setting of  $\theta$  so that the output of the network (which we will sometimes call its “prediction”) matches certain target outputs as closely as possible. In particular, given a training set  $S$  consisting of training pairs  $(x, y)$ , the goal of learning is to minimize the objective function

$$h(\theta) \equiv \frac{1}{|S|} \sum_{(x,y) \in S} L(y, f(x, \theta)), \quad (1)$$

where  $L(y, z)$  is a “loss function” which measures the amount of disagreement between  $y$  and  $z$ .

The prediction  $f(x, \theta)$  may be a guess for  $y$ , in which case  $L$  might measure the inaccuracy of this guess (e.g. using the familiar squared error  $\frac{1}{2}\|y - z\|^2$ ). Or  $f(x, \theta)$  could encode the parameters of some simple predictive distribution. For example,  $f(x, \theta)$  could be the set of probabilities which parameterize a multinomial distribution over the possible discrete values of  $y$ , with  $L(y, f(x, \theta))$  being the negative log probability of  $y$  under this distribution.

## 4. KL divergence objectives

The natural gradient method of Amari (1998) can be potentially applied to any objective function which measures the performance of some statistical model. However, it enjoys richer theoretical properties when applied to objective functions based on the KL divergence between the model’s distribution and the target distribution, or certain approximations/surrogates of these.

In this section we will establish the basic notation and properties of these objective functions, and discuss the various ways in which they can be formulated. Each of these formulations will be analogous to a particular formulation of the Fisher information matrix and natural gradient (as defined in Section 5), which will differ in subtle but important ways.

In the idealized setting, input vectors  $x$  are drawn independently from a *target* distribution  $Q_x$  with density function  $q(x)$ , and the corresponding (target) outputs  $y$  from a conditional *target* distribution  $Q_{y|x}$  with density function  $q(y|x)$ .

We define the goal of learning as the minimization of the KL divergence from target joint distribution  $Q_{x,y}$ , whose density is  $q(y, x) = q(y|x)q(x)$ , to the learned distribution  $P_{x,y}(\theta)$ , whose density is  $p(x, y|\theta) = p(y|x, \theta)q(x)$ . Note that the second  $q(x)$  is not a typo here, since we are not learning the distribution over  $x$ , only the conditional distribution of  $y$  given  $x$ . Our objective function is thus

$$\text{KL}(Q_{x,y} \| P_{x,y}(\theta)) = \int q(x, y) \log \frac{q(x, y)}{p(x, y|\theta)} dx dy.$$

This is equivalent to the expected KL divergence

$$\mathbb{E}_{Q_x}[\text{KL}(Q_{y|x} \| P_{y|x}(\theta))] \tag{2}$$

since we have

$$\begin{aligned} \mathbb{E}_{Q_x}[\text{KL}(Q_{y|x} \| P_{y|x}(\theta))] &= \int q(x) \int q(y|x) \log \frac{q(y|x)}{p(y|x, \theta)} dy dx \\ &= \int q(x, y) \log \frac{q(y|x)q(x)}{p(y|x, \theta)q(x)} dx dy \\ &= \text{KL}(Q_{x,y} \| P_{x,y}(\theta)). \end{aligned}$$

It is often the case that we only have samples from  $Q_x$  and no direct knowledge of its density function. Or the expectation w.r.t.  $Q_x$  in eqn. 2 may be too difficult to compute. In such cases, we can substitute an empirical *training* distribution  $\hat{Q}_x$  in for  $Q_x$ , which is given by a set  $S_x$  of samples from  $Q_x$ . This gives the objective

$$\mathbb{E}_{\hat{Q}_x}[\text{KL}(Q_{y|x} \| P_{y|x}(\theta))] = \frac{1}{|S|} \sum_{x \in S_x} \text{KL}(Q_{y|x} \| P_{y|x}).$$

Provided that  $q(y|x, \theta)$  is known for each  $x$  in  $S_x$  and that  $\text{KL}(Q_{y|x} \| P_{y|x})$  can be efficiently computed, we can use the above expression as our objective.

Otherwise, as is often the case, we might only have access to a single sample  $y$  from  $Q_{y|x}$  for each  $x \in S_x$ , giving an empirical *training* distribution  $\hat{Q}_{y|x}$ . Substituting this in for  $Q_{y|x}$  gives the objective function

$$\mathbb{E}_{\hat{Q}_x}[\text{KL}(\hat{Q}_{y|x} \| P_{y|x})] = \frac{1}{|S|} \sum_{(x,y) \in S} \log \frac{1}{p(y|x, \theta)} = -\frac{1}{|S|} \sum_{(x,y) \in S} \log p(y|x, \theta),$$

where we have extended  $S_x$  to a set  $S$  of the  $(x, y)$  pairs (which agrees with how  $S$  was defined in Section 3). This is the same objective as is minimized in *standard maximum likelihood learning*



This kind of objective function fits into the general supervised learning framework described in Section 3 as follows. We define the learned conditional distribution  $P_{y|x}$  to be the composition of the deterministic neural network function  $f(x, \theta)$ , and an “output” conditional distribution  $R_{y|z}$  (with associated density function  $r(y|z)$ ), so that

$$P_{y|x} = R_{y|f(x, \theta)}.$$

We then define the loss function as  $L(y, z) = -\log r(y|z)$ .

Given a loss function  $L$  which is not explicitly defined this way one can typically still find a corresponding  $R$  to make the definition apply. In particular, if  $\exp(-L(y, z))$  has the same finite integral w.r.t.  $y$  for each  $z$ , then one can define  $R$  by taking  $r(y|z) \propto \exp(-L(y, z))$ , where the proportion is w.r.t. both  $y$  and  $z$ .

## 5. Various definitions of the natural gradient and the Fisher information matrix

The usual definition of the natural gradient (Amari, 1998) which appears in the literature is

$$\tilde{\nabla} h = F^{-1} \nabla h,$$

where  $F$  is the Fisher information matrix of  $P_{x,y}(\theta)$  w.r.t.  $\theta$ .  $F$  is given by

$$F = E_{P_{x,y}} \left[ \nabla \log p(x, y|\theta) \nabla \log p(x, y|\theta)^\top \right] \quad (3)$$

$$= -E_{P_{x,y}} \left[ H_{\log p(x, y|\theta)} \right]. \quad (4)$$

where gradients and Hessians are taken w.r.t.  $\theta$ . For the purposes of brevity we will often refer to the Fisher information matrix simply as the “Fisher”.

It can be immediately seen from the first of these expressions for  $F$  that it is positive semi-definite (PSD) (since it’s the expectation of something which is trivially PSD, a vector outer-product). And from the second expression we can see that it also has the interpretation of being the negative expected Hessian of  $\log p(x, y|\theta)$ .

Because  $p(x, y|\theta) = p(y|x, \theta)q(x)$  where  $q(x)$  doesn’t depend on  $\theta$ , we have

$$\nabla \log p(x, y|\theta) = \nabla \log p(y|x, \theta) + \nabla \log q(x) = \nabla \log p(y|x, \theta),$$

and so  $F$  can also be written as the expectation (w.r.t.  $Q_x$ ) of the Fisher information matrix of  $P_{y|x}(\theta)$  as follows:

$$F = E_{Q_x} \left[ E_{P_{y|x}} \left[ \nabla \log p(y|x, \theta) \nabla \log p(y|x, \theta)^\top \right] \right] \quad \text{or} \quad F = -E_{Q_x} \left[ E_{P_{y|x}} \left[ H_{\log p(y|x, \theta)} \right] \right].$$

In Amari (1998), this version of  $F$  is computed explicitly for a basic perceptron model (basically a neural network with 0 hidden layers) in the case where  $Q_x = N(0, I)$ .

However in practice the real  $q(x)$  may be not directly available, or it may be difficult to integrate  $H_{\log p(y|x, \theta)}$  over  $Q_x$ . For example, the conditional Hessian  $H_{\log p(y|x, \theta)}$  corresponding to a multilayer neural network may be far too complicated to be analytically integrated,

even for a very simple  $Q_x$ . In such situations  $Q_x$  may be replaced with its empirical version  $\hat{Q}_x$  giving

$$F = \frac{1}{|S|} \sum_{x \in S_x} E_{P_{y|x}} \left[ \nabla \log p(y|x, \theta) \nabla \log p(y|x, \theta)^\top \right] \quad \text{or} \quad F = -\frac{1}{|S|} \sum_{x \in S_x} E_{P_{y|x}} \left[ H_{\log p(y|x, \theta)} \right].$$

This is the version of  $F$  considered in Park et al. (2000).

From these expressions we can see that when  $L(y, z) = -\log r(y|z)$  (as in Section 4), the Fisher has the interpretation of being the expectation under  $P_{x,y}$  of the Hessian of  $L(y, f(x, \theta))$ :

$$F = -\frac{1}{|S|} \sum_{x \in S_x} E_{P_{y|x}} \left[ H_{L(y, f(x, \theta))} \right].$$

Meanwhile, the Hessian  $H$  of  $h$  is also given by the expected value of the Hessian of  $L(y, f(x, \theta))$ , except under the distribution  $\hat{Q}_{x,y}$  instead of  $P_{x,y}$  (where  $\hat{Q}_{x,y}$  is given by the density  $\hat{q}(x, y) = \hat{q}(y|x)\hat{q}(x)$ ). In other words

$$H = -\frac{1}{|S|} \sum_{x \in S_x} E_{\hat{Q}_{x,y}} \left[ H_{L(y, f(x, \theta))} \right].$$

Thus  $F$  can be seen as an approximation of  $H$  in some sense.

## 6. Geometric interpretation

The negative gradient  $-\nabla h$  can be interpreted as the steepest descent direction for  $h$  in the sense that it yields the most reduction in  $h$  per unit of change in  $\theta$ , where change is measured using the standard Euclidean norm  $\|\cdot\|$ . More formally we have

$$\frac{-\nabla h}{\|\nabla h\|} = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \arg \min_{d: \|d\| \leq \epsilon} h(\theta + d).$$

This interpretation exposes the strong dependence of the gradient on the Euclidean geometry of the parameter space (as defined by the norm  $\|\cdot\|$ ).

One way to motivate the natural gradient is to show that it can be viewed as a steepest descent direction, much like the negative gradient can be, except with respect to a metric that is intrinsic to the distributions being modeled as opposed to the default Euclidean metric in parameter space. In particular, the natural gradient can be derived by adapting the steepest descent formulation to use an alternative definition of (local) distance based on the “information geometry” (Amari and Nagaoka, 2000) of the space of probability distributions (as induced by the parameters). The particular distance function<sup>3</sup> which gives rise to the natural gradient turns out to be

$$\text{KL}(P_{x,y}(\theta + d) \| P_{x,y}(\theta)).$$

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3. Note that this is not a formal “distance” function in the usual sense since it is not symmetric.

To make this formal, we will first show how the KL divergence and the Fisher are fundamentally connected. The Taylor series expansion of the above distance is

$$\text{KL}(P_{x,y}(\theta + d) \| P_{x,y}(\theta)) = \frac{1}{2} d^\top F d + O(d^3),$$

where “ $O(d^3)$ ” is short-hand to mean terms that are order 3 or higher in the entries of  $d$ . Thus  $F$  defines the local quadratic approximation of this distance, and so gives the mechanism of *local* translation between the geometry of the space of distributions, and that of the original parameter space with its default Euclidean geometry.

To make use of this connection we first observe, as in Arnold et al. (2011), that for a general positive definite matrix  $A$  we have

$$\frac{-A^{-1}\nabla h}{\|\nabla h\|_{A^{-1}}} = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \arg \min_{d: \|d\|_A \leq \epsilon} h(\theta + d)$$

where the notation  $\|v\|_B$  is defined by  $\|v\|_B = \sqrt{v^\top B v}$ .

Then taking  $A = \frac{1}{2}F$  and using the above Taylor series expansion of the KL divergence to show that  $\text{KL}(P_{x,y}(\theta + d) \| P_{x,y}(\theta)) \rightarrow \frac{1}{2} d^\top F d = \frac{1}{2} \|d\|_F^2$  as  $\epsilon \rightarrow 0$ , with some extra work (Arnold et al., 2011) it follows that

$$-\sqrt{2} \frac{\tilde{\nabla} h}{\|\nabla h\|_{F^{-1}}} = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \arg \min_{d: \text{KL}(P_{x,y}(\theta + d) \| P_{x,y}(\theta)) \leq \epsilon^2} h(\theta + d).$$

Thus the negative natural gradient is indeed the steepest descent direction in the space of distributions where distance is (approximately) measured in local neighborhoods by the KL divergence. While this might seem impossible since the KL divergence is in general not symmetric in its two arguments, it turns out that  $\text{KL}(P_{x,y}(\theta + d) \| P_{x,y}(\theta))$  is locally/asymptotically symmetric as  $d$  goes to zero, and so will be (approximately) symmetric in a local neighborhood<sup>4</sup>.

Note that both  $F$  and  $\tilde{\nabla} h$  are defined in terms of the standard basis in  $\theta$ -space, and so obviously depend on the parameterization of  $h$ . But the KL divergence does not, and instead only depends on the form of the predictive distribution  $P_{y|x}$ . Thus, the direction in distribution space defined implicitly by  $\tilde{\nabla} h$  will be invariant to our choice of parameterization (whereas the direction defined by  $\nabla h$  will not be).

By using the smoothly varying PSD matrix  $F$  to locally define a metric tensor at every point in parameter space, a Riemannian manifold can be generated over the space of distributions. Note that the associated metric of this space won’t be the KL divergence (this isn’t even a valid metric), although it will be “locally equivalent” to the square root of the KL divergence in the sense that the two will approximate each other within a small neighborhood.

## 7. 2nd-order optimization

The basic idea in 2nd-order optimization is to compute the update  $\delta$  to  $\theta \in \mathbb{R}^n$  by minimizing some local quadratic approximation  $M(\delta)$  of  $h(\theta_k + \delta)$  centered around the current iterate  $\theta_k$ .

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4. This follows from the fact the second order term of the Taylor series of  $\text{KL}(P_{x,y}(\theta) \| P_{x,y}(\theta + d))$  is *also* given by  $\frac{1}{2} d^\top F d$ .

That is, we compute  $\delta^* = \arg \min_{\delta} M(\delta)$  and then update  $\theta$  according to  $\theta_{k+1} = \theta_k + \alpha_k \delta^*$ , where  $M(\delta)$  is defined by

$$M(\delta) = \frac{1}{2} \delta^\top B \delta + \nabla h(\theta_k)^\top \delta + h(\theta_k),$$

and where  $B \in \mathbb{R}^{n \times n}$  is the “curvature matrix”, which is symmetric. The “sub-problem” of optimizing  $M(\delta)$  can be performed exactly by solving the  $n \times n$  dimensional linear system  $B\delta = -\nabla h$ , whose solution is  $\delta^* = -B^{-1}\nabla h$  when  $B$  is invertible.

Gradient descent, the canonical 1st-order method, can be viewed in the framework of 2nd-order methods as making the choice  $B = \beta I$  for some  $\beta$ , resulting in the update  $\delta^* = -\frac{1}{\beta} \nabla h(\theta_k)$ . In the case where  $h$  is convex and Lipschitz-smooth<sup>5</sup> with constant  $\mathcal{L}$ , a safe/conservative choice that will ensure convergence with  $\alpha_k = 1$  is  $\beta = \mathcal{L}$  (e.g. Nesterov, 2013). The intuition behind this choice is that  $B$  will act as a *global* upper bound on the curvature of  $h$ , in the sense that  $B = \mathcal{L}I \succeq H(\theta)$ <sup>6</sup>, so that  $\delta^*$  never extends past the point that would be safe in the worst-case scenario where the curvature sharply increases to the upper bound  $\mathcal{L}$  as one travels along  $\delta^*$ . More concretely, one can show that given this choice of  $\beta$ ,  $M(\delta)$  upper bounds  $h(\theta_k + \delta)$ , and will therefore never predict a reduction in  $h(\theta_k + \delta)$  where there is actually a sharp increase (e.g. due to  $h$  curving unexpectedly upward on the path from  $\theta_k$  to  $\theta_k + \delta$ ). Minimizing  $M(\delta)$  is therefore guaranteed not to increase  $h(\theta_k + \delta)$  beyond the current value  $h(\theta_k)$  since  $M(0) = h(\theta_k)$ . But despite these nice properties, this choice will almost always overestimate the curvature in most directions, leading to updates that move unnecessarily slowly along directions of consistent low curvature.

While neural networks haven’t been closely studied by optimization researchers, many of the local optimization issues related to neural network learning can be seen as extreme special cases of problems which arise more generally in continuous optimization. For example, tightly coupled parameters with strong local dependencies, and large variations in scale along different directions in parameter space (which may arise due to the “vanishing gradient” phenomenon (Hochreiter et al., 2000)), are precisely the sorts of issues for which 2nd-order optimization is well suited. Gradient descent on the other hand is well-known to be very sensitive to such issues, and in order to avoid large oscillations and instability must use a learning rate which is inversely proportional to the size  $\mathcal{L}$  of the curvature along the highest curvature direction. 2nd-order optimization methods provide a much more powerful and elegant solution to the problem of variations in scale/curvature along different directions, by selectively re-scaling the gradient along different eigen-directions of the curvature matrix  $B$  according to their associated curvature (eigenvalue), instead of employing a one-size-fits-all step-size.

In the classical Newton’s method we take  $B = H(\theta_k)$ , in which case  $M(\delta)$  becomes the 2nd-order Taylor-series approximation of  $h$  centered at  $\theta_k$ . This choice gives us the most accurate *local* model of the curvature possible, and allows for very rapid exploration of low-curvature directions yielding faster convergence. Unfortunately, Newton’s method runs into numerous problems when applied to neural network training objectives, such as  $H$  being sometimes indefinite (and thus  $M(\delta)$  being unbounded below in directions of negative curvature) and related issues of model trust, where the method implicitly “trusts” its own

5. By this we mean that  $\|\nabla h(\theta) - \nabla h(\theta')\| \leq \mathcal{L}\|\theta - \theta'\|$  for all  $\theta$  and  $\theta'$ .

6. Here we define  $A \succeq C$  to mean that  $A - C$  is PSD.

local quadratic model of the objective too much, causing it to generate huge and nonsensical updates that increase  $h$ . This problem is particular to 2nd-order methods because they use a much less conservative model of the curvature than gradient descent, that may start out as accurate around  $\theta_k$ , but which may quickly become a severe underestimate as one travels along  $\delta^*$ . Fortunately, using the Gauss-Newton approximation to the Hessian (as discussed in Section 8), and applying various update damping/trust-region techniques (as discussed in Section 10), these issues can be mostly overcome.

Another important issue preventing the naive application of 2nd-order methods to neural networks is the very high dimensionality of the parameter space, which prohibits the calculation/storage/inversion of the  $n^2$ -entry curvature matrix  $B$ . To address this, various approximate Newton methods have been developed within the optimization and machine learning communities. These methods work by approximating  $B$  with something easier to compute/store/invert such as a low-rank or diagonal matrix, or by performing only approximate/incomplete optimization of  $M(\delta)$ . A survey of such methods is outside the scope of this report, so we refer to the reader to Martens (2016).

## 8. The generalized Gauss-Newton matrix

The classical Gauss-Newton matrix (or more simply the Gauss-Newton matrix) is the curvature matrix  $G$  which arises in the Gauss-Newton method for non-linear least squares problems. It is applicable to our standard neural network training objective  $h$  in the case where  $L(y, z) = \frac{1}{2}\|y - z\|^2$ , and is given by

$$G = \frac{1}{|S|} \sum_{(x,y) \in S} J_f^\top J_f,$$

where  $J_f$  is the Jacobian of  $f(x, \theta)$  w.r.t. the parameters  $\theta$ . It is usually defined as the approximation to the Hessian  $H$  of  $h$  (w.r.t.  $\theta$ ) obtained by dropping the second term inside the sum of the following expression for  $H$ :

$$H = \frac{1}{|S|} \sum_{(x,y) \in S} \left( J_f^\top J_f - \sum_{j=1}^m [y - f(x, \theta)]_j H_{[f]_j} \right),$$

where  $H_{[f]_j}$  is the Hessian (w.r.t.  $\theta$ ) of the  $j$ -th component of  $f(x, \theta)$ .

An alternative way to derive the classical Gauss-Newton is to simply replace the non-linear function  $f(x, \theta)$  by its own local linear approximation, centered at the current value  $\theta_i$  of  $\theta$ . In particular, we replace  $f$  by  $\tilde{f}(x, \theta) = J_f \cdot (\theta - \theta_i) + f(x, \theta_i)$  so that  $h$  becomes a quadratic function of  $\theta$ , with derivative  $\nabla h(\theta_i)$  and Hessian given by  $G$ .

Schraudolph (2002) showed how the idea of the Gauss-Newton matrix can be generalized to the situation where  $L(y, z)$  is *any* loss function which is convex in  $z$ . The generalized formula for  $G$  is

$$G = \frac{1}{|S|} \sum_{(x,y) \in S} J_f^\top H_L J_f, \tag{5}$$

where  $H_L$  is the Hessian of  $L(y, z)$  w.r.t.  $z$ , evaluated at  $z = f(x, \theta)$ . Because  $L$  is convex,  $H_L$  will be PSD for each  $(x, y)$ , and thus so will  $G$ . We will call this  $G$  the Generalized

Gauss-Newton matrix (GGN). Analogously to the case of the classical Gauss-Newton matrix (which assumed  $L(y, z) = \frac{1}{2}\|y - z\|^2$ ), the GGN can be obtained by dropping the second term inside the sum of the following expression for the Hessian  $H$  (e.g. Nocedal and Wright, 2006):

$$H = \frac{1}{|S|} \sum_{(x,y) \in S} \left( J_f^\top H_L J_f + \sum_{j=1}^m \left[ \nabla_z L(y, z)|_{z=f(x,\theta)} \right]_j H_{[f]_j} \right). \quad (6)$$

Here,  $\nabla_z L(y, z)|_{z=f(x,\theta)}$  is the gradient of  $L(y, z)$  w.r.t.  $z$ , evaluated at  $z = f(x, \theta)$ . Note if we have for some local optimum  $\theta^*$  that  $\left[ \nabla_z L(y, z)|_{z=f(x,\theta^*)} \right]_j \approx 0$  for each  $(x, y)$  and  $j$ , which corresponds to network making an optimal prediction for each training case over each dimension, then  $G(\theta^*) = H(\theta^*)$ . In such a case, the behavior of a 2nd-order optimizer using  $G$  will approach the behavior of the ideal Newton method as it converges to  $\theta^*$ .

Like the Hessian, the GGN can be used to define a local quadratic model of  $h$ , as given by:

$$M(\delta) = \frac{1}{2} \delta^\top G \delta + \nabla h^\top \delta + h(\theta).$$

In approximate Newton/2nd-order methods based on the GGN, parameter updates are computed by minimizing  $M(\delta)$  w.r.t.  $\delta$ . The exact minimizer  $\delta^* = -G^{-1} \nabla h$  is often too difficult to compute, and so practical methods like the Hessian-free optimization of Martens (2010), or Krylov Subspace Descent (Vinyals and Povey, 2012) will only approximately minimize  $M(\delta)$ .

A key property of  $G$  which is not shared by the Hessian  $H$  is that it is PSD, and can thus be used to define a local quadratic model to the objective  $h$  which is bounded. While the unboundedness of local quadratic models defined by the Hessian can be worked around by imposing a trust region, it has nevertheless been observed by various researchers Schraudolph (2002); Martens (2010); Vinyals and Povey (2012) that  $G$  works much better in practice for neural network optimization.

Since computing the whole matrix explicitly is usually too expensive, the GGN is typically accessed via matrix-vector products. To compute such products efficiently one can use the method of Schraudolph (2002), which is a generalization of the well-known method for computing such products with the classical Gauss-Newton. The method is similar in cost and structure to standard backpropagation, although it can sometimes be tricky to implement (see Martens and Sutskever (2012)).

As pointed out in Martens and Sutskever (2011), the GGN can also be derived by generalizing the previously described alternative derivation of the classical Gauss-Newton matrix to the situation where  $L$  is an arbitrary convex loss. In particular, if we substitute the linearization  $\tilde{f}$  for  $f$  in  $h$  as before (where  $\tilde{f}(x, \theta) = J_f \cdot (\theta - \theta_i) + f(x, \theta_i)$  is the linearization of  $f$ ), it is not difficult to see that the Hessian of the resulting  $h$  will be equal to the GGN.

Schraudolph (2002) advocated that when computing the GGN,  $L$  and  $f$  be redefined so that as much as possible of the network's computation is formally performed by  $L$  instead of  $f$ , while maintaining the convexity of  $L$ . This is because, unlike  $f$ ,  $L$  is not linearly

approximated in the GGN, and so its associated second-order derivative terms are faithfully captured. What this almost always means in practice is that what is usually thought of as the final non-linearity of the network (i.e.  $\phi_\ell$ ) is folded into  $L$ , and the network itself just computes the identity function at its top layer. Interestingly, in many natural situations which occur in practice, doing this gives a much simpler and more elegant expression for  $H_L$ . Exactly when and why this happens will be made clear in Section 9.

### 8.1 Speculation on possible advantages of the GGN over the Hessian

Unlike the Hessian, the GGN is positive semi-definite (PSD). This means that it never models the curvature in any direction as negative. The most obvious problem with negative curvature is that the quadratic model will predict an unbounded quadratic improvement in the objective for moving in certain directions. Indeed, without the use of some kind of trust-region or damping technique (as discussed in Section 10) the update produced by minimizing the quadratic model will be infinitely large in any direction of negative curvature.

While curvature can indeed be negative in a local neighborhood (as measured by the Hessian), we know it must quickly become non-negative as we travel along any particular direction, given that our loss  $L(y, z)$  is convex in  $z$  and bounded below. Meanwhile, positive curvature predicts a quadratic penalty, and in the worst case merely underestimates how badly the objective will eventually increase along a particular direction.

Because contributions made to the GGN for each training case and each individual component of  $f(x, \theta)$  are PSD, there can be no cancellation between positive and negative/indefinite contributions. This means that the GGN can be more robustly estimated from subsets of the training data than the Hessian. By analogy, consider how much harder it is to estimate the scale of the mean value of a variable when that variable can take on both positive and negative values, and has a mean close to 0.

This property of being PSD for individual training cases and components of  $f(x, \theta)$  also means that positive curvature from one training case, or one component of the network’s prediction, cannot be cancelled out by negative curvature from others. If we believe that negative curvature is less “trustworthy” than positive curvature over larger distances, then it seems like a good idea to prevent positive curvature from being cancelled in this manner.

Notably the GGN is not an upper bound on the Hessian (in the PSD sense), as it fails to model *all* of the positive curvature contained in the latter. But crucially, it only fails to model the (positive or negative) curvature coming from the network function  $f(x, \theta)$ , as opposed to the curvature coming from the loss function  $L(y, z)$ . (To see this, recall the decomposition of the Hessian from eqn. 6, noting that the term dropped from the Hessian depends only on the gradients of  $L$  and the Hessian of components of  $f$ .) Curvature coming from  $f$ , whether it is positive or negative, is arguably less trustworthy/stable across long distance than curvature coming from  $L$ , as argued below.

The following decomposition of the Hessian is a generalization of eqn. 6:

$$H = \frac{1}{|S|} \sum_{(x,y) \in S} \left( J_f^\top H_L J_f + \sum_{i=1}^{\ell} \sum_{j=1}^{m_i} [\nabla_{a_i} L(y, f)]_j J_{s_i}^\top H_{[\phi_i(s_i)]_j} J_{s_i} \right).$$

Here,  $\nabla_{a_i} L(y, f)$  is the gradient of  $L(y, f)$  w.r.t.  $a_i$ ,  $H_{[\phi_i(s_i)]_j}$  is the Hessian of  $\phi_i(s_i)$  (i.e. the function which computes  $a_i$ ) w.r.t.  $s_i$ , and  $J_{s_i}$  is the Jacobian of  $s_i$  (viewed as a function of  $\theta$  and  $x$ ) w.r.t.  $\theta$ .

We can see from this equation that the curvature coming from the network function  $f$  is a sum of curvature terms coming from each neural unit, weighted by the gradient of the loss w.r.t. that unit's output  $[a_i]_j$ . It seems reasonable to expect that the sign of these terms may be subject to frequent change, due both to changes in the sign of "local Hessian"  $H_{[\phi_i(s_i)]_j}$  of  $\phi_i$  ( $\phi_i$  is typically non-convex), and to changes in the sign of the loss derivative w.r.t. that unit's output ( $[\nabla_{a_i} L(y, f)]_j$ ), which depends on the behavior of all of the layers above  $a_i$ . This is to be contrasted with the curvature term  $J_f^\top H_L J_f$  arising from the loss, which remains PSD everywhere.

Finally, it is worth noting that for networks with piece-wise linear activation functions, such as the popular RELUs (given by  $[\phi_i(s_i)]_j = \max([s_i]_j, 0)$ ), the network function  $f$  has zero curvature almost everywhere, since  $H_{[\phi_i(s_i)]_j} = 0$  when  $[\phi_i(s_i)]_j \neq 0$ , and is undefined otherwise. Thus the Hessian will coincide with the GGN for such networks at all points where the former is defined.

## 9. Computational aspects of the natural gradient and connections to the generalized Gauss-Newton matrix

### 9.1 Computing the Fisher (and matrix-vector products with it)

Note that

$$\nabla \log p(y|x, \theta) = J_f^\top \nabla_z \log r(y|z),$$

where  $J_f$  is the Jacobian of  $f(x, \theta)$  w.r.t.  $\theta$ , and  $\nabla_z \log r(y|z)$  is the gradient of  $\log r(y|z)$  w.r.t.  $z$ , evaluated at  $z = f(x, \theta)$  (with  $r$  defined as near the end of Section 4).

As was first shown by Park et al. (2000), the Fisher information matrix is thus given by

$$\begin{aligned} F &= E_{Q_x} \left[ E_{P_{y|x}} \left[ \nabla \log p(y|x, \theta) \nabla \log p(y|x, \theta)^\top \right] \right] \\ &= E_{Q_x} [E_{P_{y|x}} [J_f^\top \nabla_z \log r(y|z) \nabla_z \log r(y|z)^\top J_f]] \\ &= E_{Q_x} [J_f^\top E_{P_{y|x}} [\nabla_z \log r(y|z) \nabla_z \log r(y|z)^\top] J_f] = E_{Q_x} [J_f^\top F_R J_f], \end{aligned}$$

where  $F_R$  is the Fisher information matrix of the predictive distribution  $R_{y|z}$  at  $z = f(x, \theta)$ .

$F_R$  is itself given by

$$F_R = E_{P_{y|x}} [\nabla_z \log r(y|z) \nabla_z \log r(y|z)^\top] = E_{R_{y|f(x, \theta)}} [\nabla_z \log r(y|z) \nabla_z \log r(y|z)^\top]$$

or

$$F_R = -E_{R_{y|f(x, \theta)}} [H_{\log r}],$$

where  $H_{\log r}$  is the Hessian of  $\log r(y|z)$  w.r.t.  $z$ , evaluated at  $z = f(x, \theta)$ .

Note that even if  $Q_x$ 's density function  $q(x)$  is known, and is relatively simple, only for certain choices of  $R_{y|z}$  and  $f(x, \theta)$  will it be possible to analytically evaluate the expectation w.r.t.  $Q_x$  in the above expression for  $F$ .



For example, if we take  $Q_x = \mathcal{N}(0, I)$ ,  $R_{y|z} = \mathcal{N}(z, \sigma^2)$ , and  $f$  to be a simple neural network with no hidden units and a single tan-sigmoid output unit, then both  $F$  and its inverse can be computed efficiently (Amari, 1998). This situation is exceptional however, and for even slightly more complex models, such as neural networks with one or more hidden layers, it has never been demonstrated how to make such computations feasible in high dimensions.

Fortunately the situation improves significantly if  $Q_x$  is replaced by  $\hat{Q}_x$ , as this gives

$$F = \mathbb{E}_{\hat{Q}_x}[J_f^\top F_R J_f] = \frac{1}{|S|} \sum_{x \in S_x} J_f^\top F_R J_f, \quad (7)$$

which is easy to evaluate when  $F_R$  is. Moreover, this is essentially equivalent to the expression in eqn. 5 for the generalized Gauss-Newton matrix (GGN), except that we have the Fisher  $F_R$  of the predictive distribution ( $R_{y|z}$ ) instead of Hessian  $H_L$  of the loss ( $L$ ) as the “inner” matrix.

It also suggests a straightforward and efficient way of computing matrix-vector products with  $F$ , using an approach similar to the one in Schraudolph (2002) for computing matrix-vector products with the GGN. In particular, one can multiply by  $J_f$  using a linearized forward pass, then multiply by  $F_R$  (which will be easy if  $R_{y|z}$  is sufficiently simple), and then finally multiply by  $J_f^\top$  using a standard backwards pass.

## 9.2 Qualified equivalence of the GGN and the Fisher

As we shall see in this subsection, the connections between the GGN and the Fisher run deeper than just similar expressions and similar algorithms for computing matrix-vector products.

In Park et al. (2000) it was shown that if the density function of  $R_{y|z}$  has the form  $r(y|z) = \prod_{j=1}^m c(y_j - z_j)$  where  $c(a)$  is some univariate density function over  $\mathbb{R}$ , then  $F$  is equal to a re-scaled<sup>7</sup> version of the classical Gauss-Newton matrix for non-linear least squares, with regression function given by  $f$ . And in particular, the choice  $c(a) = \frac{1}{2}a^2$  turns the learning problem into exactly non-linear least squares, and  $F$  into precisely the classical Gauss-Newton matrix.

Heskes (2000) showed that the Fisher and the classical Gauss-Newton matrix are equivalent in the case of the squared error loss and proposed using the Fisher as an approximation to the Hessian in more general contexts. Concurrently with this work (Martens, 2014), Pascanu and Bengio (2014) showed that for several common loss functions like cross-entropy and squared error, the GGN and the Fisher are equivalent.

We will show that in fact there is a much more general equivalence between the two matrices, starting from observation that the expressions for the GGN in eqn. 5 and the Fisher in eqn. 7 are identical up to the equivalence of  $H_L$  and  $F_R$ .

First, note that  $L(y, z)$  may not even be convex in  $z$ , and so the GGN won’t necessarily be well-defined. But even if  $L(y, z)$  is convex in  $z$ , it won’t be true in general that  $F_R = H_L$ , and so the GGN and the Fisher will differ. However, there is an important class of  $R_{y|z}$ ’s for which  $F_R = H_L$  will hold, provided that we have  $L(y, z) = -\log r(y|z)$  (putting us in the framework of Section 4).

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7. Where the re-scaling constant is determined by properties of  $c(a)$ .

Notice that  $F_R = -\mathbb{E}_{R_{y|f(x,\theta)}}[H_{\log r}]$ , and  $H_L = -H_{\log r}$  (which follows from  $L(y, z) = -\log r(y|z)$ ). Thus, the two matrices being equal is equivalent to the condition

$$\mathbb{E}_{R_{y|f(x,\theta)}}[H_{\log r}] = H_{\log r}. \quad (8)$$

While this condition may seem arbitrary, it is actually very natural and holds in the important case where  $R_{y|z}$  corresponds to an exponential family model with “natural” parameters given by  $z$ . That is, when we have

$$\log r(y|z) = z^\top T(y) - \log Z(z)$$

for some function  $T$ , where  $Z(z)$  is the normalizing constant/partition function. In this case we have  $H_{\log r} = -H_{\log Z}$  which doesn’t depend on  $y$ , and so eqn. 8 holds trivially.

Examples of such  $R_{y|z}$ ’s include:

- multivariate normal distributions where  $z$  parameterizes only the mean  $\mu$
- multivariate normal distributions where  $z$  is the concatenation of  $\Sigma^{-1}\mu$  and the vectorization of  $\Sigma^{-1}$
- multinomial distributions where the softmax of  $z$  is the vector of probabilities for each class

Note that the loss function  $L$  corresponding to the multivariate normal is the familiar squared error, and the one corresponding to the multinomial distribution is the familiar cross-entropy.

As discussed in Section 8, when constructing the GGN one must pay attention to how  $f$  and  $L$  are defined with regards to what parts of the neural network’s computation are performed by each function. For example, the softmax computation performed at the final layer of a classification network is usually considered to be part of the network itself and hence to be part of  $f$ . The output  $f(x, \theta)$  of this computation are normalized probabilities, which are then fed into a cross-entropy loss of the form  $L(y, z) = -\sum_j y_j \log z_j$ . But the other way of doing it, which Schraudolph (2002) recommends, is to have the softmax function be part of  $L$  instead of  $f$ , which results in a GGN which is slightly closer to the Hessian due to “less” of the computational pipeline being linearized before taking the 2nd-order Taylor series approximation. The corresponding loss function is  $L(y, z) = -\sum_j y_j z_j + \log(\sum_j \exp(z_j))$  in this case. As we have established above, doing it this way also has the nice side effect of making the GGN equivalent to the Fisher, provided that  $R_{y|z}$  is an exponential family model with  $z$  as its natural parameters.

This (qualified) equivalence between the Fisher and the GGN suggests how the GGN can be generalized to cases where it might not otherwise be well-defined. In particular, it suggests formulating the loss as the negative log density for some distribution and then taking the Fisher of this distribution. Sometimes, this might be as simple as defining  $r(y|z) \propto \exp(-L(y, z))$  as per the discussion at the end of Section 4.

For example, suppose our loss is defined as the negative log probability of a multi-variate normal distribution  $R_{y|z} = N(\mu, \sigma^2)$  parameterized by  $\mu$  and  $\gamma = \log \sigma^2$  (so that  $z = \begin{bmatrix} \mu \\ \gamma \end{bmatrix}$ ).

In other words, suppose that

$$L(y, z) = -\log r(y|z) \propto \frac{1}{2}\gamma + \frac{1}{2\exp(\gamma)}(x - \mu)^2.$$

In this case the loss Hessian is equal to

$$H_L = \frac{1}{\exp(\gamma)} \begin{bmatrix} 1 & x - \mu \\ x - \mu & \frac{1}{2}(x - \mu)^2 \end{bmatrix}.$$

It is not hard to verify that this matrix is indefinite for certain settings of  $x$  and  $z$  (e.g.  $x = 2$ ,  $\mu = \gamma = 0$ ). Therefore  $L$  is not convex in  $z$  and we cannot define a GGN matrix from it (since the definition of the GGN requires this).

To resolve this problem we can use the Fisher  $F_R$  in place of  $H_L$  in the formula for the GGN, which by eqn. 7 yields  $F$ . Alternatively, we can insert reparameterization operations into our network to transform  $\mu$  and  $\gamma$  into the natural parameters  $\frac{\mu}{\sigma^2} = \frac{\mu}{\exp(\gamma)}$  and  $-\frac{1}{2\sigma^2} = -\frac{1}{2\exp(\gamma)}$ , and then proceed to compute the GGN as usual, noting that  $H_L = F_R$  in this case, so that  $H_L$  will be PSD (and  $L$  therefore convex in  $z$ ). Either way will yield the same curvature matrix, due to the above discussed equivalence of the Fisher and GGN matrix for natural parameterizations.

## 10. Constructing practical natural gradient methods, and the role of damping

Assuming that it is easy to compute, the simplest way to use the natural gradient in optimization is to substitute it in place of the standard gradient within a basic gradient descent approach. This gives the iteration

$$\theta_{k+1} = \theta_k - \alpha_k \tilde{\nabla} h(\theta_k), \quad (9)$$

where  $\{\alpha_i\}_i$  is a schedule of step-sizes/step-sizes.

Choosing the step-size schedule can be difficult. There are adaptive schemes which are largely heuristic in nature (Amari, 1998) and some non-adaptive prescriptions such as  $\alpha_k = c/k$ , which have certain theoretical convergence guarantees in the stochastic setting, but which won't necessarily work well in practice.

Ideally, we would want to apply the natural gradient method with infinitesimally small steps and produce a smooth idealized path through the space of realizable distributions. But since this is usually impossible in practice, and we don't have access to any other simple description of the class of distributions parameterized by  $\theta$  that we could work with more directly, we must take non-negligible discrete steps in the given parameter space<sup>8</sup>.

The fundamental problem with simple schemes such as the one in eqn. 9 is that they implicitly assume that the natural gradient is a good direction to follow over non-negligible

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8. In principle, we could move to a much more general class of distributions, such as those given by some non-parametric formulation, where we could work directly with the distributions themselves. But even assuming such an approach would be practical from a computational efficiency standpoint, we would lose the various advantages that we get from working with powerful parametric models like neural networks. In particular, we would lose their ability to generalize to unseen data by modeling the ‘‘computational process’’ which explains the data, instead of merely using smoothness and locality to generalize.

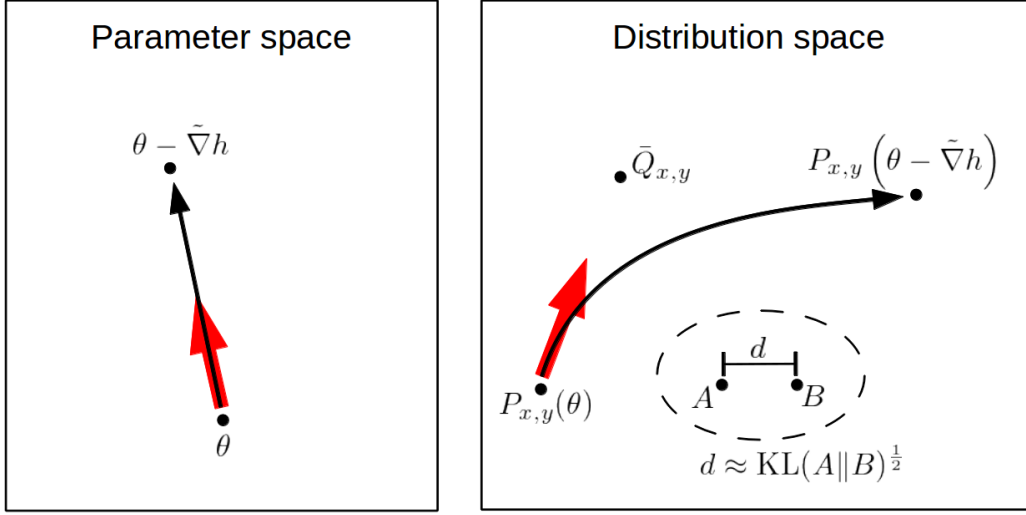


Figure 1: A typical situation encountered when performing large discrete updates in the original parameter space. The red arrow is the natural gradient direction (given by the vector  $\tilde{\nabla}h$  in parameter space) and the black arrow is the path generated by taking  $\theta - \alpha \tilde{\nabla}h$  for  $\alpha \in [0, 1]$ .

distances in the original parameter space, which will not be true in general. Traveling along a straight line in the original parameter space will not yield a straight line in distribution space, and so the resulting path may instead veer far away from the target that the natural gradient originally pointed towards. This is illustrated in Figure 1.

Fortunately, we can exploit the (qualified) equivalence between the Fisher and the GGN in order to produce natural gradient-like updates which will often be appropriate to take with  $\alpha_k = 1$ . In particular, we know from the discussion in Section 8 that the GGN matrix  $G$  can serve as a reasonable proxy for the Hessian  $H$  of  $h$ , and will often produce smaller and more “conservative” updates as it tends to model the curvature as being higher in most directions than the Hessian does. Meanwhile, the update  $\delta$  produced by minimizing the GGN-based local quadratic model  $M(\delta) = \frac{1}{2}\delta^\top G\delta + \nabla h^\top \delta + h(\theta)$  is given by  $-G^{-1}\nabla h$ , which will be equal to the natural gradient when  $F = G$ . Thus, the natural gradient, with scaling factor  $\alpha = 1$ , can be seen as the optimal update according to an approximate, and perhaps slightly conservative, 2nd-order model of  $h$ .

But just as in the case of approximate 2nd-order methods, the break-down in the accuracy of the quadratic approximation of  $h$  over long distances, combined with the potential for the natural gradient to be very large (e.g. when  $F$  contains some very small eigenvalues), can often lead to very large and very poor update proposals. And simply re-scaling the update by reducing  $\alpha$  may be too crude a mechanism to deal with this subtle problem, as it will affect all eigen-directions (of  $F$ ) equally, including those in which the natural gradient is already sensible or even overly conservative.

Instead, the connection between natural gradient descent and 2nd-order methods suggests the use of some of the various update “damping” techniques that have been developed for the latter, which work by constraining or penalizing the solution for  $\delta$  in various ways

during the optimization of  $M(\delta)$ . Examples include Tikhonov regularization/damping and the closely related trust-region method (e.g. Nocedal and Wright, 2006), and other more sophisticated ones such as the “structural damping” approach of Martens and Sutskever (2011), or the approach present in Krylov Subspace Descent (Vinyals and Povey, 2012). See Martens and Sutskever (2012) for an in-depth discussion of these and other damping techniques.

This idea is well supported by practical experience since, for example, the Hessian-free optimization approach of Martens (2010) generates its updates using an Tikhonov damping scheme applied to the GGN matrix (which for the objectives they optimized in the paper were equivalent to the Fisher), and these updates are used effectively with  $\alpha_k = 1$  and make a lot more progress on the objective than optimally re-scaled updates computed without damping (i.e. the raw natural gradient).

## 11. The empirical Fisher

An approximation of the Fisher known as the “empirical Fisher” (denoted  $\bar{F}$ ), which is often used in practical natural gradient methods, is obtained by taking the inner expectation of eqn. 3 over the target distribution  $Q_{x,y}$  (or its empirical surrogate  $\hat{Q}_{x,y}$ ) instead of the model’s distribution  $P_{x,y}$ .

In the case that one uses  $\hat{Q}_{x,y}$ , this yields the following simple form:

$$\begin{aligned}\bar{F} &= \mathbb{E}_{\hat{Q}_{x,y}} \left[ \nabla \log p(x, y|\theta) \nabla \log p(x, y|\theta)^\top \right] \\ &= \mathbb{E}_{\hat{Q}_x} \left[ \mathbb{E}_{\hat{Q}_{y|x}} \left[ \nabla \log p(y|x, \theta) \nabla \log p(y|x, \theta)^\top \right] \right] \\ &= \frac{1}{|S|} \sum_{(x,y) \in S} \nabla \log p(y|x, \theta) \nabla \log p(y|x, \theta)^\top.\end{aligned}$$

This matrix is often incorrectly referred to as the Fisher, or even the Gauss-Newton, although it is in general not equivalent to either of those matrices.

### 11.1 Comparisons to the standard Fisher

Like the Fisher  $F$ , the empirical Fisher  $\bar{F}$  is PSD. But unlike  $F$ , it is essentially free to compute, provided that one is already computing the gradient of  $h$ . It can also be applied to objective functions which might not involve a probabilistic model in any obvious way.

Compared to  $F$ , which is of rank  $\leq |S| \text{rank}(F_R)$ ,  $\bar{F}$  has a rank of  $\leq |S|$ , which can make it easier to work with in practice. For example, the problem of computing the diagonal (or various blocks) is easier for the empirical Fisher than it is for higher rank matrices like the standard Fisher (Martens et al., 2012). This has motivated its use in optimization methods such as TONGA (Le Roux et al., 2008), and as the diagonal preconditioner of choice in the Hessian-free optimization method (Martens, 2010). Interestingly however, there are stochastic estimation methods (Chapelle and Erhan, 2011; Martens et al., 2012) which can be used to efficiently estimate the diagonal (or various blocks) of the standard Fisher  $F$ , and these work quite well in practice.

Despite the various practical advantages of using  $\bar{F}$ , there are good reasons to use true Fisher  $F$  instead of  $\bar{F}$  whenever possible. In addition to Amari’s extensive theory developed

for the exact natural gradient (which uses  $F$ ), perhaps the best reason for using  $F$  over  $\bar{F}$  is that  $F$  turns out to be a reasonable approximation to the Hessian  $H$  of  $h$  in certain important special cases, which is a property that  $\bar{F}$  lacks in general.

For example, as discussed in Section 5, when the loss is given by  $-\log p(y|x)$  (as in Section 4),  $F$  can be seen as an approximation of  $H$ , because both matrices have the interpretation of being the expected Hessian of the loss under some distribution. Due to the similarity of the expression for  $F$  in eqn. 3 and the one above for  $\bar{F}$  it might be tempting to think that  $\bar{F}$  is given by the expected Hessian of the loss under  $\hat{Q}_{x,y}$  (which is actually the formula for  $H$ ) in the same way that  $F$  is given by eqn. 4, however this is not the case in general.

And as we saw in Section 9, given certain assumptions about how the GGN is computed, and some additional assumptions about the form of the loss function  $L$ ,  $F$  turns out to be equivalent to the GGN. This is very useful since the GGN can be used to define a local quadratic approximation of  $h$ , whereas  $F$  normally doesn't have such an interpretation. Moreover, Schraudolph (2002) and later Martens (2010) compared  $\bar{F}$  to the GGN and observed that the latter performed much better as a curvature matrix within various neural network optimization methods.

As concrete evidence for why the empirical Fisher is, at best, a questionable choice for the curvature matrix, consider the following example. We will set  $n = 1$ ,  $f(x, \theta) = \theta$ ,  $R_{y|z} = \mathcal{N}(z, 1)$ , and  $S = \{(0, 0)\}$ , so that  $h(\theta)$  is a simple convex quadratic function of  $\theta$  given by  $h(\theta) = \frac{1}{2}\theta^2$ . In this example we have that  $\nabla h = \theta$ ,  $\bar{F} = \theta^2$ , while  $F = 1$ . If we use  $\bar{F}^\xi$  as our curvature matrix for some exponent  $\frac{1}{2} \leq \xi \leq 1$ , then it is easy to see that an iteration of the form

$$\theta_{k+1} = \theta_k - \alpha_k (\bar{F}(\theta_k)^\xi)^{-1} \nabla h(\theta_k) = \theta_k - \alpha_k (\theta_k^2)^{-\xi} \theta_k = (1 - \alpha_k |\theta_k|^{-2\xi}) \theta_k$$

will fail to converge to the minimizer ( $\theta = 0$ ) unless  $\xi < 1$  and the step-size  $\alpha_k$  goes to 0 sufficiently fast. And even when it does converge, it will only be at a rate comparable to the speed at which  $\alpha_k$  goes to 0, which in typical situations will be either  $\mathcal{O}(1/k)$  or  $\mathcal{O}(1/\sqrt{k})$ . Meanwhile, a similar iteration of the form

$$\theta_{k+1} = \theta_k - \alpha_k F^{-1} \nabla h(\theta_k) = \theta_k - \alpha_k \theta_k = (1 - \alpha_k) \theta_k,$$

which uses the exact Fisher  $F$  as the curvature matrix, will experience very fast linear convergence<sup>9</sup> with rate  $|1 - \alpha|$ , for any fixed step-size  $\alpha_k = \alpha$  satisfying  $0 < \alpha < 2$ .

It is important to note that this example uses a noise-free version of the gradient, and that this kind of linear convergence is (provably) impossible in most realistic stochastic/online settings. Nevertheless, we would argue that a highly desirable property of any stochastic optimization method should be that it can, in principle, revert to an optimal (or nearly optimal) behavior in the deterministic setting. This might matter a lot in practice, since the gradient may end up being sufficiently well estimated in earlier stages of optimization from only a small amount of data (which is a common occurrence in our experience), or in later stages provided that larger mini-batches or other variance-reducing procedures are employed (e.g. Le Roux et al., 2012; Johnson and Zhang, 2013). More concretely, the

9. Here we mean ‘‘linear’’ in the classical sense that  $|\theta_k - 0| \leq |\theta_0 - 0| |1 - \alpha|^k$  and *not* in the sense that  $|\theta_k - 0| \in \mathcal{O}(1/k)$

pre-asymptotic convergence rate of stochastic 2nd-order optimizers can still strongly depend on the choice of the curvature matrix, as we will show in Section 12.

## 11.2 Recent diagonal methods based on the empirical Fisher

Recently, a spate of stochastic optimization methods have been proposed that are all based on diagonal approximations of the empirical Fisher  $\bar{F}$ . These include the diagonal version of AdaGrad (Duchi et al., 2011), RMSProp (Tieleman and Hinton, 2012), Adam (Ba and Kingma, 2015), etc. Such methods use iterations of the following form (possibly with some slight modifications):

$$\theta_{k+1} = \theta_k - \alpha_k (B_k + \lambda I)^{-\xi} g_k(\theta_k), \quad (10)$$

where the curvature matrix  $B_k$  is taken to be a diagonal matrix  $\text{diag}(p_k)$  with  $p_k$  adapted to maintain some kind of estimate of the diagonal of  $\bar{F}$  (possibly using information from previous iterates/mini-batches),  $g_k(\theta_k)$  is an estimate of  $\nabla h(\theta_k)$  produced from the current mini-batch,  $\alpha_k$  is a schedule of step-sizes, and  $0 < \lambda$  and  $0 < \xi \leq 1$  are hyperparameters (discussed later in this section).

There are also slightly more sophisticated methods (Schaul et al., 2013; Zeiler, 2013) which use preconditioners that combine the diagonal of  $\hat{F}$  with other quantities (such as an approximation of the diagonal of the Gauss-Newton/Fisher in the case of Schaul et al. (2013)) in order to correct for how the empirical Fisher doesn’t have the right “scale” (which is ultimately the reason why it does poorly in the example given at the end of Section 11.1).

A diagonal preconditioner of the form used in eqn. 10 was also used to accelerate the CG sub-optimizations performed within HF (Martens, 2010). In the context of CG, the improper scale of  $\bar{F}$  is not as serious an issue due to the fact that CG is invariant to the overall scale of its preconditioner (since it computes an optimal “step-size” at each step which automatically adjusts for the scale). However, it still makes more sense to use the diagonal of  $F$  as a preconditioner, and thanks to the method proposed by Chapelle and Erhan (2011), this can be estimated efficiently and accurately.

While the idea of using the diagonal of  $F$ ,  $\bar{F}$ , or the Gauss-Newton as a preconditioner for stochastic gradient descent (SGD) is sometimes incorrectly attributed to Duchi et al. (2011), it actually goes back *much* earlier, and was likely first applied to neural networks with the work of Lecun and collaborators (Becker and LeCun, 1989; LeCun et al., 1998), who proposed an iteration of the form in eqn. 10 with  $\xi = 1$  where  $p_k$  approximates the diagonal of the Hessian or the Gauss-Newton matrix (which as shown in Section 9, is actually equivalent to  $F$  for the common squared-error loss).

Following this early work of Lecun, Amari, and their collaborators, various neural network optimization methods have been developed over the last couple of decades that use diagonal, block-diagonal, low-rank, or Krylov-subspace based approximations of  $F$  or  $\bar{F}$  as a curvature matrix/preconditioner. In addition to methods based on diagonal approximations already mentioned, some methods based on non-diagonal approximations include the method of Park et al. (2000), TONGA (Le Roux et al., 2008), Natural Newton (Le Roux and Fitzgibbon, 2010), HF (Martens, 2010), KSD (Vinyals and Povey, 2012) and many more.

The idea of computing an estimate of the (empirical) Fisher using a history of previous iterates/mini-batches also appeared in various early works. The particular way of doing

this advocated by Duchi et al. (2011), which is to use an equally weighted average of all past gradients, was motivated from a regret-based asymptotic convergence analysis and tends not to work well in practice (Tieleman and Hinton, 2012). The traditional and more intuitive approach of using an exponentially decayed running average (e.g. LeCun et al., 1998; Park et al., 2000) works better, at least pre-asymptotically, as it is able to naturally “forget” very old contributions to the estimate (which are based on stale parameter values).

It is important to observe that the way  $\bar{F}$  is estimated can affect the convergence characteristics of an iteration like eqn. 10 in subtle and important ways. For example, if  $\bar{F}$  is estimated using gradients from previous iterations, and especially if it is the average of *all* past gradients as in AdaGrad, it may shrink sufficiently slowly that the convergence issues seen in the example at the end of Section 11.1 are avoided. Moreover, for reasons related to this phenomenon, it seems likely that the proofs of regret bounds in Duchi et al. (2011) and the related work of Hazan et al. (2007) could *not* be modified work if the exact  $\bar{F}$ , computed only at the current  $\theta$ , were used. Developing a better understanding of this issue, and the relationship between methods and theories such as AdaGrad developed in the convex optimization literature, and classical stochastic 2nd-order methods and theories (e.g. Murata, 1998; Bottou and LeCun, 2005) remains an interesting direction for future research.

The constants  $\lambda$  and  $\xi$  present in eqn. 10 are often thought of as “fudge factors” designed to correct for the “poor conditioning” (Becker and LeCun, 1989) of the curvature matrix, or to guarantee boundedness of the updates and prevent the optimizer from “blowing up” (LeCun et al., 1998). However, these explanations are severe oversimplifications at best. A much more compelling and *useful* explanation, at least in the case of  $\lambda$ , comes from viewing the update in eqn. 10 as being the minimizer of a local quadratic approximation  $M(\delta) = \frac{1}{2}\delta^\top B_k \delta + \nabla h(\theta)^\top \delta + h(\theta)$  to  $h(\theta_k + \delta)$ , as discussed in Section 10. In this view,  $\lambda$  plays the role of a Tikhonov damping parameter (e.g. Martens and Sutskever, 2012) which is added to  $B_k$  in order to ensure that the proposed update stays within a certain radius around zero in which  $M(\delta)$  remains a reasonable approximation to  $h(\theta + \delta)$ . Note that this explanation implies that no single fixed value of  $\lambda$  will be appropriate throughout the entire course of optimization (since the local properties of the objective will change), and so an adaptive adjustment scheme, such as the one present in HF (Martens, 2010) (based on the Levenberg-Marquardt method) should be used.

The use of the exponent  $\xi = 3/4$  first appeared in HF as part of its diagonal preconditioner for CG, and was justified as a way of making the curvature estimate “more conservative” by making it closer to a multiple of the identity, to compensate for the diagonal approximation being made (among other things). Around the same time, Duchi et al. (2011) proposed to use  $\xi = 1/2$  within an update of the form of eqn. 10, which was important in proving a certain regret bound both for the diagonal and non-diagonal versions of the method.

To shed some light on the question of  $\xi$ , we can consider the work of Hazan et al. (2007), who like Duchi et al. (2011), developed and analyzed an online approximate Newton method within the framework of online convex optimization. Like the non-diagonal version of AdaGrad, the method proposed by Hazan et al. (2007) uses an estimate of the empirical Fisher  $\bar{F}$  computed as the average of gradients from all previous iterations. While impractical for high dimensional problems like any non-diagonal method is (or at least, one that doesn’t



make some other strong approximation of the curvature matrix), this method achieves a superior upper bound on the regret than Duchi et al. (2011) was able to show for AdaGrad ( $\mathcal{O}(\log(k))$  instead of  $\mathcal{O}(\sqrt{k})$ , where  $k$  is the total number of iterations), which was possible in part due to the use of stronger hypotheses about the properties of  $h$  (e.g. that for each  $x$  and  $y$ ,  $L(y, f(x, \theta))$  is a strongly convex function of  $\theta$ ). Notably, this method uses  $\xi = 1$ , just as in standard natural gradient descent, which provides support for such a choice, especially since the  $h$  used in neural networks will typically satisfy these stronger assumptions in a local neighborhood of the optimum, at least when standard  $\ell_2$  regularization is used.

However, it is important to note that Hazan et al. (2007) also proves a  $\mathcal{O}(\log(k))$  bound on the regret for a basic version of SGD, and that what actually differentiates the various methods they analyze is the constant hidden in the big-O notation, which is much larger for the version of SGD they consider than for their approximate Newton method. In particular, the former depends on a quantity which grows with the condition number of the Hessian  $H$  at  $\theta^*$ , while the latter does not, in a way that echos the various analyses performed on stochastic gradient descent and stochastic approximations of Newton’s method in the more classical “local-convergence” setting (e.g. Murata, 1998; Bottou and LeCun, 2005).

## 12. Asymptotic convergence speed

### 12.1 Amari’s Fisher efficiency result

A property of natural gradient descent which is frequently referenced in the literature is that it is “Fisher efficient”. In particular, Amari (1998) showed that an iteration of the form

$$\theta_{k+1} = \theta_k - \alpha_k \tilde{g}_k(\theta_k) \quad (11)$$

when applied to an objective of the form discussed in Section 4, with  $\alpha_k$  shrinking as  $1/k$ , and with  $\tilde{g}_k(\theta_k) = F^{-1}g_k(\theta_k)$  where  $g_k(\theta_k)$  is a stochastic estimate of  $\nabla h(\theta_k)$  (from a single training case), will produce an estimator  $\theta_k$  which is asymptotically “Fisher efficient”. This means that  $\theta_k$  will tend to an unbiased estimator of the global optimum  $\theta^*$ , and that its expected squared error matrix (which tends to its variance) will satisfy

$$\mathbb{E}[(\theta_k - \theta^*)(\theta_k - \theta^*)^\top] = \frac{1}{k} F(\theta^*)^{-1} + \mathcal{O}\left(\frac{1}{k^2}\right), \quad (12)$$

which is (asymptotically) the smallest<sup>10</sup> possible variance matrix that any unbiased estimator computed from  $k$  training cases can have, according to the Cramér-Rao lower bound.

This result can also be straightforwardly extended to handle the case where  $g_k(\theta_k)$  is computed using a mini-batch of size  $m$  (which uses  $m$  independently sampled cases at each iteration), in which case the above asymptotic variance bound becomes

$$\frac{1}{mk} F(\theta^*)^{-1} + \mathcal{O}\left(\frac{1}{k^2}\right),$$

which again matches the Cramér-Rao lower bound.

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10. With the usual definition of  $\preceq$  for matrices:  $A \preceq C$  iff  $C - A$  is PSD.

Note that this result applies to the version of natural gradient descent where  $F$  is computed using the training distribution  $\hat{Q}_x$  (see Section 5). If we instead consider the version where  $F$  is computed using the true data distribution  $Q_x$ , then a similar result will still apply, provided that we sample  $x$  from  $Q_x$  and  $y$  from  $Q_{y|x}$  when computing the stochastic gradient  $g_k(\theta_k)$ , and that  $\theta^*$  is defined as the minimum of the idealized objective  $\text{KL}(Q_{x,y} \| P_{x,y}(\theta))$  (see Section 4).

While this Fisher efficiency result would seem to suggest that natural gradient descent is the best possible optimization method in the stochastic setting, it unfortunately comes with several important caveats, which we discuss below.

Firstly, the proof assumes that the iteration in eqn. 11 eventually converges to the global optimum  $\theta^*$  (at an unspecified speed). While this assumption can be justified when the objective  $h$  is convex (provided that  $\alpha_k$  is chosen appropriately), it won't be true in general for non-convex objectives, such as those encountered in neural network training. In practice, a reasonable local optimum  $\theta^*$  might be a good surrogate for the global optimum, in which case a property analogous to asymptotic Fisher efficiency may still hold, at least approximately.

Secondly, it is assumed in Amari's proof that  $F$  is computed using the full training distribution  $\hat{Q}_x$ , which in the case of neural network optimization usually amounts to an entire pass over the training set  $S$ . So while the proof allows for the gradient  $\nabla h$  to be stochastically estimated from a mini-batch, it doesn't allow this for the Fisher  $F$ . This is a serious challenge to the idea that (stochastic) natural gradient descent gives an estimator which makes optimal use of the training data that it sees. And note that while one can approximate  $F$  using minibatches from  $S$ , which is a solution that often works well in practice, especially when combined with a decayed-averaging scheme, a Fisher efficiency result like the one proved by Amari (1998) will likely no longer hold. Investigating the manner and degree in which it may hold *approximately* when  $F$  is estimated in this way is an interesting direction for future research.

A third issue with Amari's result is that it is given in terms of the convergence of  $\theta_k$  according to its own (arbitrary) euclidean geometry instead of the arguably more relevant objective function value. Fortunately, it is straightforward to obtain the former from the latter. In particular, by applying Taylor's theorem and using  $\nabla h(\theta^*) = 0$  we have

$$\begin{aligned} h(\theta_k) - h(\theta^*) &= \frac{1}{2}(\theta_k - \theta^*)^\top H^*(\theta_k - \theta^*) + \nabla h(\theta^*)^\top (\theta_k - \theta^*) + \mathcal{O}((\theta_k - \theta^*)^3) \\ &= \frac{1}{2}(\theta_k - \theta^*)^\top H^*(\theta_k - \theta^*) + \mathcal{O}((\theta_k - \theta^*)^3) , \end{aligned} \tag{13}$$

where  $H^* = H(\theta^*)$  and  $\mathcal{O}((\theta_k - \theta^*)^3)$  is short-hand to mean a function which is cubic in the entries of  $\theta_k - \theta^*$ . From this it follows<sup>11</sup> that

$$\begin{aligned} \mathbb{E}[h(\theta_k)] - h(\theta^*) &= \frac{1}{2} \mathbb{E}[(\theta_k - \theta^*)^\top H^* (\theta_k - \theta^*)] + \mathbb{E}[\mathcal{O}((\theta_k - \theta^*)^3)] \\ &= \frac{1}{2} \text{tr} \left( H^* \mathbb{E}[(\theta_k - \theta^*)(\theta_k - \theta^*)^\top] \right) + \mathbb{E}[\mathcal{O}((\theta_k - \theta^*)^3)] \\ &= \frac{1}{2k} \text{tr}(H^* F(\theta^*)^{-1}) + \mathbb{E}[\mathcal{O}((\theta_k - \theta^*)^3)] = \frac{n}{2k} + o\left(\frac{1}{k}\right), \end{aligned} \quad (14)$$

where we have used  $H^* = F(\theta^*)$  which follows from the “realizability” hypothesis used to prove the Fisher efficiency result (see below).

Note that while this is the same convergence rate ( $\mathcal{O}(1/k)$ ) as the one which appears in Hazan et al. (2007) (see our Section 11), the constant is much better. However, the comparison is slightly unfair, since Hazan et al. (2007) doesn’t require that the curvature matrix be estimated on the entire dataset (as discussed above).

The fourth and final caveat of Amari’s Fisher efficiency result is that Amari’s proof assumes that the training distribution  $\hat{Q}_{x,y}$  and the optimal model distribution  $P_{x,y}(\theta^*)$  coincide, a condition called “realizability” (which is also required in order for the Cramér-Rao lower bound to apply). This means, essentially, that the model perfectly captures the training distribution at  $\theta = \theta^*$ . This assumption is used in Amari’s proof of the Fisher efficiency result to show that the Fisher  $F$ , when evaluated at  $\theta = \theta^*$ , is equal to both the empirical Fisher  $\bar{F}$  and the Hessian  $H$  of  $h$ .

It is not clear from Amari’s proof what happens when this correspondence fails to hold at  $\theta = \theta^*$ , and whether a (perhaps) weaker asymptotic upper bound on the variance might still be provable. Fortunately, various authors (Murata, 1998; Bottou and LeCun, 2005; Bordes et al., 2009) building on early work of Amari (1967), provide some further insight into this question by studying asymptotic behavior of general iterations of the form<sup>12</sup>

$$\theta_{k+1} = \theta_k - \alpha_k B_k^{-1} g_k(\theta_k), \quad (15)$$

where  $B_k = B$  is a fixed<sup>13</sup> curvature matrix (which is independent of  $\theta_k$  and  $k$ ), and where  $g_k(\theta_k)$  is a stochastic estimate of  $\nabla h(\theta_k)$  (which must be unbiased, have finite variance, and have the property that  $\{g_i(\theta)\}_i$  are i.i.d. variables).

In particular, Murata (1998) gives exact (although implicit) expressions for the asymptotic mean and variance of  $\theta_k$  in the above iteration for the case where  $\alpha_k = 1/(k+1)$

11. The last line of this derivation uses  $\mathbb{E}[\mathcal{O}((\theta_k - \theta^*)^3)] = o(1/k)$ , which is an (unjustified) assumption that is used in Amari’s proof. This assumption has intuitive appeal since  $\mathbb{E}[\mathcal{O}((\theta_k - \theta^*)^2)] = \mathcal{O}(1/k)$ , and so it makes sense that  $\mathbb{E}[\mathcal{O}((\theta_k - \theta^*)^3)]$  would shrink faster. However, extreme counterexamples are possible which involve very heavy-tailed distributions on  $\theta_k$  over unbounded regions. By adding some mild hypotheses such as  $\theta_k$  being restricted to some bounded region, which is an assumption frequently used in the convex optimization literature, it is possible to justify this assumption rigorously. Rather than linger on this issue we will refer the reader to Bottou and LeCun (2005), which provides a more rigorous treatment of these kind of asymptotic results, using various generalizations of the big-O notation.

12. Note that some authors define  $B_k$  to be the matrix that multiplies the gradient, instead of its inverse (as we do instead).

13. Note that for a non-constant  $B_k$  where  $B_k^{-1}$  converges sufficiently quickly to a fixed  $B^{-1}$  as  $\theta_k$  converges to  $\theta^*$ , these analyses will likely still apply, at least approximately.

or  $\alpha_k$  is constant, thus generalizing Amari's Fisher efficiency result. These expressions describe the (asymptotic) behavior of this iteration in cases where the curvature matrix  $B$  is not the Hessian  $H$  or the Fisher  $F$ , covering the non-realizable case, as well as the case where the curvature matrix is only an approximation of the Hessian or Fisher. Bordes et al. (2009) meanwhile gives expressions for  $E[h(\theta_k)]$  in the case where  $\alpha_k$  shrinks as  $1/k$ , thus generalizing eqn. 14 in a similar manner.

In the following subsection we will examine these results in more depth, and significantly improve on those of Bordes et al. (2009) (at least in the quadratic case) by giving an *exact* asymptotic solution for  $E[h(\theta)]$ . To do this we will apply a generalization of eqn. 14 to Murata's expressions for the asymptotic mean and covariance of  $\theta_k$ , thus expressing  $E[h(\theta)]$  in terms of the trace of the solution of a certain matrix equation, and then apply some methods from the control theory literature for computing the trace of such solutions.

Some interesting consequences of this analysis are discussed in Sections 12.2.1 and 12.3.1. Among these are the observation that when an annealed step-size  $\alpha_k = 1/(k+1)$  is used, the application of stochastic 2nd-order optimization with  $B = H$ , while not improving the asymptotic dependency on  $k$  of the convergence rate vs SGD, will in realistic scenarios significantly improve the multiplicative constant on the asymptotically dominant  $\mathcal{O}(1/k)$  term in the expression for  $E[h(\theta)] - h(\theta_0)$ . We also show that when a iterate averaging scheme is used with a fixed step-size, the constant on the  $\mathcal{O}(1/k)$  term is *not* improved by the application of 2nd-order optimization, while the constant on the  $\mathcal{O}(1/k^2)$  term improves significantly. We argue that this second term, which is independent of the stochastic gradient noise and instead depends on the initial value of the objective ( $h(\theta_0)$ ), may matter more in practice given a limited iteration budget.

## 12.2 Some new results concerning asymptotic convergence speed of general stochastic 2nd-order methods

In this subsection we build on the results of Murata (1998) in order to prove Theorem 4, which is a result that gives detailed expressions for the convergence speed of stochastic 1st and 2nd-order methods based on iterations of the form in eqn. 15. Along the way, we will develop techniques for computing the asymptotic mean and covariance of  $\theta_k$ .

For an  $n$ -dimensional symmetric matrix  $A$  we will denote by  $\lambda_i(A)$  its  $i$ -th largest eigenvalue, so that  $\lambda_1(A) \geq \lambda_2(A) \geq \dots \geq \lambda_n(A)$ . Further, we will denote

$$\begin{aligned} V_k &= \text{var}(\theta_k) = \text{cov}(\theta_k, \theta_k) = E \left[ (\theta_k - E[\theta_k])(\theta_k - E[\theta_k])^\top \right] \\ \Xi_A(X) &= AX + (AX)^\top \\ \Sigma_g(\theta) &= \text{var}(g(\theta)) = \text{cov}(g(\theta), g(\theta)) = E \left[ (g(\theta) - E[g(\theta)])(g(\theta) - E[g(\theta)])^\top \right], \end{aligned}$$

where  $\Xi_A$  is a linear operator on  $n \times n$  matrices<sup>14</sup>, and  $g(\theta)$  denotes a random variable with the same distribution as each of the  $g_i(\theta)$ 's.

14. Note that it is *not* an  $n \times n$  matrix itself, although it can be represented as an  $n^2 \times n^2$  matrix using Kronecker product notation. Also note this operator can be linearly combined and composed, where we will use the standard  $\pm$  notation for linear combination, and multiplication for composition, where  $I$  will be the identity operator. So, for example,  $(I + \Xi_A^2)(X) = X + \Xi_A(\Xi_A(X))$ .

The following theorem summarizes the relevant results of Murata (1998) on the asymptotic behavior of stochastic iterations of the form in eqn. 15. Note that we use the symbols defined below in a somewhat inconsistent way from how they are used by Murata (1998) (e.g. “ $V_\infty$ ” has a different scaling).

**Theorem 1** (*Adapted from Theorems 1 and 4 of Murata (1998)*) Suppose that  $\theta_k$  is generated by the stochastic iteration in eqn. 15 while optimizing a quadratic objective

$$h(\theta) = \frac{1}{2}(\theta - \theta^*)^\top H^*(\theta - \theta^*).$$

If  $\alpha_k = \alpha$  is constant then we have that

$$\begin{aligned} \mathbb{E}[\theta_k] &= \theta^* + (I - \alpha B^{-1} H^*)^k (\theta_0 - \theta^*) \\ V_k &= \left( I - (I - \Xi_{\alpha B^{-1} H^*})^k \right) (V_\infty) + (I - \Xi_{\alpha B^{-1} H^*})^k ((\theta_0 - \theta^*)(\theta_0 - \theta^*)^\top), \end{aligned}$$

where  $V_\infty = \alpha (\Xi_{B^{-1} H^*})^{-1} (B^{-1} \Sigma_g(\theta^*) B^{-1})$ .

If on the other hand  $\alpha_k = 1/(k+1)$  and  $\lambda_n(B^{-1} H^*) > \frac{1}{2}$  then we have that

$$\begin{aligned} \mathbb{E}[\theta_k] &= \theta^* + \prod_{j=0}^{k-1} (I - \alpha_j B^{-1} H^*) (\theta_0 - \theta^*) \\ V_k &= \frac{1}{k} (\Xi_{B^{-1} H^*} - I)^{-1} (B^{-1} \Sigma_g(\theta^*) B^{-1}) - \frac{1}{k^2} (\Xi_{B^{-1} H^*} - 2I)^{-1} (B^{-1} \Sigma_g(\theta^*) B^{-1}) + \mathcal{O}\left(\frac{1}{k^3}\right). \end{aligned}$$

**Remark 2** Theorem 1 deviates from the original presentation of Murata (1998) by assuming that  $h(\theta)$  is exactly quadratic. This is done because Murata (1998) proved their more general results in a somewhat non-rigorous way by first assuming this hypothesis, and then appealing to the fact that more general objectives are well-approximated by such a convex quadratic in a close proximity to the local minimum  $\theta^*$ , as long as they are sufficiently smooth. While their proof made a cursory attempt to rigorously deal with the resulting approximation error, at least in the case where  $\alpha_k = 1/(k+1)$ , this produced an analysis that was at best flawed but repairable, and at worst wrong. These issues could likely be repaired in the case where  $\alpha_k = 1/(k+1)$  with a more careful approach that uses the fact that the error vanishes asymptotically as  $\theta_k$  converges (both with high probability). However, in the case where  $\alpha_k = \alpha$  is constant, the theorem does not strictly hold without assuming that  $h(\theta)$  is a convex quadratic, even if we only require that the expressions for the mean and variance are asymptotically accurate. Moreover, without assuming that  $h(\theta)$  is quadratic, it is unlikely that any closed-form expression could be obtained for the asymptotic covariance  $V_\infty$  in this case. See Appendix A for some additional discussion of this issue.

**Remark 3** We have taken a few additional liberties in interpreting the results in Murata (1998). For example, we give a slightly different result (which can be obtained by a minor modification of the original arguments) where we assume that the covariance of the stochastic gradients,  $\Sigma_g(\theta)$ , is constant, as opposed to assuming that  $\mathbb{E}[g(\theta)g(\theta)^\top] =$

$\Sigma_g(\theta) + \mathbb{E}[g(\theta)] \mathbb{E}[g(\theta)]^\top$  is constant as Murata (1998) does<sup>15</sup>. Note that this change doesn't affect the terms that are dominant (in  $k$ ) in any of the resulting asymptotic expressions or those which we derive from them, although it does affect the non-dominant terms, and in a way that makes the resulting expressions arguably more accurate. We have also given a more detailed expression for  $V_k$  in the  $\alpha_k = 1/(k+1)$  case which is accurate up to order  $1/k^2$  (instead of just  $1/k$ ). See Appendix A for further details.

One interesting observation we can immediately make from Theorem 1 is that, at least in the case where the objective is a convex quadratic,  $\mathbb{E}[\theta_k]$  progresses in a way that is fully independent of the amount/shape of noise which exists in the estimate of the gradient (which is captured by the  $\Sigma_g(\theta^*)$  matrix). Indeed, it proceeds as  $\theta_k$  itself would in the case of fully deterministic optimization. It is only the variance of  $\theta_k$  around  $\mathbb{E}[\theta_k]$  that depends on the gradient noise.

To see why this happens, note that if  $h(\theta)$  is quadratic then  $\nabla h(\theta)$  will be an affine function and thus commutes with expectation. This allows us to write

$$\mathbb{E}[g(\theta_k)] = \mathbb{E}[\nabla h(\theta_k)] = \nabla h(\mathbb{E}[\theta_k]).$$

Thus, provided that  $\alpha_k$  doesn't depend on  $\theta_k$  in any way (as we are implicitly assuming), we have

$$\mathbb{E}[\theta_{k+1}] = \mathbb{E}[\theta_k - \alpha_k B^{-1} g(\theta_k)] = \mathbb{E}[\theta_k] - \alpha_k B^{-1} \nabla h(\mathbb{E}[\theta_k]),$$

which is precisely the deterministic version of eqn. 15, where we treat  $\mathbb{E}[\theta_k]$  as the optimized quantity.

While Theorem 1 provides a detailed picture of how well  $\theta^*$  is estimated by  $\theta_k$ , it doesn't tell us anything directly about how quickly progress is being made on the objective, which is arguably a much more relevant concern in practice. Fortunately, as observed by Murata (1998), we have the basic identity

$$\begin{aligned} \mathbb{E}[(\theta_k - \theta^*)(\theta_k - \theta^*)^\top] &= \mathbb{E}[(\theta_k - \mathbb{E}[\theta_k])(\theta_k - \mathbb{E}[\theta_k])^\top] + \mathbb{E}[(\mathbb{E}[\theta_k] - \theta^*)(\mathbb{E}[\theta_k] - \theta^*)^\top] \\ &= V_k + (\mathbb{E}[\theta_k] - \theta^*)(\mathbb{E}[\theta_k] - \theta^*)^\top. \end{aligned}$$

And thus

$$\begin{aligned} \mathbb{E}[h(\theta_k)] - h(\theta^*) &= \frac{1}{2} \text{tr} \left( H^* \mathbb{E}[(\theta_k - \theta^*)(\theta_k - \theta^*)^\top] \right) \\ &= \frac{1}{2} \text{tr} \left( H^* \left( V_k + (\mathbb{E}[\theta_k] - \theta^*)(\mathbb{E}[\theta_k] - \theta^*)^\top \right) \right) \\ &= \frac{1}{2} \text{tr} (H^* V_k) + \frac{1}{2} \text{tr} \left( H^* (\mathbb{E}[\theta_k] - \theta^*)(\mathbb{E}[\theta_k] - \theta^*)^\top \right) \end{aligned} \quad (16)$$

15. Note that Murata (1998) only makes this assumption up to an asymptotically negligible approximation factor, and this isn't dealt with in a completely rigorous way, as per the discussion in Remark 2. Insofar as Theorem 1 can be extended to handle the non-quadratic case, it can likely also be extended to handle a non-constant gradient covariance matrix, provided that said matrix becomes approximately constant sufficiently quickly as  $\theta_k$  converges to  $\theta^*$ .

which allows us to relate the convergence of  $E[\theta_k]$  (which behaves like  $\theta_k$  in the deterministic version of the algorithm) and the size/shape of the variance of  $\theta_k$  to the convergence of  $E[h(\theta_k)]$ . In particular, we see that in this simple case where  $h(\theta)$  is quadratic,  $E[h(\theta_k)] - h(\theta^*)$  neatly decomposes as the sum of two independent terms that quantify the roles of these respective factors in the convergence of  $E[h(\theta_k)]$  to  $h(\theta^*)$ .

In the proof of the following theorem, which is located in Appendix B, we will use the above expression and Theorem 1 to precisely characterize the asymptotic convergence of  $E[h(\theta_k)]$ . Note that while Murata (1998) gives expressions for this as well, these expressions only include the asymptotically dominant terms, and cannot be directly evaluated except in certain special cases (such as when  $B = H$ ).

**Theorem 4** *Suppose that  $\theta_k$  is generated by the stochastic iteration in eqn. 15 while optimizing a quadratic objective  $h(\theta) = \frac{1}{2}(\theta - \theta^*)^\top H^*(\theta - \theta^*)$ .*

*If  $\alpha_k = \alpha$  is constant and  $2\alpha\lambda_1(B^{-1}H^*) < 1$ , then we have*

$$L(k) \leq E[h(\theta_k)] - h(\theta^*) \leq U(k),$$

where

$$U(k) = \left[1 - (1 - 2\epsilon_1)^k\right] \frac{\alpha}{4} \text{tr}(B^{-1}\Sigma_g(\theta^*)) + (1 - 2\epsilon_2)^k h(\theta_0) + (1 - \epsilon_2)^{2k} h(\theta_0)$$

and

$$L(k) = \left[1 - (1 - 2\epsilon_2)^k\right] \frac{\alpha}{4} \text{tr}(B^{-1}\Sigma_g(\theta^*)) + (1 - 2\epsilon_1)^k h(\theta_0) + (1 - \epsilon_1)^{2k} h(\theta_0),$$

with  $\epsilon_1 = \alpha\lambda_1(B^{-1}H^*)$  and  $\epsilon_2 = \alpha\lambda_n(B^{-1}H^*)$ .

*If on the other hand  $\alpha_k = 1/(k+1)$  and  $\lambda_n(B^{-1}H^*) > 1/2$  then we have*

$$\begin{aligned} E[h(\theta_k)] - h(\theta^*) &= \frac{1}{4k} \text{tr} \left( \left( I - \frac{1}{2} B^{1/2} H^{*-1} B^{1/2} \right)^{-1} B^{-1/2} \Sigma_g(\theta^*) B^{-1/2} \right) \\ &\quad - \frac{1}{8k^2} \text{tr} \left( \left( I - \frac{1}{4} B^{1/2} H^{*-1} B^{1/2} \right)^{-1} B^{-1/2} \Sigma_g(\theta^*) B^{-1/2} \right) \\ &\quad + \mathcal{O} \left( \frac{h(\theta_0)}{k^{2\lambda_n(B^{-1}H^*)}} \right) + \mathcal{O} \left( \frac{1}{k^3} \right). \end{aligned}$$

**Remark 5** *As with the theorem on which it is based (Theorem 1), the above theorem can likely be extended to handle non-quadratic objectives (at least in the case where  $\alpha_k = 1/(k+1)$ ).*

### 12.2.1 CONSEQUENCES OF THEOREM 4

In the case of a fixed step-size  $\alpha_k = \alpha$ , Theorem 4 shows that  $E[h(\theta_k)]$  will tend to  $h(\theta^*) + \frac{\alpha}{4} \text{tr}(B^{-1}\Sigma_g(\theta^*))$ . The size of this extra additive factor is correlated with the step-size  $\alpha$  and gradient noise covariance  $\Sigma_g(\theta^*)$ , and inversely correlated with the size of  $B$ . Thus,

if the covariance is relatively small compared to the step-size, this factor may not be very large in practice.

Moreover, one can use the fact that the iterates  $\{\theta_k\}_{k=1}^\infty$  are (non-independent) asymptotically unbiased estimators of  $\theta^*$  to produce an asymptotically unbiased estimator with shrinking variance by averaging them together. This is done in the averaging method (e.g. Polyak and Juditsky, 1992), which we analyze in Section 12.3.

In the scenario where  $\alpha_k = 1/(k+1)$ , if one performs stochastic 2nd-order optimization with  $B = H^*$ , Theorem 4 gives that

$$\mathbb{E}[h(\theta_k)] - h(\theta^*) = \left( \frac{1}{2k} - \frac{1}{6k^2} \right) \text{tr} \left( H^{*-1} \Sigma_g(\theta^*) \right) + \mathcal{O} \left( \frac{h(\theta_0)}{k^2} \right).$$

And if one considers the scenario corresponding to 1st-order optimization where we take  $B = \beta I$  for  $\beta < 2\lambda_n(H^*)$  (so that the condition  $\lambda_n(B^{-1}H^*) > 1/2$  holds), we get

$$\begin{aligned} \mathbb{E}[h(\theta_k)] - h(\theta^*) &= \frac{1}{4k\beta} \text{tr} \left( \left( I - \frac{\beta}{2} H^{*-1} \right)^{-1} \Sigma_g(\theta^*) \right) \\ &\quad - \frac{1}{8k^2\beta} \text{tr} \left( \left( I - \frac{\beta}{4} H^{*-1} \right)^{-1} \Sigma_g(\theta^*) \right) + \mathcal{O} \left( \frac{h(\theta_0)}{k^{2\lambda_n(H^*)/\beta}} \right) + \mathcal{O} \left( \frac{1}{k^3} \right). \end{aligned}$$

For  $\beta = \lambda_n(H^*)$ , which is the lowest value we can choose while ensuring that the starting-point dependent term  $\mathcal{O}(h(\theta_0)/k^{2\lambda_n(H^*)/\beta})$  shrinks as  $1/k^2$ , we obtain the upper bound

$$\mathbb{E}[h(\theta_k)] - h(\theta^*) \leq \frac{1}{4k\lambda_n(H^*)} \text{tr} \left( \left( I - \frac{\lambda_n(H^*)}{2} H^{*-1} \right)^{-1} \Sigma_g(\theta^*) \right) + \mathcal{O} \left( \frac{h(\theta_0)}{k^2} \right).$$

While the starting-point dependent terms (which are noise independent) are the same in either scenario (the hidden constant is the same too), the noise-dependent terms, which are the ones asymptotically dominant in  $k$ , differ. To compare the size of these terms we can apply Lemma 9 to obtain the following bounds (see Appendix C):

$$\frac{1}{2k\lambda_1(H^*)} \text{tr}(\Sigma_g(\theta^*)) \leq \frac{1}{2k} \text{tr} \left( H^{*-1} \Sigma_g(\theta^*) \right) \leq \frac{1}{2k\lambda_n(H^*)} \text{tr}(\Sigma_g(\theta^*))$$

and

$$\frac{1}{4k\lambda_n(H^*)} \text{tr}(\Sigma_g(\theta^*)) \leq \frac{1}{4k\lambda_n(H^*)} \text{tr} \left( \left( I - \frac{\lambda_n(H^*)}{2} H^{*-1} \right)^{-1} \Sigma_g(\theta^*) \right) \leq \frac{1}{2k\lambda_n(H^*)} \text{tr}(\Sigma_g(\theta^*)).$$

So while in the worst case the noise-dependent terms are closely comparable between the two scenarios, in the  $B = H^*$  scenario the term has the *potential* to be much smaller, due to the much smaller lower bound. A necessary condition for this to happen is that  $H^*$  is ill-conditioned (so that  $\lambda_1(H^*) \gg \lambda_n(H^*)$ ), although this alone is not sufficient.

To actually provide an example where the noise-dependent term is smaller in the  $B = H^*$  scenario we must make further assumptions about the nature of the gradient noise covariance matrix  $\Sigma_g(\theta^*)$ . As an important example, we consider the case where the stochastic



gradients are computed using (single) randomly sampled cases from the training set  $S$  and where we are in the realizable regime (so that  $H^* = \bar{F}^* = \Sigma_g(\theta^*)$ , see Section 12.1). In this case we have that in the  $B = H^*$  scenario the noise dependent term is

$$\frac{1}{2k} \operatorname{tr} \left( H^{*-1} \Sigma_g(\theta^*) \right) = \frac{1}{2k} \operatorname{tr} \left( H^{*-1} H^* \right) = \frac{n}{2k},$$

while in the  $B = \lambda_n(H^*)I$  scenario it is

$$\begin{aligned} \frac{1}{4k\lambda_n(H^*)} \operatorname{tr} \left( \left( I - \frac{\lambda_n(H^*)}{2} H^{*-1} \right)^{-1} \Sigma_g(\theta^*) \right) &= \frac{1}{4k\lambda_n(H^*)} \operatorname{tr} \left( \left( I - \frac{\lambda_n(H^*)}{2} H^{*-1} \right)^{-1} H^* \right) \\ &= \frac{1}{4k\lambda_n(H^*)} \sum_{i=1}^n \frac{\lambda_i(H^*)}{1 - \frac{\lambda_n(H^*)}{2\lambda_i(H^*)}} = \frac{1}{4k} \sum_{i=1}^n \frac{r_i}{1 - \frac{1}{2r_i}}, \end{aligned}$$

where we have defined  $r_i = \lambda_i(H^*)/\lambda_n(H^*)$ , and we have used the fact that all matrices involved have the same eigenvectors to go from the first to the second line. Observing that  $1 \leq r_i$  we have  $r_i \leq r_i/(1 - 1/(2r_i))$ , so that

$$\frac{1}{4k} \kappa(H^*) \leq \frac{1}{4k} \sum_{i=1}^n r_i \leq \frac{1}{4k} \sum_{i=1}^n \frac{r_i}{1 - \frac{1}{2r_i}}.$$

From these bounds we see that the noise dependent term may be much larger than  $n/(2k)$  when  $\kappa(H^*) \gg n$ , or when the spectrum of  $H^*$  covers a large range. For example, if  $\lambda_i(H^*) = n - i + 1$  then it will be  $\Omega(n^2/k)$ .

Moreover, in the non-realizable case,  $1/(2k) \operatorname{tr} (H^{*-1} \Sigma_g(\theta^*))$  turns out to be the same asymptotic rate as that achieved by the “empirical risk minimizer” (i.e. the estimator of  $\theta$  that minimizes the expected loss over the training cases processed thus far) and is thus “optimal” in a certain sense. See Frostig et al. (2014) for a good recent discussion of this.

Thus we see that, under the restriction that a  $\mathcal{O}(1/k^2)$  rate is achieved for the starting-point dependent term (which is noise *independent*), the use of 2nd-order optimization, in the case where  $\alpha_k = 1/(k+1)$ , allows us to obtain a better trade-off between the noise dependent and independent terms, which may be very significant in practice.

This result may seem counter-intuitive since 2nd-order optimization is usually thought of as speeding up deterministic optimization, and to be less important in the stochastic case. However, formal results about the effectiveness of 2nd-order optimization tend to rely on the use of a fixed step-size, and so we can identify the use of an annealed step-size schedule  $\alpha_k = 1/(k+1)$  as the source of this apparent paradox. Indeed, Theorem 4 shows that in the case of a fixed step-size  $\alpha_k = \alpha$  the noise-independent terms will shrink exponentially quickly, although at the cost of preventing the noise-dependent term from ever shrinking beyond a certain fixed size (and therefore preventing total convergence).

### 12.2.2 RELATED RESULTS

The related result most directly comparable to Theorem 4 is Theorem 1 of Bordes et al. (2009), which provides upper and lower bounds for  $\mathbb{E}[h(\theta_k)] - h(\theta^*)$  in the case where

$\alpha_k = 1/(k + k_0)$  for some  $k_0$  and  $\lambda_n(B^{-1}H^*) > 1/2$ . In particular, using a different technique from our own, Bordes et al. (2009) show that<sup>16</sup>

$$\frac{1}{k} \frac{\text{tr}(H^*B^{-1}\Sigma_g(\theta^*)B^{-1})}{4(\lambda_1(B^{-1}H^*) - \frac{1}{2})} + o\left(\frac{1}{k}\right) \leq \mathbb{E}[h(\theta_k)] - h(\theta^*) \leq \frac{1}{k} \frac{\text{tr}(H^*B^{-1}\Sigma_g(\theta^*)B^{-1})}{4(\lambda_n(B^{-1}H^*) - \frac{1}{2})} + o\left(\frac{1}{k}\right).$$

Apart from the minor assumption that  $k_0 = 1$  which is inherited from Theorem 1, as well as the much more significant additional hypothesis that  $h(\theta)$  is quadratic (which could possibly be removed as per Remark 2), Theorem 4 represents a strict improvement to the above result since it gives the exact asymptotic value of  $\mathbb{E}[h(\theta_k)] - h(\theta^*)$  instead of a bound (and is therefore more precise even in just the  $\mathcal{O}(1/k)$  term), where we note<sup>17</sup> that  $\mathcal{O}(h(\theta_0)/k^{2\lambda_n(B^{-1}H^*)}) = o(h(\theta_0)/k)$ .

### 12.3 An analysis of averaging

In this subsection we will extend the analysis from Subsection 12.2 to incorporate basic iterate averaging of the standard type (e.g. Polyak and Juditsky, 1992). In particular, we will bound  $\mathbb{E}[h(\bar{\theta}_k)]$  where

$$\bar{\theta}_k = \frac{1}{k+1} \sum_{i=0}^k \theta_i.$$

Note that while this type of averaging leads to elegant bounds (as we will see), a form of averaging based on an exponentially-decayed moving average typically works much better in practice. This is given by

$$\bar{\theta}_k = (1 - \beta_k)\theta_k + \beta_k\bar{\theta}_{k-1} \quad \bar{\theta}_0 = \theta_0$$

for  $\beta_k = \min\{1 - 1/k, \beta_{\max}\}$  with  $0 < \beta_{\max} < 1$  close to 1 (e.g.  $\beta_{\max} = 0.99$ ). This type of averaging has the advantage that it more quickly “forgets” the very early  $\theta_i$ ’s (since their “weight” in the average decays exponentially quickly), at the cost of preventing the variance from fully converging towards zero.

The main result of this subsection is stated as follows:

**Theorem 6** *Suppose that  $\theta_k$  is generated by the stochastic iteration in eqn. 15 with constant step-size  $\alpha_k = \alpha$  while optimizing a quadratic objective  $h(\theta) = \frac{1}{2}(\theta - \theta^*)^\top H^*(\theta - \theta^*)$ . Further suppose that  $2\alpha\lambda_1(B^{-1}H^*) < 1$ , and define  $\bar{\theta}_k = \frac{1}{k+1} \sum_{i=0}^k \theta_i$ .*

*Then we have the following bound:*

$$\begin{aligned} \mathbb{E}[h(\bar{\theta}_k)] - h(\theta^*) &\leq \min \left\{ \frac{1}{k+1} \text{tr} \left( H^{*-1} \Sigma_g(\theta^*) \right), \frac{\alpha}{2} \text{tr} \left( B^{-1} \Sigma_g(\theta^*) \right) \right\} \\ &\quad + \min \left\{ \frac{1}{(k+1)^2 \alpha^2} \left\| H^{*-1/2} B(\theta_0 - \theta^*) \right\|^2, \frac{1}{(k+1)\alpha} \left\| B^{1/2}(\theta_0 - \theta^*) \right\|^2, 3h(\theta_0) \right\}. \end{aligned}$$

16. Note that the notation ‘ $B$ ’ as it is used by Bordes et al. (2009) means the *inverse* of the matrix  $B$  as it appears in this paper. And while Bordes et al. (2009) presents their bounds with  $\bar{F}$  in place of  $\Sigma_g$ , these are the same matrix when evaluated at  $\theta = \theta^*$  as we have  $\mathbb{E}[g(\theta^*)] = 0$  (since  $\theta^*$  is a local optimum).

17. Note that Bordes et al. (2009) treats  $h(\theta_0)$  as a constant in their asymptotic expressions, which is why the term  $o(1/k)$  appears in their bound instead of  $o(h(\theta_0)/k)$ .

The proof of Theorem 6 is located in Appendix D.

Note that asymptotically as  $k \rightarrow \infty$  this bound can be written as

$$\mathbb{E}[h(\bar{\theta}_k)] - h(\theta^*) \leq \mathcal{O}\left(\frac{1}{k+1} \text{tr}\left(H^{*-1}\Sigma_g(\theta^*)\right)\right)$$

which notably doesn't depend on either  $\alpha$  or  $B$ . This is a somewhat surprising property of averaging to be sure, and can be explained intuitively as follows. Increasing the step-size along any direction  $d$  (as measured by  $\alpha d^\top B^{-1}d$ ) will increase the variance in that direction for each iterate (since the step-size multiplies the stochastic gradient and hence the noise), but will also cause the iterates to decorrelate faster in that direction (as can be seen from eqn. 44). Increased decorrelation in the iterates leads to lower variance in their average, which counteracts the aforementioned increased variance. As it turns out, these competing effects will exactly cancel in the asymptotic limit, which the proof of Theorem 6 rigorously establishes.

### 12.3.1 CONSEQUENCES OF THEOREM 6

In the case of stochastic 2nd-order optimization where we take  $B = H^*$  (which allows us to use an  $\alpha$  close to  $1/2$ ) this gives

$$\mathbb{E}[h(\bar{\theta}_k)] - h(\theta^*) \leq \frac{\text{tr}\left(H^{*-1}\Sigma_g(\theta^*)\right)}{k+1} + \frac{2h(\theta_0)}{(k+1)^2\alpha^2}.$$

Then choosing the maximum allowable value of  $\alpha$  this becomes

$$\mathbb{E}[h(\bar{\theta}_k)] - h(\theta^*) \leq \frac{\text{tr}\left(H^{*-1}\Sigma_g(\theta^*)\right)}{k+1} + \frac{8h(\theta_0)}{(k+1)^2},$$

which is a similar bound to the one described in Section 12.2.1 for stochastic 2nd-order optimization (with  $B = H^*$ ) using an annealed step-size  $\alpha_k = 1/(k+1)$ .

For the sake of comparison, applying Theorem 6 with  $B = I$  gives that

$$\mathbb{E}[h(\bar{\theta}_k)] - h(\theta^*) \leq \frac{\text{tr}\left(H^{*-1}\Sigma_g(\theta^*)\right)}{k+1} + \frac{\left\|H^{*-1/2}(\theta_0 - \theta^*)\right\|^2}{(k+1)^2\alpha^2} \quad (17)$$

under the assumption that  $2\alpha\lambda_1(H^*) < 1$ . For the maximum allowable value of  $\alpha$  this becomes

$$\mathbb{E}[h(\bar{\theta}_k)] - h(\theta^*) \leq \frac{\text{tr}\left(H^{*-1}\Sigma_g(\theta^*)\right)}{k+1} + \frac{\lambda_1(H^*)^2 \left\|H^{*-1/2}(\theta_0 - \theta^*)\right\|^2}{(k+1)^2}.$$

An interesting observation we can make about these bounds is that they *do not* demonstrate any improvement through the use of 2nd-order optimization on the asymptotically dominant noise-dependent term in the bound. Moreover, in the case where the stochastic gradients (the  $g_k(\theta_k)$ 's) are sampled using random training cases in the usual way so that  $\Sigma_g(\theta) = \bar{F}(\theta)$ , and the realizability hypothesis is satisfied so that  $H^* = F(\theta^*) = \bar{F}(\theta^*)$  (see Section 12.1), we can see that simple stochastic gradient descent with averaging achieves a

similar *asymptotic* convergence speed (given by  $n/(k+1) + o(1/k)$ ) to that possessed by Fisher efficient methods like stochastic natural gradient descent (c.f. eqn. 14), despite not involving the use of curvature matrices.

However, these bounds *do* demonstrate an improvement to the noise-independent term (which depends on the starting point  $\theta_0$ ) through the use of 2nd-order optimization, since when  $H^*$  is ill-conditioned and  $\theta_0 - \theta^*$  has a large component in the direction of eigenvectors of  $H^*$  with small eigenvalues, we will have

$$\lambda_1(H^*)^2 \|H^{*-1/2}(\theta_0 - \theta^*)\|^2 \gg h(\theta_0).$$

Crucially, this noise-independent term may often matter more in practice, as  $\lambda_1(H^*)^2 \|H^{*-1/2}(\theta_0 - \theta^*)\|^2$  may be very large compared to  $\Sigma_g(\theta^*)$ , and we may be interested in stopping the optimization long before the more slowly shrinking noise-dependent term begins to dominate asymptotically (e.g. if we have a fixed iteration budget or are employing early-stopping). This is especially likely to be the case if the gradient noise is mitigated through the use of large mini-batches.

It is also worth pointing out that compared to standard stochastic 2nd-order optimization with a fixed step-size (as considered by the first part of Theorem 4), the noise-independent term shrinks much more slowly when we use averaging (quadratically vs exponentially), or for that matter when we use an annealed step-size  $\alpha_k = 1/(k+1)$  (see Section 12.2.1). This seems to be the price one has to pay in order to ensure that the noise-dependent term shrinks as  $1/k$ . (Although in practice one can potentially obtain a more favorable dependence on the starting point by adopting the “forgetful” version of averaging discussed at the beginning of this subsection.)

### 12.3.2 RELATED RESULTS

Under weaker assumptions about the nature of the stochastic gradient noise (strictly weaker than our own), Polyak and Juditsky (1992) showed that

$$\mathbb{E}[(\bar{\theta}_k - \theta^*)(\bar{\theta}_k - \theta^*)^\top] = \frac{1}{k+1} H^{*-1/2} \Sigma_g(\theta^*) H^{*-1/2} + o\left(\frac{1}{k}\right),$$

which using the first line of eqn. 16 yields,

$$\mathbb{E}[h(\bar{\theta}_k)] - h(\theta^*) = \frac{\text{tr}(H^{*-1} \Sigma_g(\theta^*))}{k+1} + o\left(\frac{1}{k}\right).$$

While consistent with Theorem 6, this bound gives a less detailed picture of convergence, and in particular it fails to quantify the relative contribution of the noise-dependent and independent terms and thus doesn’t properly distinguish between the behavior of stochastic 1st or 2nd-order optimization methods (i.e.  $B = I$  vs  $B = H^*$ ).

Assuming a model for the gradient noise which is consistent with linear least-squares regression and  $B = I$ , Défossez and Bach (2014) showed that

$$\mathbb{E}[h(\bar{\theta}_k)] - h(\theta^*) \approx \frac{\text{tr}(H^{*-1} \Sigma_g(\theta^*))}{k+1} + \frac{\|H^{*-1/2}(\theta_0 - \theta^*)\|^2}{(k+1)^2 \alpha^2},$$

holds in the asymptotic limit as  $\alpha \rightarrow 0$  and  $k \rightarrow \infty$ .

This expression is similar to the one generated by Theorem 6 (see eqn. 17), although it only holds in the asymptotic limit of small  $\alpha$  and large  $k$ , and assumes a particular kind of noise which is more narrowly specialized than our general formulation. Notably however, our formulation does not capture this kind of noise precisely either, since for least-squares linear regression the covariance of the noise  $\Sigma_g(\theta)$  will depend on  $\theta$ , which is contrary to our assumption that it remains constant (with value  $\Sigma_g(\theta^*)$ ). An interesting question for future research is whether Theorem 1 could be extended in way that would allow  $\Sigma_g(\theta)$  to vary with  $\theta$ , and whether this would allow us to prove a more general version of Theorem 6 that would cover the case of linear least-squares.

A result which is more directly comparable to Theorem 6 is Theorem 3 of Flammarion and Bach (2015), which when applied to the same general case considered in Theorem 6 gives the following upper bound (assuming that  $B = I^{18}$  and  $\alpha\lambda_1(H^*) \leq 1$ ):

$$\mathbb{E}[h(\bar{\theta}_k)] - h(\theta^*) \leq 4\alpha \text{tr}(\Sigma_g(\theta^*)) + \frac{\|\theta_0 - \theta^*\|^2}{(k+1)\alpha}.$$

Unlike the bound proved in Theorem 6, this bound fails to establish that  $\mathbb{E}[h(\bar{\theta}_k)]$  even converges, since the term  $4\alpha \text{tr}(\Sigma_g(\theta^*))$  is constant in  $k$ .

### 13. A critical analysis of parameterization invariance

One of the main selling points of the natural gradient is its invariance to reparameterizations. In particular, the smooth path through the space of distributions generated by the idealized natural gradient method with infinitesimally small steps will be invariant to any smooth invertible reparameterization of the model.

More precisely, it can be said that this path will be the same whether we use the default parameterization (given by  $P_{y|x}(\theta)$ ), or parameterize our model as  $P_{y|x}(\zeta(\gamma))$ , where  $\zeta : \mathbb{R}^n \rightarrow \mathbb{R}^n$  is a smooth invertible “reparameterization function” which relates  $\theta$  to  $\gamma$  as  $\theta = \zeta(\gamma)$ .

In this section we will examine this “smooth path parameterization invariance” property more closely in order to answer the following questions:

- How can we characterize it using only basic properties of the curvature matrix?
- Does it have a more elementary proof that can be applied to more general settings?
- What other kinds of curvature matrices give rise to it, and is the Hessian included among these?
- Will this invariance property imply that *practical* optimization algorithms based on the natural gradient (i.e. those that use large discrete steps) will behave in a way that is invariant to the parameterization?

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18. Note that the assumption that  $B = I$  doesn’t actually limit this result since stochastic 2nd-order optimization of a quadratic using a *fixed*  $B$  can be understood as stochastic gradient descent applied to a transformed version of the original quadratic (with an appropriately transformed gradient noise matrix  $\Sigma_g$ ).

Let  $\zeta$  be as above, and let  $d_\theta$  and  $d_\gamma$  be updates given in  $\theta$ -space and  $\gamma$ -space (resp.). Additively updating  $\gamma$  by  $d_\gamma$  and translating it back to  $\theta$ -space via  $\zeta$  gives  $\zeta(\gamma + d_\gamma)$ . Measured by some non-specific norm  $\|\cdot\|$ , this differs from  $\theta + d_\theta$  by:

$$\|\zeta(\gamma + d_\gamma) - (\theta + d_\theta)\|.$$

This can be rewritten and bounded as

$$\|(\zeta(\gamma + d_\gamma) - (\zeta(\gamma) + J_\zeta d_\gamma)) + (J_\zeta d_\gamma - d_\theta)\| \leq \|\zeta(\gamma + d_\gamma) - (\zeta(\gamma) + J_\zeta d_\gamma)\| + \|J_\zeta d_\gamma - d_\theta\|, \quad (18)$$

where  $J_\zeta$  is the Jacobian of  $\zeta$  and we have used  $\theta = \zeta(\gamma)$ .

The first term on the RHS of eqn. 18 measures the extent to which  $\zeta(\gamma + d_\gamma)$  fails to be predicted by the first-order Taylor series approximation of  $\zeta$  centered at  $\gamma$  (i.e. the locally optimal affine approximation of  $\zeta$  at  $\gamma$ ). This quantity will depend on the size of  $d_\gamma$  and the degree of smoothness of  $\gamma$ , and in case where  $\zeta$  is affine, it will be exactly 0. We can further bound it by applying Taylor's theorem, which gives

$$\|\zeta(\gamma + d_\gamma) - (\zeta(\gamma) + J_\zeta d_\gamma)\| \leq \frac{1}{2} \left\| \begin{bmatrix} d_\gamma^\top H_{[\zeta]_1}(\gamma + c_1 d_\gamma) d_\gamma \\ d_\gamma^\top H_{[\zeta]_2}(\gamma + c_2 d_\gamma) d_\gamma \\ \vdots \\ d_\gamma^\top H_{[\zeta]_n}(\gamma + c_n d_\gamma) d_\gamma \end{bmatrix} \right\| \quad (19)$$

for some  $c_i \in (0, 1)$ . If we assume that there is some  $C > 0$  so that for all  $\gamma$  and  $i$ ,  $\|H_{[\zeta]_i}(\gamma)\|_2 \leq C$ , then using the fact that  $|d_\gamma^\top H_{[\zeta]_i}(\gamma + c_i d_\gamma) d_\gamma| \leq \frac{1}{2} \|H_{[\zeta]_i}(\gamma + c_i d_\gamma)\|_2 \|d_\gamma\|_2^2$  we can further upper bound this by  $\frac{1}{2} C \|d_\gamma\|_2^2 \mathbf{1}_n$ .

The second term on the RHS of eqn. 18 will be zero when

$$J_\zeta d_\gamma = d_\theta, \quad (20)$$

which (as we will see) is a condition that is satisfied in certain natural situations.

A slightly weakened version of this condition is that  $J_\zeta d_\gamma \propto d_\theta$ . Because we have

$$\lim_{\epsilon \rightarrow 0} \frac{\zeta(\gamma + \epsilon d_\gamma) - \zeta(\gamma)}{\epsilon} = J_\zeta d_\gamma$$

this condition can thus be interpreted as saying that that  $d_\gamma$ , when translated appropriately via  $\zeta$ , points in the same direction away from  $\theta$  that  $d_\theta$  does. In the smooth path case, where the optimizer only moves an infinitesimally small distance in the direction of  $d_\gamma$  (or  $d_\theta$ ) at each iteration before recomputing it at the new  $\gamma$  (or  $\theta$ ), this condition is sufficient to establish that the path in  $\gamma$  space, when mapped back to  $\theta$  space via the  $\zeta$  function, will be the same as the path which would have been taken if the optimizer had worked directly in  $\theta$  space.

However, for a practical update scheme where we move the entire distance of  $d_\gamma$  or  $d_\theta$  before recomputing the update vector, such as the one in eqn. 9, this kind of invariance will not strictly hold even when  $J_\zeta d_\gamma = d_\theta$ . But given that  $J_\zeta d_\gamma = d_\theta$ , the per-iteration error will be bounded by the first term on the RHS of eqn. 18, and will thus be small provided that  $d_\gamma$  is sufficiently small and  $\zeta$  is sufficiently smooth (as shown above).

Now, suppose we generate the updates  $d_\theta$  and  $d_\gamma$  from curvature matrices  $B_\theta$  and  $B_\gamma$  according to  $d_\theta = -\alpha B_\theta^{-1} \nabla h$  and  $d_\gamma = -\alpha B_\gamma^{-1} \nabla_\gamma h$ , where  $\nabla_\gamma h$  is the gradient of  $h(\zeta(\gamma))$  w.r.t.  $\gamma$ . Then noting that  $\nabla_\gamma h = J_\zeta^\top \nabla h$ , the condition in eqn. 20 becomes equivalent to

$$J_\zeta B_\gamma^{-1} J_\zeta^\top \nabla h = B_\theta^{-1} \nabla h.$$

For this to hold, a *sufficient* condition is that  $B_\theta^{-1} = J_\zeta B_\gamma^{-1} J_\zeta^\top$ . Since  $J_\zeta$  is invertible (because  $\zeta$  is) an equivalent condition is

$$J_\zeta^\top B_\theta J_\zeta = B_\gamma. \quad (21)$$

The following theorem summarizes our results so far.

**Theorem 7** *Suppose that  $B_\theta$  and  $B_\gamma$  are invertible matrices satisfying*

$$J_\zeta^\top B_\theta J_\zeta = B_\gamma$$

*Then we have that additively updating  $\theta$  by  $d_\theta = -\alpha B_\theta^{-1} \nabla h$  is **approximately** equivalent to additively updating  $\gamma$  by  $d_\gamma = -\alpha B_\gamma^{-1} \nabla_\gamma h$ , in the sense that  $\zeta(\gamma + d_\gamma) \approx \theta + d_\theta$ , with error bounded as*

$$\|\zeta(\gamma + d_\gamma) - (\theta + d_\theta)\| \leq \|\zeta(\gamma + d_\gamma) - (\zeta(\gamma) + J_\zeta d_\gamma)\|.$$

*Moreover, this error can be further bounded as in eqn. 19, and will be exactly 0 if  $\zeta$  is affine.*

Extending Theorem 7 in the obvious way from the case of a single update to one of an entire optimization path/trajectory gives the following corollary:

**Corollary 8** *Suppose either that  $\zeta$  is affine, or that  $\alpha$  goes to zero (so that the optimizer follows an idealized smooth path). Further suppose that  $B_\theta$  and  $B_\gamma$  are invertible matrices satisfying*

$$J_\zeta^\top B_\theta J_\zeta = B_\gamma$$

*for all values of  $\theta$ . Then the path followed by an iterative optimizer working in  $\theta$  space and using additive updates of the form  $d_\theta = -\alpha B_\theta^{-1} \nabla h$  is the same as the path followed by an iterative optimizer working in  $\gamma$  space using additive updates of the form  $d_\gamma = -\alpha B_\gamma^{-1} \nabla_\gamma h$ , provided that the optimizers use equivalent starting points (i.e.  $\theta_0 = \zeta(\gamma_0)$ ).*

So from these results we see that practical natural gradient-based methods will *not* be invariant to smooth invertible reparameterizations  $\zeta$ , although they will be *approximately* invariant, and in a way that depends on the smoothness of  $\zeta$  and the size  $\alpha$  of the step-size.

### 13.1 When is the condition $J_\zeta^\top B_\theta J_\zeta = B_\gamma$ satisfied?

Suppose the curvature matrix  $B_\theta$  has the form

$$B_\theta = \mathbb{E}_{D_{x,y}} [J_f^\top A J_f],$$

where  $D_{x,y}$  is some arbitrary distribution over  $x$  and  $y$  (such as the training distribution), and  $A \in \mathbb{R}^{m \times m}$  is some arbitrary invertible matrix (which can depend on  $x$ ,  $y$  and  $\theta$ ). Note that this type of curvature matrix includes as special cases the Generalized Gauss-Newton (whether or not it is equivalent to the Fisher), the Fisher, and the empirical Fisher (discussed in Section 11).

To obtain the analogous curvature matrix  $B_\gamma$  for the  $\gamma$  parameterization we replace  $f$  by  $f \circ \zeta$  which gives

$$B_\gamma = \mathbb{E}_{D_{x,y}}[(J_f J_\zeta)^\top A (J_f J_\zeta)].$$

Then noting that  $J_{f \circ \zeta} = J_f J_\zeta$ , where  $J_\zeta$  is the Jacobian of  $\zeta$ , we have

$$B_\gamma = \mathbb{E}_{D_{x,y}}[(J_f J_\zeta)^\top A (J_f J_\zeta)] = J_\zeta^\top \mathbb{E}_{D_{x,y}}[J_f^\top A J_f] J_\zeta = J_\zeta^\top B_\theta J_\zeta.$$

(Here we have used the fact that the reparameterization function  $\zeta$  is independent of  $x$  and  $y$ .)

Thus, this type of curvature matrix satisfies the sufficient condition in eqn. 21.

The Hessian on the other hand does not satisfy this sufficient condition, except in certain narrow special cases. To see this, note that taking the curvature matrix to be the Hessian gives

$$B_\gamma = J_\zeta^\top H J_\zeta + \frac{1}{|S|} \sum_{(x,y) \in S} \sum_{j=1}^n [\nabla h]_j H_{[\zeta]_j},$$

where  $H = B_\theta$  is the Hessian of  $h$  w.r.t.  $\theta$ . Thus, when the curvature matrix is the Hessian, the sufficient condition  $J_\zeta^\top B_\theta J_\zeta = J_\zeta^\top H J_\zeta \propto B_\gamma$  holds if and only if

$$\frac{1}{|S|} \sum_{(x,y) \in S} \sum_{j=1}^n [\nabla h]_j H_{[\zeta]_j} = J_\zeta^\top H J_\zeta,$$

where  $\nabla L$  is the gradient of  $L(y, z)$  w.r.t.  $z$  (evaluated at  $z = f(x, \theta)$ ), and we allow a proportionality constant of 0. Rearranging this gives

$$\frac{1}{|S|} \sum_{(x,y) \in S} \sum_{j=1}^n [\nabla h]_j J_\zeta^{-\top} H_{[\zeta]_j} J_\zeta^{-1} = H.$$

This relation is unlikely to be satisfied unless the left hand side is equal to 0. One situation where this will occur is when  $H_{[\zeta]_j} = 0$  for each  $j$ , which holds when  $[\zeta]_j$  is an affine function of  $\gamma$ . Another situation is where we have  $\nabla h = 0$  for each  $(x, y) \in S$ .

## 14. A new interpretation of the natural gradient

As discussed in Section 10, the natural gradient is given by the minimizer of a local quadratic approximation  $M(\delta)$  to  $h$  whose curvature matrix is the Fisher  $F$ . And if we have that the



gradient  $\nabla h$  and  $F$  are computed on the same set  $S$  of data points,  $M(\delta)$  can be written as

$$\begin{aligned}
 M(\delta) &= \frac{1}{2} \delta^\top F \delta + \nabla h^\top \delta + h(\theta) \\
 &= \frac{1}{|S|} \sum_{(x,y) \in S} \left[ \frac{1}{2} \delta^\top J_f^\top F_R J_f \delta + (J_f^\top \nabla_z \log r(y|z))^\top \delta \right] + h(\theta) \\
 &= \frac{1}{|S|} \sum_{(x,y) \in S} \left[ \frac{1}{2} (J_f \delta)^\top F_R (J_f \delta) + \nabla_z \log r(y|z)^\top F_R^{-1} F_R (J_f \delta) \right. \\
 &\quad \left. + \frac{1}{2} (\nabla_z \log r(y|z))^\top F_R^{-1} F_R F_R^{-1} \nabla_z \log r(y|z) \right. \\
 &\quad \left. - \frac{1}{2} (\nabla_z \log r(y|z))^\top F_R^{-1} F_R F_R^{-1} \nabla_z \log r(y|z) \right] + h(\theta) \\
 &= \frac{1}{|S|} \sum_{(x,y) \in S} \frac{1}{2} (J_f \delta + F_R^{-1} \nabla_z \log r(y|z))^\top F_R (J_f \delta + F_R^{-1} \nabla_z \log r(y|z)) + c \\
 &= \frac{1}{|S|} \sum_{(x,y) \in S} \frac{1}{2} \|J_f \delta + F_R^{-1} \nabla_z \log r(y|z)\|_{F_R}^2 + c,
 \end{aligned}$$

where  $F_R$  is the Fisher of the predictive distribution  $R_{y|z}$  (as originally defined in Section 9),  $\|v\|_{F_R} = \sqrt{v^\top F_R v}$ , and  $c = h(\theta) - \frac{1}{2} (\sum_{(x,y) \in S} \nabla_z \log r(y|z)^\top F_R^{-1} \nabla_z \log r(y|z)) / |S|$  is a constant (independent of  $\delta$ ).

Note that for a given  $(x, y) \in S$ ,  $F_R^{-1} \nabla_z \log r(y|z)$  can be interpreted as the natural gradient direction in  $z$ -space for an objective corresponding to the KL divergence between the predictive distribution  $R_{y|z}$  and a delta distribution on the given  $y$ . In other words, it points in the direction which moves  $R_{y|z}$  most quickly towards to said delta distribution, as measured by the KL divergence (see Section 6). And assuming that the GGN interpretation of  $F$  holds (as discussed in Section 9), we know that it also corresponds to the optimal change in  $z$  according to the 2nd-order Taylor series approximation of the loss function  $L(y, z)$ .

Thus,  $M(\delta)$  can be interpreted as the sum of squared distances (as measured using the Fisher metric tensor) between these “optimal” changes in the  $z$ ’s, and the changes in the  $z$ ’s which result from adding  $\delta$  to  $\theta$ , as predicted using 1st-order Taylor-series approximations to  $f$ .

In addition to giving us a new interpretation for the natural gradient, this expression also gives us an easy-to-compute bound on the largest possible improvement to  $h$  (as predicted by  $M(\delta)$ ). In particular, since the squared error terms are non-negative, we have

$$M(\delta) - h(\theta) \geq -\frac{1}{2|S|} \sum_{(x,y) \in S} \nabla_z \log r(y|z)^\top F_R^{-1} \nabla_z \log r(y|z).$$

Given  $F_R = H_L$ , this quantity has the simple interpretation of being the optimal improvement in  $h$  (as predicted by a 2nd-order order model of  $L(y, z)$  for each case in  $S$ ) achieved in the hypothetical scenario where we can change the  $z$ ’s independently for each case.

The existence of this bound shows that the natural gradient can be meaningfully defined even when  $F^{-1}$  may not exist, provided that we compute  $F$  and  $\nabla h$  on the *same data*, and

that each  $F_R$  is invertible. In particular, it can be defined as the minimizer of  $M(\delta)$  that has minimum norm (which must exist since  $M(\delta)$  is bounded below). In practice this could be computed by using the pseudo-inverse of  $F$  in place of  $F^{-1}$ .

## 15. Conclusions and open questions

In this report we have examined several aspects of the natural gradient method, such as its relationship to 2nd-order methods, its local convergence speed, and its invariance properties.

The link we have established between natural gradient descent and approximate (stochastic) 2nd-order optimization with the Generalized Gauss-Newton matrix (GGN) provides intuition for why it might work well with large step-sizes, and gives prescriptions for how to make it work robustly in practice (by using of damping/regularization techniques).

However, even in the case of squared loss (where the GGN becomes the standard Gauss-Newton matrix), we don't yet have a completely rigorous understanding of 2nd-order optimization with the GGN. A rigorous account of its global convergence remains elusive (even if we can assume convexity), and local results such as those proved in Section 12 don't even provide a complete picture of its *local* convergence.

For example, these kinds of local convergence bounds, which assume the objective is quadratic (or is well-approximated as such), are always improved by using the Hessian instead of the GGN, and thus fail to explain the empirically observed superiority of the GGN over the Hessian for neural network training. This is likely because they assume that the objective function has constant curvature (given by the Hessian at the optimum) so that optimization could not possibly be helped by using a more "conservative" curvature matrix like the GGN (e.g. for the reasons discussed in Section 8.1). Similarly they fail to explain why damping/regularization methods are so crucial to robust global optimization performance.

And for local convergence, the bounds we have proved in Section 12 may be hard to interpret when the curvature matrix is GGN/Fisher (i.e.  $B = F$ ). For example, if we pay attention only to the noise-independent/starting point-dependent term in the bound in Theorem 6, which is given by

$$\frac{1}{(k+1)^2\alpha^2} \left\| H^{*-1/2} B(\theta_0 - \theta^*) \right\|^2,$$

and plug in  $B = F$  and the maximum-allowable learning rate  $\alpha = 1/(2\lambda_1(B^{-1}H^*))$ , we get the somewhat opaque expression

$$\frac{4\lambda_1(F^{-1}H^*)^2}{(k+1)^2} \left\| H^{*-1/2} F(\theta_0 - \theta^*) \right\|^2.$$

It is not immediately obvious how we can further bound this expression in the non-realizable case (i.e. where we don't necessarily have  $F = H^*$ ) using easily accessible/interpretable properties of the objective function. This is due to the complicated nature of the relationship between the GGN and the Hessian, which we haven't explored in this report beyond the speculative discussion in Section 8.1.

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## Appendix A. Extra derivations for Theorem 1

Given  $\alpha_k = 1/(k+1)$  and  $\lambda_n(B^{-1}H^*) > \frac{1}{2}$  Murata (1998) shows that

$$V_k = \frac{1}{k} (\Xi_{B^{-1}H^*} - I)^{-1} (B^{-1}\Sigma_g(\theta^*)B^{-1}) + o\left(\frac{1}{k}\right).$$

In this section we will derive the following more detailed asymptotic expression for  $V_k$  which is accurate up to terms of order  $1/k^2$ :

$$V_k = \frac{1}{k} (\Xi_{B^{-1}H^*} - I)^{-1} (B^{-1}\Sigma_g(\theta^*)B^{-1}) - \frac{1}{k^2} (\Xi_{B^{-1}H^*} - 2I)^{-1} (B^{-1}\Sigma_g(\theta^*)B^{-1}) + \mathcal{O}\left(\frac{1}{k^3}\right).$$

To derive this expression we will make use of the following recursive expression for  $V_k$  (which holds under the hypotheses of Theorem 1 concerning the objective function  $h$ ):

$$\begin{aligned} V_{k+1} &= V_k - \alpha_k (B^{-1}H^*V_k + V_kH^*B^{-1}) + \alpha_k^2 B^{-1}\Sigma_g(\theta^*)B^{-1} \\ &= (I - \Xi_{\alpha_k B^{-1}H^*}) (V_k) + \alpha_k^2 B^{-1}\Sigma_g(\theta^*)B^{-1}. \end{aligned} \quad (22)$$

A similar expression to this one is derived by Murata (1998) in their Lemmas 2 & 3, but included several extra terms on the RHS. The presence of the first set of terms is due to the approximation of  $h$  by its own 2nd-order Taylor series expansion, and we can drop these since we are assuming that  $h$  is *exactly* quadratic. Note that Murata (1998) also drops these terms when giving their Lemma 3, although they only justify this in a non-rigorous way by claiming that these terms can be ignored in the subsequent analysis. While this is likely true for some of the subsequent results like their Theorem 4 (covering the  $\alpha_k = 1/(k+1)$  case), it is likely false for their Theorem 1 (covering the constant  $\alpha_k$  case).

The second extra term is of the form  $-\alpha_k^2 B^{-1}H^*(E[\theta_t] - \theta^*)(E[\theta_t] - \theta^*)^\top H^*B^{-1}$ , and appears in Lemma 3 of Murata (1998). The presence of this extra term is due to our use of a slightly different assumption regarding the gradient noise made than is made by Murata (1998). In particular, Murata (1998) assumes that the second order statistics of the gradient, i.e.  $E[g(\theta)g(\theta)^\top] = \Sigma_g(\theta) + E[g(\theta)]E[g(\theta)]^\top$ , is constant, whereas we assume that the covariance  $\Sigma_g(\theta)$  is constant. Our assumption is arguably more realistic and also happens to simplify the analysis. By adopting it and making minor modifications to the proof of Lemma 3 of Murata (1998) as appropriate, one can easily derive our eqn. 22.

In the remainder of this subsection we will compute the asymptotic value of  $V_k$  and also compute the constant on the  $\mathcal{O}(1/k^2)$  term, which will be useful in the proof of Theorem 4 (note that an expression for this term doesn't appear in Murata (1998)).

We start by expanding

$$V_k = \frac{1}{k}C_1 + \frac{1}{k^2}C_2 + \frac{1}{k^3}C_3 + \mathcal{O}\left(\frac{1}{k^4}\right).$$

Plugging this into eqn. 22 and using  $\alpha_k = 1/(k+1)$  we have

$$\begin{aligned} &\frac{1}{k+1}C_1 + \frac{1}{(k+1)^2}C_2 + \frac{1}{(k+1)^3}C_3 + \mathcal{O}\left(\frac{1}{k^4}\right) \\ &= \left(I - \frac{1}{k+1}\Xi_{B^{-1}H^*}\right) \left(\frac{1}{k}C_1 + \frac{1}{k^2}C_2 + \frac{1}{k^3}C_3 + \mathcal{O}\left(\frac{1}{k^4}\right)\right) + \frac{1}{(k+1)^2}B^{-1}\Sigma_g(\theta^*)B^{-1}. \end{aligned}$$

Rearrangement gives

$$\begin{aligned} & \left( \frac{1}{k(k+1)} \Xi_{B^{-1}H^*} + \left( \frac{1}{k+1} - \frac{1}{k} \right) I \right) (C_1) + \left( \frac{1}{k^2(k+1)} \Xi_{B^{-1}H^*} + \left( \frac{1}{(k+1)^2} - \frac{1}{k^2} \right) I \right) (C_2) \\ & \quad + \left( \frac{1}{k^3(k+1)} \Xi_{B^{-1}H^*} + \left( \frac{1}{(k+1)^3} - \frac{1}{k^3} \right) I \right) (C_3) \\ & = \frac{1}{(k+1)^2} B^{-1} \Sigma_g(\theta^*) B^{-1} + \mathcal{O}\left(\frac{1}{k^4}\right). \end{aligned}$$

Because  $1/(k+1)^3 - 1/k^3 = \mathcal{O}(1/k^4)$  we note that the term depending on  $C_3$  can thus be absorbed into the  $\mathcal{O}(1/k^4)$  term. This, combined with the fact that  $1/(k+1) - 1/k = -1/(k(k+1))$  and  $1/(k+1)^2 - 1/k^2 = -(2k+1)/(k^2(k+1))$ , lets us rewrite the above equation as

$$\begin{aligned} & \left( \frac{1}{k(k+1)} \Xi_{B^{-1}H^*} - \frac{1}{k(k+1)} I \right) (C_1) + \left( \frac{1}{k^2(k+1)} \Xi_{B^{-1}H^*} - \frac{2k+1}{k^2(k+1)^2} I \right) (C_2) \\ & = \frac{1}{(k+1)^2} B^{-1} \Sigma_g(\theta^*) B^{-1} + \mathcal{O}\left(\frac{1}{k^4}\right). \end{aligned}$$

Multiplying both sides of this by  $k(k+1)$  yields

$$\begin{aligned} & (\Xi_{B^{-1}H^*} - I) (C_1) + \left( \frac{1}{k} \Xi_{B^{-1}H^*} - \frac{2k+1}{k(k+1)} I \right) (C_2) \\ & = \frac{k}{k+1} B^{-1} \Sigma_g(\theta^*) B^{-1} + \mathcal{O}\left(\frac{1}{k^2}\right) = B^{-1} \Sigma_g(\theta^*) B^{-1} - \frac{1}{k+1} B^{-1} \Sigma_g(\theta^*) B^{-1} + \mathcal{O}\left(\frac{1}{k^2}\right). \end{aligned}$$

Noting that  $1/k - 1/(k+1) = \mathcal{O}(1/k^2)$  and  $(2k+1)/(k(k+1)) - 2/(k+1) = \mathcal{O}(1/k^2)$  we have

$$\begin{aligned} & \left( \frac{1}{k} \Xi_{B^{-1}H^*} - \frac{2k+1}{k(k+1)} I \right) (C_2) = \left( \frac{1}{k+1} \Xi_{B^{-1}H^*} - \frac{2}{k+1} I \right) (C_2) + \mathcal{O}\left(\frac{1}{k^2}\right) \\ & = \frac{1}{k+1} (\Xi_{B^{-1}H^*} - 2I) (C_2) + \mathcal{O}\left(\frac{1}{k^2}\right), \end{aligned}$$

which combined with the previous equation yields

$$(\Xi_{B^{-1}H^*} - I) (C_1) + \frac{1}{k+1} (\Xi_{B^{-1}H^*} - 2I) (C_2) = B^{-1} \Sigma_g(\theta^*) B^{-1} - \frac{1}{k+1} B^{-1} \Sigma_g(\theta^*) B^{-1} + \mathcal{O}\left(\frac{1}{k^2}\right).$$

Comparing coefficients gives

$$\begin{aligned} & (\Xi_{B^{-1}H^*} - I) (C_1) = B^{-1} \Sigma_g(\theta^*) B^{-1} \\ & (\Xi_{B^{-1}H^*} - 2I) (C_2) = -B^{-1} \Sigma_g(\theta^*) B^{-1}, \end{aligned}$$

or in other words

$$\begin{aligned} & C_1 = (\Xi_{B^{-1}H^*} - I)^{-1} (B^{-1} \Sigma_g(\theta^*) B^{-1}) \\ & C_2 = -(\Xi_{B^{-1}H^*} - 2I)^{-1} (B^{-1} \Sigma_g(\theta^*) B^{-1}). \end{aligned}$$

Thus we may conclude that

$$\begin{aligned} V_k &= \frac{1}{k} C_1 + \frac{1}{k^2} C_2 + \mathcal{O}\left(\frac{1}{k^3}\right) \\ &= \frac{1}{k} (\Xi_{B^{-1}H^*} - I)^{-1} (B^{-1} \Sigma_g(\theta^*) B^{-1}) - \frac{1}{k^2} (\Xi_{B^{-1}H^*} - 2I)^{-1} (B^{-1} \Sigma_g(\theta^*) B^{-1}) + \mathcal{O}\left(\frac{1}{k^3}\right). \end{aligned}$$

## Appendix B. Proof of Theorem 4

First we will consider the case where  $\alpha_k = \alpha$  is constant.

Note that for any matrix  $X$  we have

$$\begin{aligned} H^{*1/2} (I - \Xi_{\alpha B^{-1}H^*}) (X) H^{*1/2} &= H^{*1/2} \left( X - \alpha B^{-1} H^* X - \alpha X^\top H^* B^{-1} \right) H^{*1/2} \\ &= H^{*1/2} X H^{*1/2} - \alpha H^{*1/2} B^{-1} H^{*1/2} (H^{*1/2} X H^{*1/2}) - \alpha (H^{*1/2} X H^{*1/2})^\top H^{*1/2} B^{-1} H^{*1/2} \\ &= (I - \Xi_{\alpha H^{*1/2} B^{-1} H^{*1/2}}) (H^{*1/2} X H^{*1/2}) = (I - \Xi_C) (H^{*1/2} X H^{*1/2}), \end{aligned}$$

where we have defined

$$C = \alpha H^{*1/2} B^{-1} H^{*1/2}.$$

Applying this recursively we obtain

$$H^{*1/2} (I - \Xi_{\alpha B^{-1}H^*})^k (X) H^{*1/2} = (I - \Xi_C)^k (H^{*1/2} X H^{*1/2}).$$

Then using the expression for  $V_k$  from Theorem 1 it follows that

$$\begin{aligned} H^{*1/2} V_k H^{*1/2} &= H^{*1/2} \left( V_\infty - (I - \Xi_{\alpha B^{-1}H^*})^k (V_\infty) + (I - \Xi_{\alpha B^{-1}H^*})^k \left( (\theta_0 - \theta^*)(\theta_0 - \theta^*)^\top \right) \right) H^{*1/2} \\ &= \left( I - (I - \Xi_C)^k \right) (H^{*1/2} V_\infty H^{*1/2}) + (I - \Xi_C)^k \left( H^{*1/2} (\theta_0 - \theta^*)(\theta_0 - \theta^*)^\top H^{*1/2} \right). \end{aligned} \quad (23)$$

And thus

$$\begin{aligned} \frac{1}{2} \text{tr}(H^* V_k) &= \frac{1}{2} \text{tr} \left( H^{*1/2} V_k H^{*1/2} \right) \\ &= \frac{1}{2} \text{tr} \left( H^{*1/2} V_\infty H^{*1/2} \right) - \frac{1}{2} \text{tr} \left( (I - \Xi_C)^k (H^{*1/2} V_\infty H^{*1/2}) \right) \\ &\quad + \frac{1}{2} \text{tr} \left( (I - \Xi_C)^k \left( H^{*1/2} (\theta_0 - \theta^*)(\theta_0 - \theta^*)^\top H^{*1/2} \right) \right). \end{aligned} \quad (24)$$

Next, observe that for any matrix  $X$ , and any symmetric matrix  $Y$

$$\begin{aligned} \text{tr}(Y(I - \Xi_C)(X)) &= \text{tr}(YX - YCX - Y(CX)^\top) = \text{tr}(YX) - \text{tr}(YCX) - \text{tr}(YX^\top C) \\ &= \text{tr}(YX) - \text{tr}(YCX) - \text{tr}((YX^\top C)^\top) = \text{tr}(YX) - \text{tr}(YCX) - \text{tr}(CXY) \\ &= \text{tr}(YX) - \text{tr}(YCX) - \text{tr}(YCX) = \text{tr}(YX - YCX - YCX) = \text{tr}(Y(I - 2C)X), \end{aligned}$$

from which it follows that

$$\text{tr}(Y(I - \Xi_C)^i(X)) = \text{tr}(Y(I - 2C)^i X) \quad (25)$$



for any non-negative integer  $i$ .

Noting that the eigenvalues of a product of square matrices is invariant under cyclic permutation of those matrices we have  $2\lambda_1(C) = 2\lambda_1(\alpha H^{*1/2} B^{-1} H^{*1/2}) = 2\alpha\lambda_1(B^{-1} H^*) < 1$  so that  $I - 2C$  is PSD, and it thus follows that  $\lambda_i((I - 2C)^k) = (1 - 2\lambda_{n-i+1}(C))^k$ . Then assuming  $X$  is also PSD we can use Lemma 9 (given below) to get

$$(1 - 2\lambda_1(C))^k \operatorname{tr}(X) \leq \operatorname{tr}((I - 2C)^k X) \leq (1 - 2\lambda_n(C))^k \operatorname{tr}(X).$$

**Lemma 9** (Adapted from Lemma 1 from Wang et al. (1986)) Suppose  $X$  and  $S$  are  $n \times n$  matrices such that  $S$  is symmetric and  $X$  is PSD. Then we have

$$\lambda_n(S) \operatorname{tr}(X) \leq \operatorname{tr}(SX) \leq \lambda_1(S) \operatorname{tr}(X).$$

Applying this to eqn. 24 we thus have the upper bound

$$\begin{aligned} \frac{1}{2} \operatorname{tr}(H^* V_k) &\leq \frac{1}{2} \operatorname{tr}(H^* V_\infty) - (1 - 2\alpha\lambda_1(B^{-1} H^*))^k \frac{1}{2} \operatorname{tr}(H^* V_\infty) + (1 - 2\alpha\lambda_n(B^{-1} H^*))^k h(\theta_0) \\ &= \left[1 - (1 - 2\alpha\lambda_1(B^{-1} H^*))^k\right] \frac{1}{2} \operatorname{tr}(H^* V_\infty) + (1 - 2\alpha\lambda_n(B^{-1} H^*))^k h(\theta_0), \end{aligned} \quad (26)$$

and the lower bound

$$\begin{aligned} \frac{1}{2} \operatorname{tr}(H^* V_k) &\geq \frac{1}{2} \operatorname{tr}(H^* V_\infty) - (1 - 2\alpha\lambda_n(B^{-1} H^*))^k \frac{1}{2} \operatorname{tr}(H^* V_\infty) + (1 - 2\alpha\lambda_1(B^{-1} H^*))^k h(\theta_0) \\ &= \left[1 - (1 - 2\alpha\lambda_n(B^{-1} H^*))^k\right] \frac{1}{2} \operatorname{tr}(H^* V_\infty) + (1 - 2\alpha\lambda_1(B^{-1} H^*))^k h(\theta_0), \end{aligned} \quad (27)$$

where we have used the following equality:

$$\begin{aligned} \frac{1}{2} \operatorname{tr}\left(H^{*1/2}(\theta_0 - \theta^*)(\theta_0 - \theta^*)^\top H^{*1/2}\right) &= \operatorname{tr}\left((\theta_0 - \theta^*)^\top H^*(\theta_0 - \theta^*)\right) \\ &= \frac{1}{2}(\theta_0 - \theta^*)^\top H^*(\theta_0 - \theta^*) = h(\theta_0). \end{aligned}$$

Next we will compute/bound the term  $\operatorname{tr}(H^*(\mathbb{E}[\theta_k] - \theta^*)(\mathbb{E}[\theta_k] - \theta^*)^\top)$ .

Theorem 1 tells us that

$$\mathbb{E}[\theta_k] - \theta^* = (I - \alpha B^{-1} H^*)^k (\theta_0 - \theta^*).$$

Then observing

$$H^{*1/2}(I - \alpha B^{-1} H^*) = \left(I - \alpha H^{*1/2} B^{-1} H^{*1/2}\right) H^{*1/2} = (I - C) H^{*1/2}$$

it follows that

$$\begin{aligned} H^{*1/2}(\mathbb{E}[\theta_k] - \theta^*) &= H^{*1/2}(I - \alpha B^{-1} H^*)^k (\theta_0 - \theta^*) \\ &= (I - C)^k H^{*1/2}(\theta_0 - \theta^*). \end{aligned} \quad (28)$$

Thus we have

$$\begin{aligned} \frac{1}{2} \operatorname{tr} \left( H^* (\mathbb{E}[\theta_k] - \theta^*) (\mathbb{E}[\theta_k] - \theta^*)^\top \right) &= \frac{1}{2} \operatorname{tr} \left( (I - C)^k H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} (I - C)^{k^\top} \right) \\ &= \frac{1}{2} \operatorname{tr} \left( (I - C)^{2k} \left( H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} \right) \right). \end{aligned}$$

Applying Lemma 9 in a similar manner to before we have the upper bound

$$\frac{1}{2} \operatorname{tr} \left( H^* (\mathbb{E}[\theta_k] - \theta^*) (\mathbb{E}[\theta_k] - \theta^*)^\top \right) \leq (1 - \alpha \lambda_n (B^{-1} H^*))^{2k} h(\theta_0), \quad (29)$$

and the lower bound

$$\frac{1}{2} \operatorname{tr} \left( H^* (\mathbb{E}[\theta_k] - \theta^*) (\mathbb{E}[\theta_k] - \theta^*)^\top \right) \geq (1 - \alpha \lambda_1 (B^{-1} H^*))^{2k} h(\theta_0). \quad (30)$$

Combining eqn. 16, eqn. 26, eqn. 27, eqn. 29, and eqn. 30 we thus have

$$L(k) \leq \mathbb{E}[h(\theta_k)] - h(\theta^*) \leq U(k), \quad (31)$$

where

$$U(k) = \left[ 1 - (1 - 2\epsilon_1)^k \right] \frac{1}{2} \operatorname{tr} (H^* V_\infty) + (1 - 2\epsilon_2)^k h(\theta_0) + (1 - \epsilon_2)^{2k} h(\theta_0)$$

and

$$L(k) = \left[ 1 - (1 - 2\epsilon_2)^k \right] \frac{1}{2} \operatorname{tr} (H^* V_\infty) + (1 - 2\epsilon_1)^k h(\theta_0) + (1 - \epsilon_1)^{2k} h(\theta_0),$$

with  $\epsilon_1 = \alpha \lambda_1 (B^{-1} H^*)$  and  $\epsilon_2 = \alpha \lambda_n (B^{-1} H^*)$ .

It remains to compute  $\frac{1}{2} \operatorname{tr} (H^* V_\infty)$ .

From Theorem 1,  $V_\infty$  is given by  $\alpha \Xi_{B^{-1} H^*}^{-1} (B^{-1} \Sigma_g(\theta^*) B^{-1})$ , so that we have

$$\Xi_{B^{-1} H^*} (V_\infty) = \alpha B^{-1} \Sigma_g(\theta^*) B^{-1}.$$

Written as a matrix equation this is

$$B^{-1} H^* V_\infty + V_\infty H^* B^{-1} = \alpha B^{-1} \Sigma_g(\theta^*) B^{-1}. \quad (32)$$

Defining

$$\begin{aligned} A &= -B^{-1} H^* \\ P &= V_\infty \\ Q &= \alpha B^{-1} \Sigma_g(\theta^*) B^{-1} \end{aligned} \quad (33)$$

we can write this as

$$-A^\top P - P A = Q,$$

which after rearrangement becomes

$$A^\top P + P A + Q = 0.$$

This is known in the control theory literature as a Continuous Algebraic Lyapunov Equation (CALE) whenever  $Q$  is PSD (as it is in our case). The control theory community has developed efficient algorithms for solving such equations for  $P = V_\infty$  (e.g Bartels and Stewart, 1972), although for the purposes of computing a bound we don't actually need this quantity, as the following lemma establishes.

**Lemma 10** Suppose  $A^\top P + PA + Q = 0$  is a CALE and  $P$  is invertible. Then we have

$$\text{tr}(A) = -\frac{1}{2} \text{tr}(P^{-1}Q).$$

**Proof** Pre-multiplying both sides of  $A^\top P + PA + Q = 0$  by  $P^{-1}$  and taking the trace yields  $\text{tr}(P^{-1}A^\top P) + \text{tr}(A) + \text{tr}(P^{-1}Q) = 0$ . Then noting that  $\text{tr}(P^{-1}A^\top P) = \text{tr}(PP^{-1}A^\top) = \text{tr}(A^\top) = \text{tr}(A)$  this becomes  $2\text{tr}(A) + \text{tr}(P^{-1}Q) = 0$ , from which the claim follows. ■

To apply this lemma we observe that eqn. 32 can be alternately written as a CALE  $A^\top P + PA + Q = 0$  where

$$\begin{aligned} A &= -H^*V_\infty \\ P &= B^{-1} \\ Q &= \alpha B^{-1}\Sigma_g(\theta^*)B^{-1}. \end{aligned} \tag{34}$$

and so

$$\text{tr}(H^*V_\infty) = \text{tr}(-A) = \frac{1}{2} \text{tr}(P^{-1}Q) = \frac{1}{2} \text{tr}((B^{-1})^{-1}\alpha B^{-1}\Sigma_g(\theta^*)B^{-1}) = \frac{\alpha}{2} \text{tr}(B^{-1}\Sigma_g(\theta^*)). \tag{35}$$

Next we will examine the second case considered in Theorem 1, where  $\alpha_k = 1/(k+1)$  and  $\lambda_n(B^{-1}H^*) > 1/2$ . From eqn. 16 we have

$$\mathbb{E}[h(\theta_k)] - h(\theta^*) = \frac{1}{2} \text{tr}(H^*V_k) + \frac{1}{2} \text{tr}\left(H^*(\mathbb{E}[\theta_k] - \theta^*)(\mathbb{E}[\theta_k] - \theta^*)^\top\right). \tag{36}$$

And by the expression for  $V_k$  from Theorem 1 we have that

$$\frac{1}{2} \text{tr}(H^*V_k) = \frac{1}{2} \text{tr}\left(H^*\left(\frac{1}{k}C_1 + \frac{1}{k^2}C_2 + \mathcal{O}\left(\frac{1}{k^3}\right)\right)\right) = \frac{1}{2k} \text{tr}(H^*C_1) + \frac{1}{2k^2} \text{tr}(H^*C_2) + \mathcal{O}\left(\frac{1}{k^3}\right), \tag{37}$$

where  $C_1 = (\Xi_{B^{-1}H^*} - I)^{-1}(B^{-1}\Sigma_g(\theta^*)B^{-1})$  and  $C_2 = -(\Xi_{B^{-1}H^*} - 2I)^{-1}(B^{-1}\Sigma_g(\theta^*)B^{-1})$ .

Since  $(\Xi_{B^{-1}H^*} - I)(C_1) = B^{-1}\Sigma_g(\theta^*)B^{-1}$  we have that  $C_1$  is given by the matrix equation

$$B^{-1}H^*C_1 + C_1H^*B^{-1} - C_1 = B^{-1}\Sigma_g(\theta^*)B^{-1}. \tag{38}$$

We can rewrite eqn. 38 as

$$C_1H^*\left(B^{-1} - \frac{1}{2}H^{*-1}\right) + \left(B^{-1} - \frac{1}{2}H^{*-1}\right)H^*C_1 = B^{-1}\Sigma_g(\theta^*)B^{-1}, \tag{39}$$

which after simple rearrangement is a CALE  $A^\top P + PA + Q = 0$  with

$$\begin{aligned} A &= -H^* C_1 \\ P &= \left( B^{-1} - \frac{1}{2} H^{*-1} \right) \\ Q &= B^{-1} \Sigma_g(\theta^*) B^{-1}, \end{aligned} \tag{40}$$

In order to compute  $\text{tr}(H^* C_1)$  we can thus apply Lemma 10.

However we must first verify that our  $P$  is invertible. To this end we will show that  $B^{-1} - \frac{1}{2} H^{*-1}$  is positive definite. This is equivalent to the condition that  $H^{*1/2}(B^{-1} - \frac{1}{2} H^{*-1})H^{*1/2} = H^{*1/2} B^{-1} H^{*1/2} - \frac{1}{2} I$  is positive definite, or in other words that  $\lambda_n(H^{*1/2} B^{-1} H^{*1/2}) = \lambda_n(H^* B^{-1}) > 1/2$ , which is true by hypothesis.

Thus Lemma 10 is applicable, and yields

$$\begin{aligned} \text{tr}(H^* C_1) &= \text{tr}(-P) = \frac{1}{2} \text{tr}(A^{-1} Q) = \frac{1}{2} \text{tr} \left( \left( B^{-1} - \frac{1}{2} H^{*-1} \right)^{-1} B^{-1} \Sigma_g(\theta^*) B^{-1} \right) \\ &= \frac{1}{2} \text{tr} \left( \left( I - \frac{1}{2} B^{1/2} H^{*-1} B^{1/2} \right)^{-1} B^{-1/2} \Sigma_g(\theta^*) B^{-1/2} \right). \end{aligned} \tag{41}$$

To compute  $\text{tr}(H^* C_2)$ , we observe that

$$C_2 = -(\Xi_{B^{-1}H^*} - 2I)^{-1} (B^{-1} \Sigma_g(\theta^*) B^{-1}) = -\frac{1}{2} \left( \Xi_{B^{-1}\frac{1}{2}H^*} - I \right)^{-1} (B^{-1} \Sigma_g(\theta^*) B^{-1}),$$

and so we may adapt our previous analysis with  $H^*$  replaced by  $\frac{1}{2}H^*$ , which yields

$$\text{tr}(H^* C_2) = -\frac{1}{4} \text{tr} \left( \left( I - \frac{1}{4} B^{1/2} H^{*-1} B^{1/2} \right)^{-1} B^{-1/2} \Sigma_g(\theta^*) B^{-1/2} \right). \tag{42}$$

It remains to compute/bound the term  $\text{tr}(H^*(\mathbb{E}[\theta_k] - \theta^*)(\mathbb{E}[\theta_k] - \theta^*)^\top)$ . From Theorem 1 we have

$$\mathbb{E}[\theta_k] - \theta^* = \prod_{j=0}^{k-1} (I - \alpha_j B^{-1} H^*) (\theta_0 - \theta^*).$$

Observing

$$H^{*1/2}(I - \alpha_i B^{-1} H^*) = (I - \alpha_i H^{*1/2} B^{-1} H^{*1/2}) H^{*1/2}$$

it follows that

$$\begin{aligned} H^{*1/2}(\mathbb{E}[\theta_k] - \theta^*) &= H^{*1/2} \prod_{j=0}^{k-1} (I - \alpha_j B^{-1} H^*) (\theta_0 - \theta^*) \\ &= \prod_{j=0}^{k-1} \left( I - \alpha_j H^{*1/2} B^{-1} H^{*1/2} \right) H^{*1/2} (\theta_0 - \theta^*) \\ &= \psi_k \left( H^{*1/2} B^{-1} H^{*1/2} \right) H^{*1/2} (\theta_0 - \theta^*), \end{aligned}$$

where  $\psi_k$  is a polynomial defined by

$$\psi_k(x) = \prod_{j=0}^{k-1} (1 - \alpha_j x) = \prod_{j=0}^{k-1} \left(1 - \frac{x}{j+1}\right).$$

As argued by Murata (1998) (in the discussion after their Theorem 4), we have  $\psi_k(x) = \mathcal{O}(1/k^x)$ . Then recalling the fact that the eigenvalues of  $\psi_k(X)$  for any matrix  $X$  are given by  $\{\psi_k(\lambda_i(X))\}_i$ , it follows that

$$\lambda_1 \left( \psi_k \left( H^{*1/2} B^{-1} H^{*1/2} \right) \right) = \mathcal{O} \left( \frac{1}{k^{\lambda_n(B^{-1} H^*)}} \right).$$

Thus we have by Lemma 9 that

$$\begin{aligned} \frac{1}{2} \operatorname{tr} \left( H^* (\mathbb{E}[\theta_k] - \theta^*) (\mathbb{E}[\theta_k] - \theta^*)^\top \right) &= \frac{1}{2} \operatorname{tr} \left( H^{*1/2} (\mathbb{E}[\theta_k] - \theta^*) (\mathbb{E}[\theta_k] - \theta^*)^\top H^{*1/2} \right) \\ &= \frac{1}{2} \operatorname{tr} \left( \psi_k \left( H^{*1/2} B^{-1} H^{*1/2} \right)^2 \left( H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} \right) \right) \\ &\leq \lambda_1 \left( \psi_k \left( H^{*1/2} B^{-1} H^{*1/2} \right) \right)^2 \frac{1}{2} \operatorname{tr} \left( H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} \right) \\ &= \mathcal{O} \left( \frac{1}{k^{\lambda_n(B^{-1} H^*)}} \right)^2 h(\theta_0) = \mathcal{O} \left( \frac{h(\theta_0)}{k^{2\lambda_n(B^{-1} H^*)}} \right). \end{aligned}$$

Combining eqn. 36, eqn. 37, eqn. 41, eqn. 42 and the above asymptotic expression we thus have

$$\begin{aligned} \mathbb{E}[h(\theta_k)] - h(\theta^*) &= \frac{1}{4k} \operatorname{tr} \left( \left( I - \frac{1}{2} B^{1/2} H^{*-1} B^{1/2} \right)^{-1} B^{-1/2} \Sigma_g(\theta^*) B^{-1/2} \right) \\ &\quad - \frac{1}{8k^2} \operatorname{tr} \left( \left( I - \frac{1}{4} B^{1/2} H^{*-1} B^{1/2} \right)^{-1} B^{-1/2} \Sigma_g(\theta^*) B^{-1/2} \right) + \mathcal{O} \left( \frac{h(\theta_0)}{k^{2\lambda_n(B^{-1} H^*)}} \right) + \mathcal{O} \left( \frac{1}{k^3} \right). \end{aligned}$$

### Appendix C. Derivations of bounds for Section 12.2.1

By Lemma 9

$$\operatorname{tr} \left( H^{*-1} \Sigma_g(\theta^*) \right) \geq \lambda_n \left( H^{*-1} \right) \operatorname{tr}(\Sigma_g(\theta^*)) = \frac{1}{\lambda_1(H^*)} \operatorname{tr}(\Sigma_g(\theta^*))$$

and

$$\operatorname{tr} \left( H^{*-1} \Sigma_g(\theta^*) \right) \leq \lambda_1 \left( H^{*-1} \right) \operatorname{tr}(\Sigma_g(\theta^*)) = \frac{1}{\lambda_n(H^*)} \operatorname{tr}(\Sigma_g(\theta^*)),$$

so that

$$\frac{1}{2k\lambda_1(H^*)} \operatorname{tr}(\Sigma_g(\theta^*)) \leq \frac{1}{2k} \operatorname{tr} \left( H^{*-1} \Sigma_g(\theta^*) \right) \leq \frac{1}{2k\lambda_n(H^*)} \operatorname{tr}(\Sigma_g(\theta^*)).$$

Meanwhile, by Lemma 9

$$\begin{aligned}
\text{tr} \left( \left( I - \frac{\lambda_n(H^*)}{2} H^{*-1} \right)^{-1} \Sigma_g(\theta^*) \right) &\geq \lambda_n \left( \left( I - \frac{\lambda_n(H^*)}{2} H^{*-1} \right)^{-1} \right) \text{tr}(\Sigma_g(\theta^*)) \\
&= \frac{1}{\lambda_1 \left( I - \frac{\lambda_n(H^*)}{2} H^{*-1} \right)} \text{tr}(\Sigma_g(\theta^*)) \\
&= \frac{1}{1 - \frac{\lambda_n(H^*)}{2} \lambda_n(H^{*-1})} \text{tr}(\Sigma_g(\theta^*)) \\
&= \frac{1}{1 - \frac{1}{2\kappa(H^*)}} \text{tr}(\Sigma_g(\theta^*)) \geq \text{tr}(\Sigma_g(\theta^*)),
\end{aligned}$$

where  $\kappa(H^*) = \lambda_1(H^*)/\lambda_n(H^*)$  is the condition number of  $H^*$ . Similarly, by Lemma 9 we have

$$\begin{aligned}
\text{tr} \left( \left( I - \frac{\lambda_n(H^*)}{2} H^{*-1} \right)^{-1} \Sigma_g(\theta^*) \right) &\leq \lambda_1 \left( \left( I - \frac{\lambda_n(H^*)}{2} H^{*-1} \right)^{-1} \right) \text{tr}(\Sigma_g(\theta^*)) \\
&= \frac{1}{\lambda_n \left( I - \frac{\lambda_n(H^*)}{2} H^{*-1} \right)} \text{tr}(\Sigma_g(\theta^*)) \\
&= \frac{1}{1 - \frac{\lambda_n(H^*)}{2} \lambda_1(H^{*-1})} \text{tr}(\Sigma_g(\theta^*)) \\
&= \frac{1}{1 - \frac{\lambda_n(H^*)}{2\lambda_n(H^*)}} \text{tr}(\Sigma_g(\theta^*)) = 2 \text{tr}(\Sigma_g(\theta^*)),
\end{aligned}$$

and thus

$$\frac{1}{4k\lambda_n(H^*)} \text{tr}(\Sigma_g(\theta^*)) \leq \frac{1}{4k\lambda_n(H^*)} \text{tr} \left( \left( I - \frac{\lambda_n(H^*)}{2} H^{*-1} \right)^{-1} \Sigma_g(\theta^*) \right) \leq \frac{1}{2k\lambda_n(H^*)} \text{tr}(\Sigma_g(\theta^*)).$$

## Appendix D. Proof of Theorem 6

To begin, we observe that analogously to eqn. 16 we have

$$\mathbb{E}[h(\bar{\theta}_k)] - h(\theta^*) = \frac{1}{2} \text{tr} (H^* \bar{V}_k) + \frac{1}{2} \text{tr} \left( H^* (\mathbb{E}[\bar{\theta}_k] - \theta^*) (\mathbb{E}[\bar{\theta}_k] - \theta^*)^\top \right), \quad (43)$$

where

$$\bar{V}_k = \text{var}(\bar{\theta}_k) = \text{cov}(\bar{\theta}_k, \bar{\theta}_k) = \mathbb{E} \left[ (\bar{\theta}_k - \mathbb{E}[\bar{\theta}_k]) (\bar{\theta}_k - \mathbb{E}[\bar{\theta}_k])^\top \right].$$

Our first major task is to find an expression for  $\bar{V}_k$  in order to bound the term  $\frac{1}{2} \text{tr} (H^* \bar{V}_k)$ . To this end we observe that

$$\bar{V}_k = \frac{1}{(k+1)^2} \sum_{i=0}^k \sum_{j=0}^k \text{cov}(\theta_i, \theta_j).$$

For  $j > i$  we have

$$\text{cov}(\theta_i, \theta_j) = \text{cov}(\theta_i, \theta_{j-1} - \alpha B^{-1} g_{j-1}(\theta_{j-1})) = \text{cov}(\theta_i, \theta_{j-1}) - \alpha \text{cov}(\theta_i, g_{j-1}(\theta_{j-1})) B^{-1},$$

where

$$\begin{aligned} \text{cov}(\theta_i, g_{j-1}(\theta_{j-1})) &= \mathbb{E} \left[ (\theta_i - \mathbb{E}[\theta_i])(g_{j-1}(\theta_{j-1}) - \mathbb{E}[g_{j-1}(\theta_{j-1})])^\top \right] \\ &= \mathbb{E}_{\theta_i, \theta_{j-1}} \left[ \mathbb{E}_{g_{j-1}(\theta_{j-1}) | \theta_{j-1}} \left[ (\theta_i - \mathbb{E}[\theta_i])(g_{j-1}(\theta_{j-1}) - \mathbb{E}[g_{j-1}(\theta_{j-1})])^\top \right] \right] \\ &= \mathbb{E}_{\theta_i, \theta_{j-1}} \left[ (\theta_i - \mathbb{E}[\theta_i])(\nabla h(\theta_{j-1}) - \mathbb{E}[g_{j-1}(\theta_{j-1})])^\top \right] \\ &= \mathbb{E} \left[ (\theta_i - \mathbb{E}[\theta_i])(\nabla h(\theta_{j-1}) - \mathbb{E}[g_{j-1}(\theta_{j-1})])^\top \right]. \end{aligned}$$

Here we have used the fact that  $g_{j-1}(\theta_{j-1})$  is conditionally independent of  $\theta_i$  given  $\theta_{j-1}$  for  $j-1 \geq i$  (which allows us to take the conditional expectation over  $g_{j-1}(\theta_{j-1})$  inside), and is an unbiased estimator of  $\nabla h(\theta_{j-1})$ .

Then noting that  $\mathbb{E}[g_{j-1}(\theta_{j-1})] = \mathbb{E}[\nabla h(\theta_{j-1})] = \mathbb{E}[H^*(\theta_{j-1} - \theta^*)] = H^*(\mathbb{E}[\theta_{j-1}] - \theta^*)$ , we have

$$\begin{aligned} \nabla h(\theta_{j-1}) - \mathbb{E}[g_{j-1}(\theta_{j-1})] &= H^*(\theta_{j-1} - \theta^*) - H^*(\mathbb{E}[\theta_{j-1}] - \theta^*) \\ &= H^*(\theta_{j-1} - \mathbb{E}[\theta_{j-1}]) \end{aligned}$$

so that

$$\begin{aligned} \text{cov}(\theta_i, g_{j-1}(\theta_{j-1})) &= \mathbb{E} \left[ (\theta_i - \mathbb{E}[\theta_i])(\nabla h(\theta_{j-1}) - \mathbb{E}[g_{j-1}(\theta_{j-1})])^\top \right] \\ &= \mathbb{E} \left[ (\theta_i - \mathbb{E}[\theta_i])(H^*(\theta_{j-1} - \mathbb{E}[\theta_{j-1}]))^\top \right] \\ &= \mathbb{E} \left[ (\theta_i - \mathbb{E}[\theta_i])(\theta_{j-1} - \mathbb{E}[\theta_{j-1}])^\top \right] H^* = \text{cov}(\theta_i, \theta_{j-1}) H^*. \end{aligned}$$

From this we conclude that

$$\begin{aligned} \text{cov}(\theta_i, \theta_j) &= \text{cov}(\theta_i, \theta_{j-1}) - \alpha \text{cov}(\theta_i, g_{j-1}(\theta_{j-1})) B^{-1} \\ &= \text{cov}(\theta_i, \theta_{j-1}) - \alpha \text{cov}(\theta_i, \theta_{j-1}) H^* B^{-1} \\ &= \text{cov}(\theta_i, \theta_{j-1}) (I - \alpha B^{-1} H^*)^\top. \end{aligned}$$

Applying this recursively we have that for  $j \geq i$

$$\text{cov}(\theta_i, \theta_j) = V_i (I - \alpha B^{-1} H^*)^{j-i\top}. \quad (44)$$

Taking transposes and switching the roles of  $i$  and  $j$  we similarly have for  $i \geq j$

$$\text{cov}(\theta_i, \theta_j) = (I - \alpha B^{-1} H^*)^{i-j} V_j.$$

Thus we have the following expression for the variance  $\bar{V}_k$  of the averaged parameter  $\bar{\theta}_k$ :

$$\begin{aligned} \bar{V}_k &= \frac{1}{(k+1)^2} \sum_{i=0}^k \sum_{j=0}^k \text{cov}(\theta_i, \theta_j) \\ &= \frac{1}{(k+1)^2} \sum_{i=0}^k \left( \sum_{j=0}^i (I - \alpha B^{-1} H^*)^{i-j} V_j + \sum_{j=i+1}^k V_i (I - \alpha B^{-1} H^*)^{j-i\top} \right), \end{aligned}$$

which by reordering the sums and re-indexing can be written as

$$\bar{V}_k = \frac{1}{(k+1)^2} \sum_{i=0}^k \left( \sum_{j=0}^{k-i} (I - \alpha B^{-1} H^*)^j V_i + \sum_{j=1}^{k-i} V_i (I - \alpha B^{-1} H^*)^{j^\top} \right).$$

Having computed  $\bar{V}_k$  we now deal with the term  $\frac{1}{2} \text{tr} (H^* \bar{V}_k)$ . Observing that

$$H^{*1/2} (I - \alpha B^{-1} H^*) = \left( I - \alpha H^{*1/2} B^{-1} H^{*1/2} \right) H^{*1/2} = (I - C) H^{*1/2},$$

where  $C = \alpha H^{*1/2} B^{-1} H^{*1/2}$  (as it is defined in Subsection 12), we have

$$H^{*1/2} \bar{V}_k H^{*1/2} = \frac{1}{(k+1)^2} \sum_{i=0}^k \left( \sum_{j=0}^{k-i} (I - C)^j (H^{*1/2} V_i H^{*1/2}) + \sum_{j=1}^{k-i} (H^{*1/2} V_i H^{*1/2}) (I - C)^j \right).$$

It thus follows that

$$\frac{1}{2} \text{tr} (H^* \bar{V}_k) = \frac{1}{2} \text{tr} (H^{*1/2} \bar{V}_k H^{*1/2}) = \frac{1}{2(k+1)^2} \sum_{i=0}^k \text{tr} \left( \left( I + 2 \sum_{j=1}^{k-i} (I - C)^j \right) H^{*1/2} V_i H^{*1/2} \right).$$

Recall that from eqn. 23 we have

$$H^{*1/2} V_i H^{*1/2} = \left( I - (I - \Xi_C)^i \right) \left( H^{*1/2} V_\infty H^{*1/2} \right) + (I - \Xi_C)^i \left( H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} \right).$$

Plugging this into the previous equation and exploiting linearity gives

$$\begin{aligned} \frac{1}{2} \text{tr} (H^* \bar{V}_k) &= \frac{1}{2(k+1)^2} \text{tr} \left( \sum_{i=0}^k \left( I + 2 \sum_{j=1}^{k-i} (I - C)^j \right) \left( I - (I - \Xi_C)^i \right) \left( H^{*1/2} V_\infty H^{*1/2} \right) \right) \\ &\quad + \frac{1}{2(k+1)^2} \text{tr} \left( \sum_{i=0}^k \left( I + 2 \sum_{j=1}^{k-i} (I - C)^j \right) (I - \Xi_C)^i \left( H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} \right) \right). \end{aligned}$$

Then applying eqn. 25 to this we obtain

$$\begin{aligned} \frac{1}{2} \text{tr} (H^* \bar{V}_k) &= \frac{1}{2(k+1)^2} \text{tr} \left( \sum_{i=0}^k \left( I + 2 \sum_{j=1}^{k-i} (I - C)^j \right) \left( I - (I - 2C)^i \right) H^{*1/2} V_\infty H^{*1/2} \right) \\ &\quad + \frac{1}{2(k+1)^2} \text{tr} \left( \sum_{i=0}^k \left( I + 2 \sum_{j=1}^{k-i} (I - C)^j \right) (I - 2C)^i H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} \right). \end{aligned} \tag{45}$$

Because  $C$  and  $I - 2C$  are PSD (which follows from the hypothesis  $2\alpha\lambda_1(B^{-1}H^*) < 1$ ), as are  $I - C$ ,  $I - (I - 2C) = 2C$  and  $I - (I - C) = C$  by consequence, we have the following



basic matrix inequalities

$$I + 2 \sum_{j=1}^{k-i} (I - C)^j \preceq 2 \sum_{j=0}^{\infty} (I - C)^j = 2C^{-1} \quad (46)$$

$$I + 2 \sum_{j=1}^{k-i} (I - C)^j \preceq 2(k+1)I \quad (47)$$

$$\sum_{i=0}^k (I - 2C)^i \preceq \sum_{i=0}^{\infty} (I - 2C)^i = \frac{1}{2}C^{-1} \quad (48)$$

$$\sum_{i=0}^k (I - 2C)^i \preceq (k+1)I \quad (49)$$

$$\sum_{i=0}^k \left( I - (I - 2C)^i \right) \preceq (k+1)I, \quad (50)$$

where  $X \preceq Y$  means that  $Y - X$  is PSD.

To exploit these inequalities we will make use of the following lemma

**Lemma 11** *If  $A$ ,  $S$ ,  $T$ , and  $X$  are matrices such that  $A$ ,  $S$  and  $T$  commute with each other,  $S \preceq T$ , and  $A$  and  $X$  are PSD, then we have*

$$\text{tr}(ASX) \leq \text{tr}(ATX).$$

**Proof** Since  $A$ ,  $S$  and  $T$  are commuting PSD matrices they have the same eigenvectors, as does  $A^{1/2}$  (which thus also commutes).

Meanwhile,  $S \preceq T$  means that  $T - S$  is PSD, and thus so is  $A^{1/2}(T - S)A^{1/2}$ . Because the trace of the product of two PSD matrices is non-negative (e.g. by Lemma 9), it follows that  $\text{tr}((A^{1/2}(T - S)A^{1/2})X) \geq 0$ . Adding  $\text{tr}(A^{1/2}SA^{1/2}X)$  to both sides of this we get  $\text{tr}(A^{1/2}TA^{1/2}X) \geq \text{tr}(A^{1/2}SA^{1/2}X)$ . Because  $A^{1/2}$  commutes with  $T$  and  $S$  we have  $\text{tr}(A^{1/2}TA^{1/2}X) = \text{tr}(ATX)$  and  $\text{tr}(A^{1/2}SA^{1/2}X) = \text{tr}(ASX)$ , and so the result follows. ■

As the right and left side of all the previously stated matrix inequalities are commuting matrices (because they all share their eigenvectors with  $C$ ), we can apply this lemma to eqn. 45 to obtain various simplifying upper bounds on  $\frac{1}{2} \text{tr}(H^* \bar{V}_k)$ .

For the first term on the RHS of eqn. 45 we can apply Lemma 11 using eqn. 46 and then eqn. 50, which gives an upper bound on this term of

$$\frac{1}{2(k+1)^2} \text{tr} \left( 2C^{-1} (k+1)I H^{*1/2} V_{\infty} H^{*1/2} \right) = \frac{1}{k+1} \text{tr} \left( C^{-1} H^{*1/2} V_{\infty} H^{*1/2} \right) = \frac{1}{(k+1)\alpha} \text{tr}(BV_{\infty}).$$

Or we can apply the lemma using eqn. 47 and then eqn. 50, which gives a different upper bound of

$$\frac{1}{2(k+1)^2} \text{tr} \left( 2(k+1)I (k+1)I H^{*1/2} V_{\infty} H^{*1/2} \right) = \text{tr}(H^* V_{\infty}).$$

For the second term we can apply Lemma 11 using eqn. 46 and then eqn. 48, which gives an upper bound on this term of

$$\frac{1}{2(k+1)^2} \operatorname{tr} \left( 2C^{-1} \frac{1}{2} C^{-1} H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} \right) = \frac{1}{2(k+1)^2 \alpha^2} \left\| H^{*-1/2} B (\theta_0 - \theta^*) \right\|^2.$$

Or we can apply the lemma using eqn. 47 and then eqn. 48, which gives a different upper bound of

$$\frac{1}{2(k+1)^2} \operatorname{tr} \left( 2(k+1)I \frac{1}{2} C^{-1} H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} \right) = \frac{1}{2(k+1)\alpha} \left\| B^{1/2} (\theta_0 - \theta^*) \right\|^2.$$

Or finally, we can apply the lemma using eqn. 47 and then eqn. 49, which gives a third upper bound of

$$\frac{1}{2(k+1)^2} \operatorname{tr} \left( 2(k+1)I (k+1)I H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} \right) = 2h(\theta_0).$$

Applying these bounds to eqn. 45 yields

$$\begin{aligned} \frac{1}{2} \operatorname{tr} (H^* \bar{V}_k) \leq & \min \left\{ \frac{1}{(k+1)\alpha} \operatorname{tr} (BV_\infty), \operatorname{tr} (H^* V_\infty) \right\} \\ & + \min \left\{ \frac{1}{2(k+1)^2 \alpha^2} \left\| H^{*-1/2} B (\theta_0 - \theta^*) \right\|^2, \frac{1}{2(k+1)\alpha} \left\| B^{1/2} (\theta_0 - \theta^*) \right\|^2, 2h(\theta_0) \right\}. \end{aligned} \quad (51)$$

To compute  $\operatorname{tr} (BV_\infty)$ , we have from eqn. 32 that

$$B^{-1} H^* V_\infty + V_\infty H^* B^{-1} = \alpha B^{-1} \Sigma_g(\theta^*) B^{-1}.$$

Left multiplying both sides by  $H^{*-1}B$  and right multiplying both sides by  $BH^{*-1}$  gives

$$V_\infty B H^{*-1} + H^{*-1} B V_\infty = \alpha H^{*-1} \Sigma_g(\theta^*) H^{*-1},$$

which after simple rearrangement can be written as a pseudo-CALE  $A^\top P + P A + Q = 0$  with

$$\begin{aligned} A &= -BV_\infty \\ P &= H^{*-1} \\ Q &= \alpha H^{*-1} \Sigma_g(\theta^*) H^{*-1}. \end{aligned} \quad (52)$$

Thus applying Lemma 10 we get that

$$\operatorname{tr} (BV_\infty) = \operatorname{tr} (-A) = \frac{1}{2} \operatorname{tr} (P^{-1}Q) = \frac{1}{2} \operatorname{tr} \left( (H^{*-1})^{-1} \alpha H^{*-1} \Sigma_g(\theta^*) H^{*-1} \right) = \alpha \operatorname{tr} \left( H^{*-1} \Sigma_g(\theta^*) \right). \quad (53)$$

It remains to bound the term  $\frac{1}{2} \text{tr} (H^* (\mathbb{E}[\bar{\theta}_k] - \theta^*) (\mathbb{E}[\bar{\theta}_k] - \theta^*)^\top)$ . First we observe that by Theorem 1

$$\mathbb{E}[\bar{\theta}_k] - \theta^* = \frac{1}{k+1} \sum_{i=0}^k (\mathbb{E}[\theta_i] - \theta^*) = \frac{1}{k+1} \sum_{i=0}^k (I - \alpha B^{-1} H^*)^i (\theta_0 - \theta^*).$$

Applying eqn. 28 then gives

$$H^{*1/2} (\mathbb{E}[\bar{\theta}_k] - \theta^*) = \frac{1}{k+1} \sum_{i=0}^k (I - C)^i H^{*1/2} (\theta_0 - \theta^*).$$

And thus we have

$$\begin{aligned} \frac{1}{2} \text{tr} (H^* (\mathbb{E}[\bar{\theta}_k] - \theta^*) (\mathbb{E}[\bar{\theta}_k] - \theta^*)^\top) &= \frac{1}{2} \text{tr} (H^{*1/2} (\mathbb{E}[\bar{\theta}_k] - \theta^*) (\mathbb{E}[\bar{\theta}_k] - \theta^*)^\top H^{*1/2}) \\ &= \frac{1}{2(k+1)^2} \text{tr} \left( \left( \sum_{i=0}^k (I - C)^i \right) H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} \left( \sum_{i=0}^k (I - C)^i \right) \right) \end{aligned} \quad (54)$$

Similarly to eqn. 46-50 we have the following matrix inequalities

$$\sum_{i=0}^k (I - C)^i \preceq \sum_{i=0}^{\infty} (I - C)^i = C^{-1} \quad (55)$$

$$\sum_{i=0}^k (I - C)^i \preceq (k+1)I. \quad (56)$$

Applying Lemma 11 using eqn. 55 twice we obtain an upper bound on the RHS of eqn. 54 of

$$\frac{1}{2(k+1)^2} \text{tr} (C^{-1} H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} C^{-1}) = \frac{1}{2(k+1)^2 \alpha^2} \|H^{*-1/2} B (\theta_0 - \theta^*)\|^2.$$

Applying the lemma using eqn. 55 and eqn. 56 gives a different upper bound of

$$\frac{1}{2(k+1)^2} \text{tr} (C^{-1} H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} (k+1)I) = \frac{1}{2(k+1)\alpha} \|B^{1/2} (\theta_0 - \theta^*)\|^2.$$

And finally, applying the lemma using eqn. 56 twice gives an upper bound of

$$\frac{1}{2(k+1)^2} \text{tr} ((k+1)I H^{*1/2} (\theta_0 - \theta^*) (\theta_0 - \theta^*)^\top H^{*1/2} (k+1)I) = h(\theta_0).$$

Combining these various upper bounds gives us

$$\begin{aligned} &\frac{1}{2} \text{tr} (H^* (\mathbb{E}[\bar{\theta}_k] - \theta^*) (\mathbb{E}[\bar{\theta}_k] - \theta^*)^\top) \\ &\leq \min \left\{ \frac{1}{2(k+1)^2 \alpha^2} \|H^{*-1/2} B (\theta_0 - \theta^*)\|^2, \frac{1}{2(k+1)\alpha} \|B^{1/2} (\theta_0 - \theta^*)\|^2, h(\theta_0) \right\}. \end{aligned} \quad (57)$$

Theorem 6 now follows from eqn. 43, eqn. 51, eqn. 57, eqn. 53 and eqn. 35.