New Insights and Perspectives on the Natural Gradient Method

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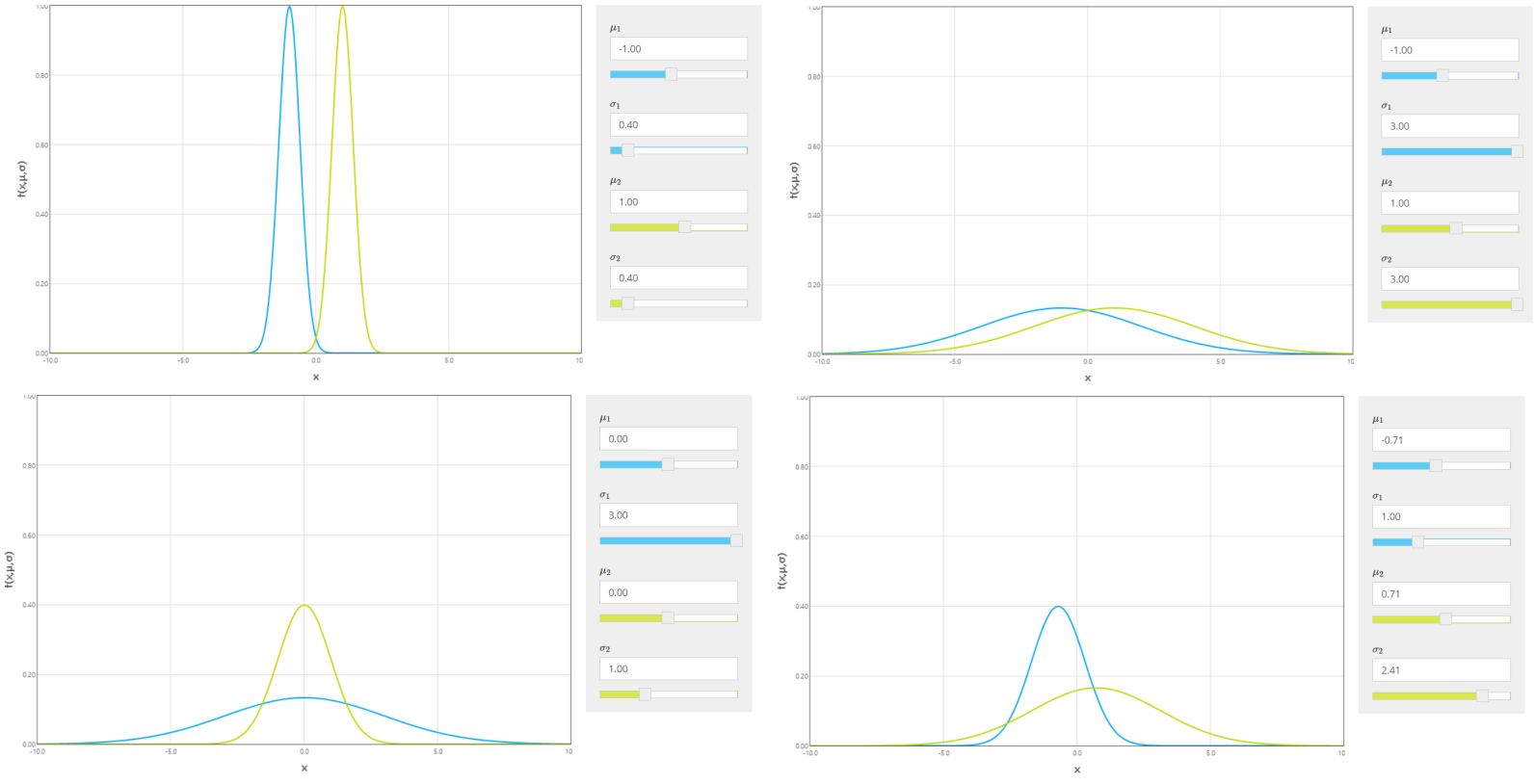
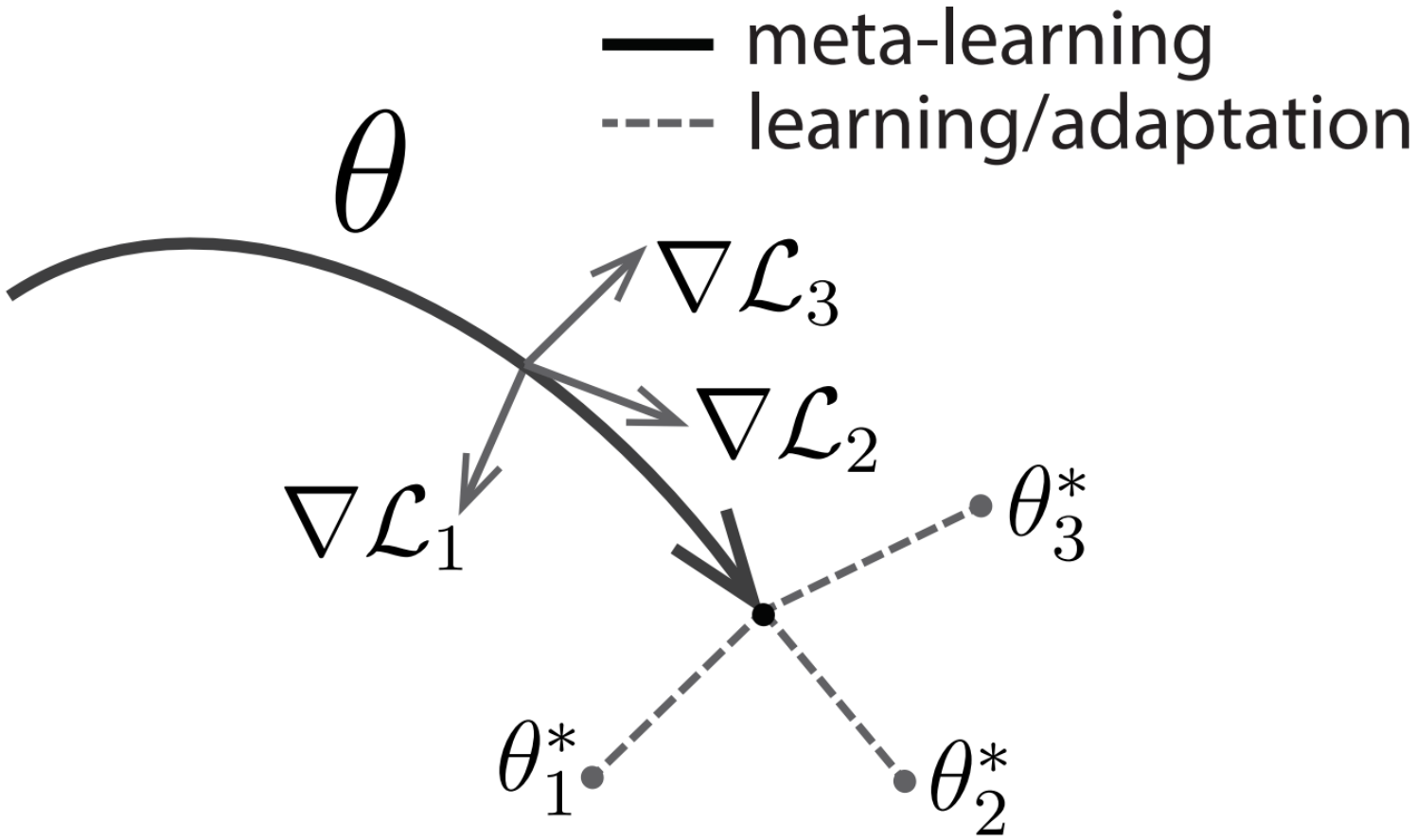
Motivation



In parameter space (μ, σ), each pair of distributions have the same distance.

Motivation



We often talk about the **parameter space** of a neural network, instead of the **functions** that those parameters represent.

Gradient Descent

The gradient descent update

$$\Delta\theta = -\alpha \nabla_\theta \mathcal{L}$$

is the solution to the following optimization problem:

$$\arg\min_{\Delta\theta} [\nabla_\theta \mathcal{L}(\theta) \cdot \Delta\theta]$$
$$s.t. \|\Delta\theta\| \leq \delta.$$

We are optimizing a linear approximation of $\mathcal{L}$ within a trust region defined by the Euclidean metric in parameter space.

Natural Gradient

Consider a family of density functions $\mathcal{F} : \theta \to p(\mathbf{z})$ where $\theta \in \mathbb{R}^n$:

$$p_\theta(\mathbf{z}) := \mathcal{F}(\theta)(\mathbf{z}).$$

We naturally obtain a notion of closeness among different values of θ:

$$d(\theta_1, \theta_2) := KL(p_{\theta_1}(\mathbf{z}) || p_{\theta_2}(\mathbf{z})).$$

Natural Gradient

$$d(\theta_1, \theta_2) := KL(p_{\theta_1}(\mathbf{z}) || p_{\theta_2}(\mathbf{z})).$$

Let's see how d behaves near a given θ.

$$\begin{aligned} KL(p_\theta(\mathbf{z}) || p_{\theta+\Delta\theta}(\mathbf{z})) &= \mathbb{E}_{\mathbf{z}}\left[\log p_\theta\right] - \mathbb{E}_{\mathbf{z}}\left[\log p_\theta\right] \\ &\quad -\mathbb{E}_{\mathbf{z}}\left[\nabla \log p_\theta\right] \Delta\theta + O(\Delta\theta^2) \\ &= O(\Delta\theta^2), \end{aligned}$$

so no useful information from first order approximation.

Natural Gradient

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Let's see how d behaves near a given θ.

$$\begin{aligned} KL(p_\theta(\mathbf{z}) || p_{\theta+\Delta\theta}(\mathbf{z})) &= -\frac{1}{2}\Delta\theta^\top \mathbb{E}_{\mathbf{z}}\left[\nabla^2 \log p_\theta\right]\Delta\theta + O(\Delta\theta^3) \\ &\approx \frac{1}{2}\Delta\theta^\top F_\theta \Delta\theta, \end{aligned}$$

where

$$F_\theta = \mathbb{E}_{\mathbf{z}}\left[-\nabla^2 \log p_\theta\right] = \mathbb{E}_{\mathbf{z}}\left[\nabla \log p_\theta \nabla \log p_\theta^\top\right].$$

The Fisher Information Matrix is the expected negative Hessian of $\log p$.

Natural Gradient

We change the constraint of

$$\arg\min_{\Delta\theta} [\nabla_\theta \mathcal{L}(\theta) \cdot \Delta\theta]$$
$$s.t.\ \|\Delta\theta\| = const$$

to

$$s.t. KL(p_\theta(\mathbf{z}) || p_{\theta+\Delta\theta}(\mathbf{z})) = const.$$

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Solution after using Lagrange multiplier

$$\nabla_\theta \mathcal{L}(\theta) \cdot \Delta\theta + \frac{1}{2}\lambda \Delta\theta^\top F_\theta \Delta\theta$$

is

$$\Delta\theta \propto F_\theta^{-1} \nabla_\theta \mathcal{L}$$

Natural Gradient

For η defined as

$$\eta - \eta_0 = F^{\frac{1}{2}}(\theta - \theta_0),$$

the Fisher ball is a unit circle. Thus in the parameter space of η, the natural gradient is the same as the gradient.

Second-order Optimization

$$\Delta\theta = \arg\min_{\delta} M(\delta), \qquad M(\delta) := \frac{1}{2}\delta^\top B\delta + \nabla h(\theta)^\top \delta + h(\theta)$$

The solution is $\Delta\theta = -B^{-1}\nabla h$.

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- $B = \beta\mathcal{I}$: Gradient Descent.
- $B = H(\theta)$: Newton's Method.

Newton's method assumes h is convex, and fails otherwise.

Second-order Optimization

The Generalized Gauss-Newton Matrix

Let our loss function be $L(f(x,\theta))$.

$$
\begin{aligned}
H_{ij} &= \frac{\partial}{\partial\theta_j}\frac{\partial L(f(x,\theta))}{\partial\theta_i} \\
&= \sum_{k=0}^{n}\frac{\partial}{\partial\theta_j}\left(\frac{\partial L\left(f(x,\theta)\right)}{\partial f_k(x,\theta)}\frac{\partial f_k(x,\theta)}{\partial\theta_i}\right) \\
&= \sum_{k=0}^{n}\left(\sum_{l=0}^{n}\frac{\partial L^2\left(f(x,\theta)\right)}{\partial f_k(x,\theta)\partial f_l(x,\theta)}\frac{\partial f_k(x,\theta)}{\partial\theta_j}\right)\frac{\partial f_k(x,\theta)}{\partial\theta_i} \\
&+ \sum_{k=0}^{n}\frac{\partial L\left(f(x,\theta)\right)}{\partial f_k(x,\theta)}\frac{\partial f_k(x,\theta)^2}{\partial\theta_j\partial\theta_i} \\
\therefore H &= J_f^\top H_L J_f + \sum_{k=0}^{n}\frac{\partial L}{\partial f_k}H_{f_k} \approx J_f^\top H_L J_f = G
\end{aligned}
$$

Second-order Optimization

Why G instead of H

- G is positive semidefinite, H is not.
- Let's expand H further, assuming f is a feedforward neural network:

$$\cdots \xrightarrow{W_i} s_i \xrightarrow{\phi} a_i \xrightarrow{W_{i+1}} s_{i+1} \cdots$$

$$H - G = \sum_{i=1}^{l} \sum_{j=1}^{m_i} (\nabla a_i L)\, J_{s_i}^{\top} H_{[\phi(s_i)]_j} J_{s_i}$$

  The remaining term is the sum of curvature terms coming from each intermediate activation. These curvature terms are subject to more frequent change.
- In ReLU networks, $H_{[\phi(s_i)]} = 0$ a.e..

F and G

Define the conditional distribution r to be

$$r(y|z) = r(y|f(x,\theta))$$

We have

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

$$\begin{aligned} F &= \mathbb{E}_x \left[\nabla \log p(y; x, \theta) \nabla \log p(y; x, \theta)^\top \right] \\ &= \mathbb{E}_x \left[J_f^\top \nabla_z \log r(y|z) \nabla_z \log r(y|z)^\top J_f \right] \\ &= \mathbb{E}_x \left[J_f^\top F_R J_f \right] \\ G &= \mathbb{E}_x \left[J_f^\top H_L J_f \right] \end{aligned}$$

$\therefore F = G$ when $F_R = H_L$.

F and G

We know that $F = G$ when $F_R = H_L$. When does this occur?
Let $L(y, z) = -\log r(y|z)$.

$$\begin{aligned} F_R &= -\mathbb{E}_{R_{y|f(x,\theta)}}\left[H_{\log r}\right] \\ H_L &= -\mathbb{E}_{(x,y)}\left[H_{\log r}\right] \end{aligned}$$

$\therefore F_R = H_L$ holds when $\mathbb{E}_{R_{y|f(x,\theta)}}\left[H_{\log r}\right] = \mathbb{E}_{(x,y)}\left[H_{\log r}\right]$

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This holds when $r(y|z)$ is an exponential family:

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

since in this case, the hessian $H_{\log r}$ does not depend on y.
Most commonly-used losses satisfy this property, including the MSE loss and cross-entropy loss.

Summary

- Roughly speaking, the natural gradient is the direction of steepest change of loss in function space.
- The natural gradient is invariant under reparameterization.
- For most neural networks of interest, natural gradient descent is identical to a second-order method (GGN).

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Thank You