Natural gradient descent with momentum

Séminaire d'Analyse Numérique et Calcul Scientifique
Besançon, 2025

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Outline

1. **What is natural gradient and why we may need it?**
   - Problem setting
   - From gradient descent to Newton's method.
   - From Newton's method to natural gradient.
   - Toy examples to gain intuition.
2. **What is momentum and when we may need it?**
3. **How to combine momentum and natural gradient.**
   - Two toy examples
   - Three less toy examples

Problem formulation

Objective: approximate target function $u \in V$ by $v \in \mathcal{M} \subset V$

Target function $\quad u : \mathbb{R}^d \to \mathbb{R} \in V$

Hilbert space
$L^2(\Omega), H^1(\Omega), \ldots$

Problem formulation

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Target function $\quad u : \mathbb{R}^d \to \mathbb{R} \in V$

Hilbert space $L^2(\Omega), H^1(\Omega), \ldots$

Approximation manifold $\quad \mathcal{M} := \{v_\theta(x) = A(\theta)(x);\ \theta \in \mathbb{R}^p\}$

Linear model

$$A(\theta)(x) = \theta_1 \phi_1(x) + \cdots + \theta_p \phi_p(x)$$
$$= \theta^T \mathbf{\Phi}(x)$$

Problem formulation

Objective: approximate target function $u \in V$ by $v \in \mathcal{M} \subset V$

Target function	$u : \mathbb{R}^d \to \mathbb{R} \in V$	Hilbert space $L^2(\Omega), H^1(\Omega), \ldots$
Approximation manifold	$\mathcal{M} := \{v_\theta(x) = A(\theta)(x);\ \theta \in \mathbb{R}^p\}$	Linear model, Neural network, ...

Minimization problem

Objective: approximate $u \in V$ by $v \in \mathcal{M}$.

Continuous problem

$$
\begin{aligned}
\mathcal{L}_u(v) &= \frac{1}{2}\|u - v\|_V^2 \\
&= \frac{1}{2}\langle u - v, u - v\rangle_V \\
&= \frac{1}{2}\int (u(x) - v(x))^2 \mathrm{d}\mu(x)
\end{aligned}
$$

Minimization problem

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Discrete problem

$$\begin{aligned}\mathcal{L}_u(v) &= \frac{1}{2}\|u - v\|_m^2 \\ &= \frac{1}{2}\langle u - v, u - v\rangle_m \\ &= \frac{1}{2m}\sum_{i=1}^{m}(u(x_i) - v(x_i))^2\end{aligned}$$

Minimization problem

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Functional perspective

$$v^* = \arg\min_{v \in \mathcal{M}} \mathcal{L}_u(v)$$

Parameter perspective

$$\theta^* = \arg\min_{\theta \in \mathbb{R}^p} \mathcal{L}_u(A(\theta))$$

$$\mathcal{L}_u(A(\theta)) = (\mathcal{L}_u \circ A)(\theta) =: \mathcal{L}(\theta)$$

Gradient descent

Iteratively improve approximation by minimizing $\mathcal{L}(\theta_k)$.

Taylor expansion around current iterate θ_k.

$$\mathcal{L}(\theta) \approx \mathcal{L}(\theta_k) + \langle \nabla_\theta \mathcal{L}(\theta_k), \theta - \theta_k \rangle_{\mathbb{R}^p}$$

Gradient descent

Iteratively improve approximation by minimizing $\mathcal{L}(\theta_k)$.

Taylor expansion around current iterate θ_k plus penalization on the distance traveled on each step.

$$\mathcal{L}(\theta) \approx \mathcal{L}(\theta_k) + \langle \nabla_\theta \mathcal{L}(\theta_k), \theta - \theta_k \rangle_{\mathbb{R}^p} + \frac{1}{2s}\rho(\theta, \theta_k)$$

Gradient descent

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Taylor expansion around current iterate θ_k plus penalization on the distance traveled on each step.

$$0 = \nabla_\theta \left[\mathcal{L}(\theta_k) + \langle \nabla_\theta \mathcal{L}(\theta_k), \theta - \theta_k \rangle_{\mathbb{R}^p} + \frac{1}{2s} \rho(\theta, \theta_k) \right]$$

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$$\frac{1}{2}\nabla_\theta \rho(\theta, \theta_k) = -s\nabla_\theta \mathcal{L}(\theta_k)$$

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Gradient descent

$$\rho(\theta, \theta_k) = \|\theta - \theta_k\|^2_{\mathbb{R}^p}$$

$$\nabla_\theta \rho(\theta, \theta_k) = 2(\theta - \theta_k)$$

$$\theta = \theta_k - s\nabla_\theta \mathcal{L}(\theta_k)$$

Preconditioned gradient

Iteratively improve approximation by minimizing $\mathcal{L}(\theta_k)$.

Taylor expansion around current iterate θ_k plus penalization on the distance traveled on each step.

$$\frac{1}{2}\nabla_\theta \rho(\theta, \theta_k) = -s\nabla_\theta \mathcal{L}(\theta_k)$$

Gradient descent	Preconditioned gradient
$\rho(\theta, \theta_k) = \|\theta - \theta_k\|^2_{\mathbb{R}^p}$	$\rho(\theta, \theta_k) = \|\theta - \theta_k\|^2_M$
$\nabla_\theta \rho(\theta, \theta_k) = 2(\theta - \theta_k)$	$\nabla_\theta \rho(\theta, \theta_k) = 2M(\theta - \theta_k)$
$\theta = \theta_k - s\nabla_\theta \mathcal{L}(\theta_k)$	$\theta = \theta_k - sM^{-1}\nabla_\theta \mathcal{L}(\theta_k)$

Newton's method

Iteratively improve approximation by minimizing $\mathcal{L}(\theta_k)$.

Taylor expansion around current iterate θ_k plus penalization on the distance traveled on each step.

$$\frac{1}{2}\nabla_\theta \rho(\theta, \theta_k) = -s\nabla_\theta \mathcal{L}(\theta_k)$$

Gradient descent	Newton's method
$\rho(\theta, \theta_k) = \|\theta - \theta_k\|^2_{\mathbb{R}^p}$	$\rho(\theta, \theta_k) = \|\theta - \theta_k\|^2_H$
$\nabla_\theta \rho(\theta, \theta_k) = 2(\theta - \theta_k)$	$\nabla_\theta \rho(\theta, \theta_k) = 2H(\theta - \theta_k)$
$\theta = \theta_k - s\nabla_\theta \mathcal{L}(\theta_k)$	$\theta = \theta_k - sH^{-1}\nabla_\theta \mathcal{L}(\theta_k)$

Functional gradient and geometric intuition

Some properties [Gruhlke, Robert, Anthony Nouy, and Philipp Trunschke. 2024].

$$H_{ij} = \frac{\partial^2 \mathcal{L}}{\partial\theta_i \partial\theta_j} = \frac{\partial}{\partial\theta_i}\left[\frac{\partial \mathcal{L}}{\partial\theta_j}\right] = \frac{\partial}{\partial\theta_i}\left[\frac{\partial}{\partial\theta_j}(\mathcal{L}_u \circ A)\right] = \frac{\partial}{\partial\theta_i}\left[\int_\Omega \nabla\mathcal{L}_u(v_\theta)(x)\frac{\partial A}{\partial\theta_j}(x)\mathrm{d}\mu(x)\right]$$

$$= \frac{\partial}{\partial\theta_i}\left[\left\langle \nabla\mathcal{L}_u, \frac{\partial A}{\partial\theta_j}\right\rangle_V\right]$$

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$$= \frac{\partial}{\partial\theta_i}\left[\left\langle \nabla\mathcal{L}_u, \frac{\partial A}{\partial\theta_j}\right\rangle_V\right]$$

$$\mathcal{L}_u(v) = \frac{1}{2}\|u - v\|^2_{L^2(\Omega)}$$

$$V \ni \nabla\mathcal{L}_u = u - v$$

Natural gradient from Newton's method

[Amari, Shun-ichi. 1998] [Martens, James 2020].

$$
\begin{aligned}
H_{ij} = \frac{\partial^2 \mathcal{L}}{\partial\theta_i \partial\theta_j} = \frac{\partial}{\partial\theta_i}\left[\frac{\partial \mathcal{L}}{\partial\theta_j}\right] &= \frac{\partial}{\partial\theta_i}\left[\frac{\partial}{\partial\theta_j}(\mathcal{L}_u \circ A)\right] = \frac{\partial}{\partial\theta_i}\left[\int_\Omega \nabla\mathcal{L}_u(v_\theta)(x)\frac{\partial A}{\partial\theta_j}(x)\mathrm{d}\mu(x)\right] \\
&= \frac{\partial}{\partial\theta_i}\left[\left\langle \nabla\mathcal{L}_u, \frac{\partial A}{\partial\theta_j}\right\rangle_V\right] \\
&= \left\langle H_V\mathcal{L}\frac{\partial A}{\partial\theta_i}, \frac{\partial A}{\partial\theta_j}\right\rangle_V + \left\langle \nabla\mathcal{L}_u, \frac{\partial^2 A}{\partial\theta_i\partial\theta_j}\right\rangle_V \\
&= G^{H_\mathcal{L}} + \langle \nabla\mathcal{L}_u, H_A\rangle_V
\end{aligned}
$$

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&= G^{H_\mathcal{L}} + \langle \nabla\mathcal{L}_u, H_A\rangle_V
\end{aligned}
$$

$$
G_{ij}^{H_\mathcal{L}} = \int \frac{\partial A}{\partial\theta_i}(x)[H_V\mathcal{L}(v)](x)\frac{\partial A}{\partial\theta_j}(x)\mathrm{d}\mu(x).
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$$

$$
\mathcal{L}_u(v) = \frac{1}{2}\|u - v\|^2_{L^2(\Omega)} \qquad \longrightarrow \qquad H_V\mathcal{L}(v)(x) = 1
$$

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G_{ij}^{H_\mathcal{L}} = \int \frac{\partial A}{\partial\theta_i}(x)[H_V\mathcal{L}(v)](x)\frac{\partial A}{\partial\theta_j}(x)\mathrm{d}\mu(x).
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G_{ij} = \int \left[\frac{\partial A}{\partial\theta_i}\frac{\partial A}{\partial\theta_j}\right](x)\mathrm{d}x
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$$= G^{H_\mathcal{L}} \cancel{+ \langle \nabla\mathcal{L}_u, H_A\rangle_V}$$

Model linearization

$$G^{H_\mathcal{L}}_{ij} = \int \frac{\partial A}{\partial\theta_i}(x)[H_V\mathcal{L}(v)](x)\frac{\partial A}{\partial\theta_j}(x)\mathrm{d}\mu(x).$$

$$\mathcal{L}_u(v) = \frac{1}{2}\|u - v\|^2_{L^2(\Omega)} \qquad \longrightarrow \qquad H_V\mathcal{L}(v)(x) = 1$$

$$G_{ij} = \int \left[\frac{\partial A}{\partial\theta_i}\frac{\partial A}{\partial\theta_j}\right](x)\mathrm{d}x$$

Natural gradient flow dynamics

$$\rho(\theta, \theta_k) = \|\theta - \theta_k\|_G^2 \qquad \longrightarrow \qquad \theta = \theta_k - sG^{-1}\nabla\mathcal{L}(\theta_k)$$

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Preconditioned gradient flow
in **parameter space**

$$\frac{\partial\theta}{\partial s} = -M^{-1}\nabla_\theta\mathcal{L}$$

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Preconditioned gradient flow
in **parameter space**

$$\frac{\partial \theta}{\partial s} = -M^{-1}\nabla_\theta \mathcal{L}$$

$$\begin{aligned}
\frac{\partial v_\theta}{\partial s} = \frac{\partial v_\theta}{\partial \theta}\frac{\partial \theta}{\partial s} = \frac{\partial A}{\partial \theta}^T M^{-1}\nabla_\theta \mathcal{L} &= -\frac{\partial A}{\partial \theta}^T M^{-1}\left\langle \nabla\mathcal{L}, \frac{\partial A}{\partial \theta}\right\rangle_V \\
&= -\left(G^{-\frac{1}{2}}\frac{\partial A}{\partial \theta}\right)^T G^{\frac{1}{2}} M^{-1} G^{\frac{1}{2}}\left\langle \nabla\mathcal{L}, G^{-\frac{1}{2}}\frac{\partial A}{\partial \theta}\right\rangle_V \\
&= -E^T G^{\frac{1}{2}} M^{-1} G^{\frac{1}{2}} \left\langle \nabla\mathcal{L}, E\right\rangle_V
\end{aligned}$$

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&= -E^T G^{\frac{1}{2}} M^{-1} G^{\frac{1}{2}} \langle \nabla\mathcal{L}, E\rangle_V
\end{aligned}$$

$$\langle E, E\rangle_V = \int_\Omega \left(G^{-\frac{1}{2}}\frac{\partial A}{\partial \theta}\right)^T \left(G^{-\frac{1}{2}}\frac{\partial A}{\partial \theta}\right) \mathrm{d}\mu(x) \quad = \int_\Omega \frac{\partial A}{\partial \theta}^T G^{-1}\frac{\partial A}{\partial \theta}\mathrm{d}\mu(x) = I$$

Natural gradient flow dynamics

$$\rho(\theta, \theta_k) = \|\theta - \theta_k\|_G^2 \qquad \longrightarrow \qquad \theta = \theta_k - sG^{-1}\nabla\mathcal{L}(\theta_k)$$

Preconditioned gradient flow in **parameter space**

$$\frac{\partial \theta}{\partial s} = -M^{-1}\nabla_\theta \mathcal{L}$$

Preconditioned gradient flow in **functional space**

$$\frac{\partial v_\theta}{\partial s} = -E^T G^{\frac{1}{2}} M^{-1} G^{\frac{1}{2}} \langle \nabla\mathcal{L}, E \rangle_V$$

Natural gradient flow dynamics

$$\rho(\theta, \theta_k) = \|\theta - \theta_k\|_G^2 \qquad \longrightarrow \qquad \theta = \theta_k - sG^{-1}\nabla\mathcal{L}(\theta_k)$$

Preconditioned gradient flow
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Gradient descent $M = I$
in **functional space**

$$\frac{\partial v_\theta}{\partial s} = -E^T G^{\frac{1}{2}} I^{-1} G^{\frac{1}{2}} \langle \nabla\mathcal{L}, E\rangle_V$$

Natural gradient flow dynamics

$$\rho(\theta, \theta_k) = \|\theta - \theta_k\|_G^2 \qquad \longrightarrow \qquad \theta = \theta_k - sG^{-1}\nabla\mathcal{L}(\theta_k)$$

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Gradient descent $M = I$
in **functional space**

$$\frac{\partial v_\theta}{\partial s} = -E^T G \langle \nabla\mathcal{L}, E\rangle_V$$

Natural gradient $M = G$
in **functional space**

$$\frac{\partial v_\theta}{\partial s} = -E^T G^{\frac{1}{2}} G^{-1} G^{\frac{1}{2}} \langle \nabla\mathcal{L}, E\rangle_V$$

Natural gradient flow dynamics

$$\rho(\theta, \theta_k) = \|\theta - \theta_k\|_G^2 \qquad \longrightarrow \qquad \theta = \theta_k - sG^{-1}\nabla\mathcal{L}(\theta_k)$$

Preconditioned gradient flow
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Gradient descent $M = I$
in **functional space**

$$\frac{\partial v_\theta}{\partial s} = -E^T G \langle \nabla\mathcal{L}, E\rangle_V$$

Natural gradient $M = G$
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Gradient descent $M = I$
in **functional space**

$$\frac{\partial v_\theta}{\partial s} = -E^T G \langle \nabla\mathcal{L}, E\rangle_V$$

Natural gradient $M = G$
in **functional space**

$$\frac{\partial v_\theta}{\partial s} = -P_{\mathcal{T}_k}^{H_\mathcal{L}} \nabla\mathcal{L}$$

Toy example

Gradient descent trajectory.

$$u \in L^2([-1,1])$$
$$\mathcal{L}_u(v) = \frac{1}{2}\|u - v\|^2$$
$$v_\theta(x) = A(\theta)(x) = \theta^T \Phi(x)$$
$$= \theta^T \begin{bmatrix} \sin(2\pi x) \\ \cos(2\pi x) \end{bmatrix}$$

$$\frac{\partial A}{\partial \theta_i}(\theta)(x) = \Phi_i(x)$$
$$G_{ij} = \int [\Phi_i \Phi_j](x)\mathrm{d}x = \delta_{ij}$$

Toy example

Gradient descent is biased in functional space.

$$u \in L^2([-1,1])$$

$$\mathcal{L}_u(v) = \frac{1}{2}\|u - v\|^2$$

$$v_\theta(x) = A(\theta)(x) = \theta^T B \Phi(x)$$

$$= \theta^T B \begin{bmatrix} \sin(2\pi x) \\ \cos(2\pi x) \end{bmatrix}$$

$$\mathbb{R}^{p\times p} \ni B = \begin{bmatrix} 1 & 0 \\ 0 & 0.2 \end{bmatrix}$$

$$\frac{\partial A}{\partial \theta_i}(\theta)(x) = B_i \Phi(x)$$

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Toy example

Natural gradient descent.

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Toy example

Non isotropic loss.

$$u \in L^2([-1,1])$$

$$\mathcal{L}_u(v) = \frac{1}{2}\|u - v\|_K^2$$

$$v_\theta(x) = A(\theta)(x) = \theta^T B \Phi(x)$$

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$$\frac{\partial A}{\partial \theta_i}(\theta)(x) = B_i \Phi(x)$$

$$G_{ij} = \int \left[\Phi^T B_i^T K B_j \Phi\right](x)\mathrm{d}x = B_i^T K B_j$$

Toy example

Natural gradient descent with loss hessian.

$$u \in L^2([-1,1])$$

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$$v_\theta(x) = A(\theta)(x) = \theta^T B \Phi(x)$$

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Toy example

Natural gradient and Newton method are equivalent for linear models.

$$u \in L^2([-1,1])$$

$$\mathcal{L}_u(v) = \frac{1}{2}\|u - v\|_K^2$$

$$v_\theta(x) = A(\theta)(x) = \theta^T B \Phi(x)$$

$$= \theta^T B \begin{bmatrix} \sin(2\pi x) \\ \cos(2\pi x) \end{bmatrix}$$

$$\mathbb{R}^{p\times p} \ni B = \begin{bmatrix} 1 & 0 \\ 0 & 0.2 \end{bmatrix}$$

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$$G_{ij} = \int \left[\Phi^T B_i^T K B_j \Phi\right](x)\mathrm{d}x = B_i^T K B_j$$

Toy example

Nonlinear manifold.

$$u \in L^2([-1,1])$$
$$\mathcal{L}_u(v) = \frac{1}{2}\|u - v\|_K^2$$
$$v_\theta(x) = A(\theta)(x) = \theta^T(B + Q\theta)\Phi(x)$$

$$\mathbb{R}^{p\times p} \ni B = \begin{bmatrix} 1 & 0 \\ 0 & 0.2 \end{bmatrix}, Q \in \mathbb{R}^{p\times p\times p}$$
$$\frac{\partial A}{\partial \theta_i}(\theta)(x) = (B_i + Q_i\theta)\Phi_i(x)$$
$$G_{ij}(\theta) = [(B + Q_i\theta)^T K (B + Q_i\theta)]_{ij}$$

Why we need momentum

Using momentum to **scape local minima** and **correct the biased step** of NGD.

Beyond L^2 loss

Classification
KL-div

$$\int \left[v \log \frac{v}{u} \right](x)\mathrm{d}x$$

PDE residual

$$\begin{aligned}\mathcal{L}(v) &= \|R(v)\|^2 \\ &= \| -\epsilon \partial_{xx} v + \partial_x v - 1\|^2\end{aligned}$$

Non-linear model

$$\theta_{k+1} = \theta_k - s G_k^{-1} \nabla_\theta \mathcal{L}(\theta_k)$$

$$\theta_s = \theta_k - \int_0^s G_k^{-1}(\theta_\ell) \nabla_\theta \mathcal{L}(\theta_\ell) \mathrm{d}\ell$$

Inacurate estimation of update

Stochastic setting
empirical loss

$$\mathcal{L}_u(v_k) = \|u - v_k\|_m^2$$

Solving NGD system

$$G^{-1} \begin{cases} \xrightarrow{Penrose} V(\Sigma_{\sigma > \varepsilon})^{-1} V^T \\ \xrightarrow{Tikhonov} (G + \varepsilon I)^{-1} \end{cases}$$

Escape local minima

$$\frac{\partial v_\theta}{\partial s} = -P_{\mathcal{T}_k} \nabla \mathcal{L}$$

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Momentum dynamics

From gradient flow to momentum [Polyak, B.T. 1964] [Nesterov, Yurii. 1983].

$$\frac{\partial \theta}{\partial s} = -\nabla_\theta \mathcal{L} \quad \longrightarrow \quad \frac{\partial^2 \theta}{\partial s^2} = -\gamma \frac{\partial \theta}{\partial s} - \nabla_\theta \mathcal{L}$$

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Heavy-ball

$$\begin{aligned} \theta_{k+1} &= \theta_k + p_k \\ p_k &= \beta p_{k-1} - \alpha \nabla_\theta \mathcal{L}_u(\theta_k) \end{aligned}$$

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$$\begin{aligned} y_k &= \theta_k + \beta(\theta_k - \theta_{k-1}) \\ \theta_{k+1} &= y_k - \alpha \nabla_\theta \mathcal{L}_u(y_k) \end{aligned}$$

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$$\theta_{k+1} = \theta_k + \beta(\theta_k - \theta_{k-1}) - \alpha \nabla_\theta \mathcal{L}_u(y_k)$$

Momentum dynamics in functional space

From momentum in parameter space to functional space.

Heavy-ball: "momentum variable"

$$\theta_{k+1} - \theta_k = \beta p_{k-1} - \alpha \nabla_\theta \mathcal{L}_u(\theta_k)$$

Heavy-ball: iterates difference

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$$P_{\mathcal{T}_k} \nabla \mathcal{L}(v_k)$$

$$P_{\mathcal{T}_k} p_{k-1}$$

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$$P_{\mathcal{T}_k} \nabla \mathcal{L}(v_k)$$

$$G_k^{-1} \nabla_\theta \mathcal{L}(\theta_k)$$

$$P_{\mathcal{T}_k} p_{k-1}$$

$$G_k^{-1} G_{k,k-1} p_{k-1}$$

$$G_{k,k-1} = \int \left[\left.\frac{\partial A}{\partial \theta}\right|_{\theta_k} \left.\frac{\partial A}{\partial \theta}\right|_{\theta_{k-1}} \right](x)\mathrm{d}x$$

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$$\theta_{k+1} - \theta_k = \beta(\theta_k - \theta_{k-1}) - \alpha \nabla_\theta \mathcal{L}_u(\theta_k)$$

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$$P_{\mathcal{T}_k}(v_k - v_{k-1})$$

$$G_k^{-1} \int \left[\left.\frac{\partial A}{\partial \theta}\right|_{\theta_k} (v_k - v_{k-1}) \right](x)\mathrm{d}x$$

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$$\theta_{k+1} - \theta_k = \beta p_{k-1} - \alpha \nabla_\theta \mathcal{L}_u(\theta_k)$$

$$\mathcal{T}_k \ni \mathrm{d}v_k = \beta P_{\mathcal{T}_k} p_{k-1} - \alpha P_{\mathcal{T}_k}^{H_\mathcal{L}} \nabla \mathcal{L}(v_k)$$

$$P_{\mathcal{T}_k}^{H_\mathcal{L}} \nabla \mathcal{L}(v_k)$$

$$(G_k^{H_\mathcal{L}})^{-1} \nabla_\theta \mathcal{L}(\theta_k)$$

$$P_{\mathcal{T}_k} p_{k-1}$$

$$G_k^{-1} G_{k,k-1} p_{k-1}$$

$$G_k^{H_\mathcal{L}} = \int \left[\frac{\partial A}{\partial \theta} H_\mathcal{L} \frac{\partial A}{\partial \theta} \right](x)\mathrm{d}x$$

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$$P_{\mathcal{T}_k}(v_k - v_{k-1})$$

$$G_k^{-1} \int \left[\left.\frac{\partial A}{\partial \theta}\right|_{\theta_k} (v_k - v_{k-1}) \right](x)\mathrm{d}x$$

Toy example

Escaping local minima.

$$u \in L^2([0,1])$$

$$\mathcal{L}_u(v) = \frac{1}{2}\|u - v\|_K^2$$

$$v_\theta(x) = \theta_1 b^T \Phi(x) + \theta_1^2 b^{\perp T} \Phi(x)$$

$$\mathrm{d}v_k^{HB} = P_{\mathcal{T}_k}[\beta p_{k-1} - \alpha \nabla \mathcal{L}(v_k)]$$

$$\mathrm{d}v_k^{N} = P_{\mathcal{T}_k}[\beta(v_k - v_{k-1}) - \alpha \nabla \mathcal{L}(y_k)]$$

Mackey Glass

A less toy example [Park, H, S.-I Amari, and K Fukumizu (2000)].

Mackey Glass caotic time series:

- $z(t+1) = (1-b)z(t) + a\frac{z(t-\tau)}{1+z(t-\tau)^{10}}$
- Input: $z(t), z(t-6), z(t-12), z(t-18)$
- Output: $z(t+6)$

Model NN: $v_\theta : \mathbb{R}^4 \to \mathbb{R}$

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Model NN: $v_\theta : \mathbb{R}^4 \to \mathbb{R}$

Classification task

Another less toy example from [Park, H, S.-I Amari, a
K Fukumizu (2000)].

Mackey Glass caotic time series:

- Input: $z \in \mathbb{R}^2$
- Output: $c \in \{0, 1\}$

$$\mathcal{L}_u(v) = \int -u \log(v) - (1-u)\log(1-v)$$

Model (Shallow NN): $v_\theta : \mathbb{R}^2 \to [0, 1]$

Physics informed learning.

Physics informed neural networks (PINNs)
[Müller J., Zeinhofer M. (2023)]
[Schwencke N., Furtlehner C. (2024)].

$$\mathcal{L}(v) = \|R(v)\|^2$$
$$\mathcal{L}(v) = \| - \epsilon \partial_{xx} v + \partial_x v - 1\|^2$$

Conclusion

What is done, what is still to be done.

We saw how to build a **Natural inertial dynamics** for gradient optimization on non linear approximation manifolds.

Some directions

- Step-size adaptivity
- Natural inertial dynamics and linesearch
- Theoretical questions: convergence? optimality?

Thank you!

(2024) Schwencke N., Furtlehner C.	
(2023) Müller J., Zeinhofer M.	NGD and PINNs.
(2024) R. Gruhlke, A. Nouy, P. Trunschke.	NGD and optimal sampling.
(2020) J. Martens.	NGD Review.
(2000) H. Park, S. Amari, K. Fukumizu.	NGD Experiments.
(1998) S. Amari.	NGD Initial paper.
(1983) Y. Nesterov.	Nestorov acceleration.
(1964) B.T. Polyak.	Heavy Ball acceleration.

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