What Makes a Good Preconditioner for Data Science?

Mitchell T. Scott

Department of Mathematics, Emory University

Preconditioning techniques for scientific and industrial applications
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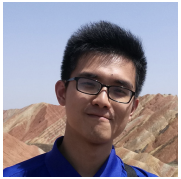
Collaborators and Acknowledgments

Yousef Saad,
Minnesota



Tianshi Xu,
Emory

Yuanzhe Xi,
Emory

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I want to minimize some loss, but the dataset is so large, the gradient computation takes forever!
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Definition (Preconditioned Stochastic Gradient Descent)

To minimize the stochastic optimization problem, we can write the resulting algorithm as

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \alpha_k \mathbf{M}^{-1} g(\mathbf{w}_k, \boldsymbol{\xi}_k), \tag{1}$$

where $g(\mathbf{w}_k, \boldsymbol{\xi}_k) = \nabla_w F_k(\mathbf{w})$ is the stochastic gradient, α_k is the learning rate, $\boldsymbol{\xi}_k$ is an i.i.d. sample drawn at iteration k, and $\mathbf{M}$ is the preconditioner.

Common preconditioners for SGD can consider isotropy and curvature.

Example (Adam [1])

Define $\mathbf{s}_k$ is an exponential moving average of squared gradients up until iteration k, then

$$\mathbf{M}_{\text{Adam}} = \text{diag}\left(\sqrt{\mathbf{s}_k} + \boldsymbol{\varepsilon}\right),$$

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Example (Full or mini-batch Hessian)

The Hessian, or mini-batch approximation to the Hessian, matrix of the loss function,

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Example (Fisher Information Matrix)

Using the Fisher Information Matrix as a preconditioner corresponds to natural gradient descent [2]

$$\mathbf{F} = \mathbb{E}\left[\frac{d \log p(y|x,\theta)}{d\theta} \frac{d \log p(y|x,\theta)}{d\theta}^\top\right] := \mathbb{E}[\mathcal{D}\boldsymbol{\theta}\mathcal{D}\boldsymbol{\theta}^\top] = \mathbb{C}\text{ov}(\mathcal{D}\boldsymbol{\theta}, \mathcal{D}\boldsymbol{\theta})$$

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Classical Convergence Results for SGD

Theorem (Convergence of SGD [3])

Assume that a loss function F where $F_* := F(\mathbf{w}^*)$, has L-Lipschitz gradients and $\mathbb{E}\left[\|\nabla F(\mathbf{w})\|^2\right] \leq \sigma^2$, then SGD converges

$$\mathbb{E}\left[F(\mathbf{w}_k) - F_*\right] \leq \frac{F(\mathbf{w}_1) - F_*}{2\overline{\alpha}k}$$

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Theorem (Strongly Convex Objective, Fixed Stepsize (Thm 4.6, [4]))

Adding in stronger bounds on the gradient's first and second moments, and c-strong convexity. Running SGD with a small fixed step size $\overline{\alpha}$ satisfy

$$\mathbb{E}[F(\mathbf{w}_k) - F_*] \leq (1 - \overline{\alpha}c\mu)^{k-1}\left(F(\mathbf{w}_1) - F_* - \frac{\overline{\alpha}LK}{2c\mu}\right) + \frac{\overline{\alpha}LK}{2c\mu}, \tag{2}$$

where μ, K are constants associated with the stochastic gradients and variance, respectively.

Two important quantities for data science preconditioning.

Remark (Two stage convergence)

This highlights two late-stage drivers: a linear contraction factor $(1 - \alpha c\mu)$ *and a stochastic error floor*

$$\frac{\alpha L K}{2c\mu} = \frac{\alpha}{2\mu}\,\kappa\,K,$$

where $\kappa := \frac{L}{c}$ *is the (Euclidean) condition number associated with curvature.*

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Definition (Conditional Variance)

$$\mathbb{V}_{\boldsymbol{\xi}_k}\big[g(\mathbf{w}_k, \boldsymbol{\xi}_k), \|\cdot\|_{\mathbf{M}^{-1}}\big] := \mathbb{E}_{\boldsymbol{\xi}_k}\left[\|g(\mathbf{w}_k, \boldsymbol{\xi}_k)\|^2_{\mathbf{M}^{-1}}\right] - \left\|\mathbb{E}_{\boldsymbol{\xi}_k}[g(\mathbf{w}_k, \boldsymbol{\xi}_k)]\right\|^2_{\mathbf{M}^{-1}} = \operatorname{tr}\big(\mathbf{M}^{-1}\boldsymbol{\Sigma}(\mathbf{w})\big), \tag{3}$$

where $\boldsymbol{\Sigma}(\mathbf{w}) := \mathbb{C}\mathrm{ov}(g(\mathbf{w}, \boldsymbol{\xi}) \mid \mathbf{w})$. For late stage convergence

$$\mathbb{V}_{\boldsymbol{\xi}_k}\big[g(\mathbf{w}_k, \boldsymbol{\xi}_k), \|\cdot\|_{\mathbf{M}^{-1}}\big] \;\leq\; K + \mathcal{O}(\overline{\alpha} K),$$

Preconditioning helps convex problems converge faster with a lower loss.

Theorem (S., *et al.*, '26, [5])

Running (1) *with small* $\alpha_k = \overline{\alpha}$ *under preconditioned analogues of common assumptions, then, for all* $k \in \mathbb{N}$,

$$\mathbb{E}[F(\mathbf{w}_k) - F_*] \leq \frac{\overline{\alpha}\,\hat{L}\,K}{2\,\hat{c}\,\mu} + (1 - \overline{\alpha}\,\hat{c}\,\mu)^{k-1}\left(F(\mathbf{w}_1) - F_* - \frac{\overline{\alpha}\,\hat{L}\,K}{2\,\hat{c}\,\mu}\right) \xrightarrow{k\to\infty} \frac{\overline{\alpha}\,\hat{L}\,K}{2\,\hat{c}\,\mu}. \tag{4}$$

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Theorem

Now suppose (1) *has a decaying learning rate, then, for all* $k \in \mathbb{N}$,

$$\mathbb{E}[F(\mathbf{w}_k) - F_*] \;\leq\; \frac{\nu}{\gamma + k}, \qquad \nu := \max\left\{\frac{\beta^2 \hat{L} K}{2(\beta\hat{c}\mu - 1)}, (\gamma+1)\big(F(\mathbf{w}_1) - F_*\big)\right\}. \tag{5}$$

Polyak-Łojasiewicz functions are structured but nonconvex.

Assumption (Local PŁ functions on $\mathcal{N}$)

There exists $\hat{\mu}_{\mathrm{PL}} > 0$ *such that, for all* $\mathbf{w} \in \mathcal{N}$: $\quad 2\hat{\mu}_{\mathrm{PL}}\big(F(\mathbf{w}) - F_*\big) \;\leq\; \|\nabla F(\mathbf{w})\|^2$.

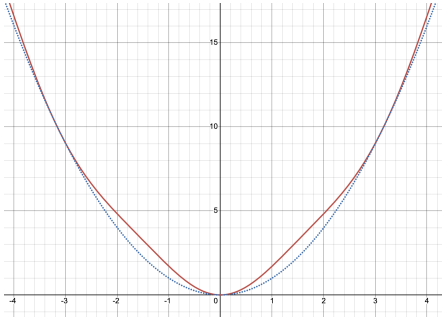

Figure 1: Comparing a convex function $F(x) = x^2$ with a $\mu-$PŁ function $F(x) = x^2 + \sin^2(x)$. [6]

Preconditioning helps in the nonconvex case, more realistic for SciML problems.

Theorem (S., *et al.*, '26 (Informal) [5])

Assume $\mathbf{w}_1$ *is in a quadratically growing local basin of radius* r, $\mathcal{N}_r$. *Let* $\tau := \inf\{k \geq 1 : \mathbf{w}_k \notin \mathcal{N}_r\}$.

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We stay in the basin w.h.p. depending on $1 - \mathcal{O}\left(\hat{L}K\right) - \sum_k \delta_k$, *where* δ_k *is the "escape probability".*

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Diagnostic quadratic model allows for explicit control of preconditioned spectra.

Example (Quadratic model)

Let $\mathbf{w}_0 \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \mathbf{w}_* = \mathbf{0}, F_* = 0$ for the quadratic model:

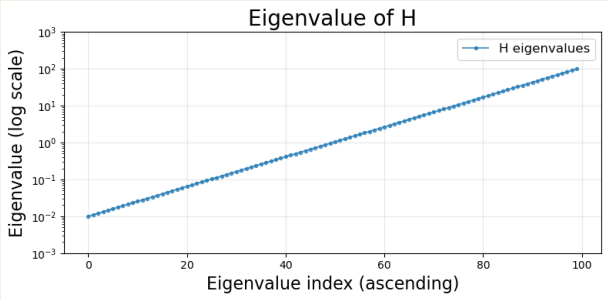
$$F(\mathbf{w}) = \frac{1}{2}(\mathbf{w} - \mathbf{w}_*)^\top \mathbf{H}(\mathbf{w} - \mathbf{w}_*),$$

where $\mathbf{H} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^\top$ has log-uniform spectrum from $[10^{-2}, 10^2]$, namely $\mathbf{H} \succ 0$.

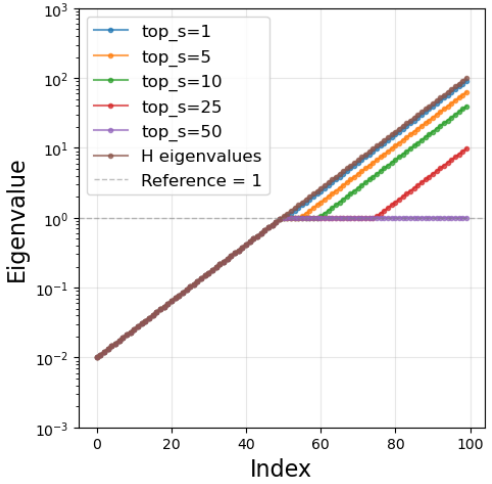
We add stochastic noise, so

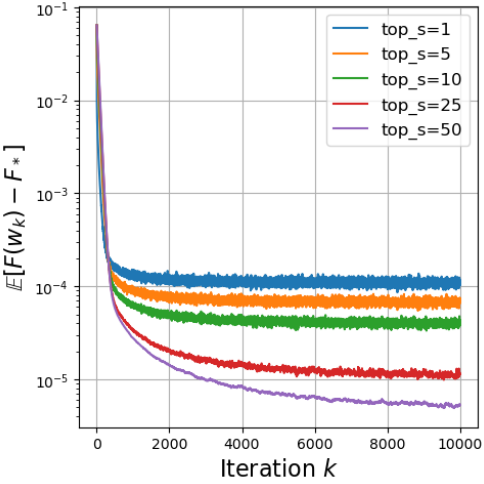
$$\nabla F(\mathbf{w}) = g(\mathbf{w}) + \boldsymbol{\epsilon}, \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

and run (preconditioned) SGD.

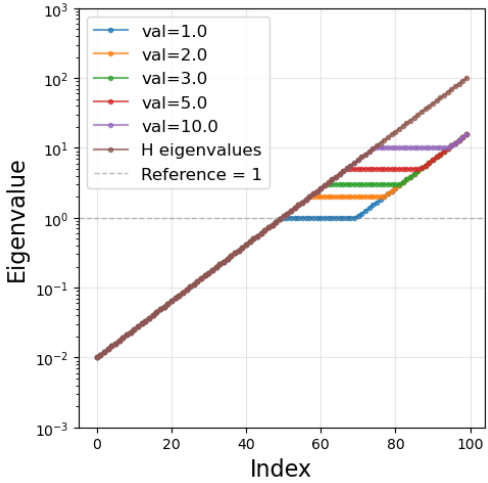


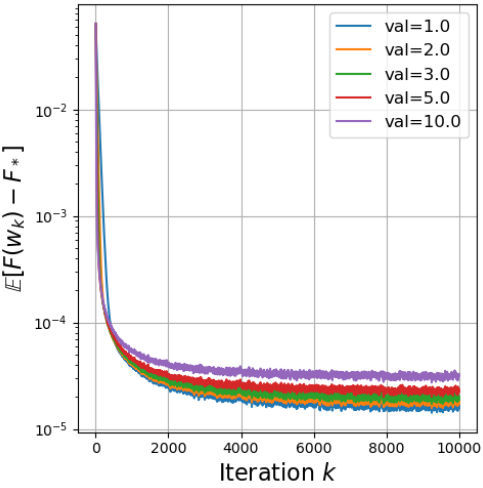
Deflation preconditioners lead to faster convergence and lower loss floor.





Generic deflation preconditioners demonstrate that a lower trace leads to a lower loss floor.

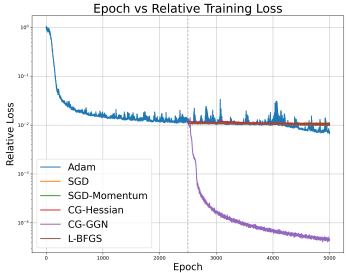


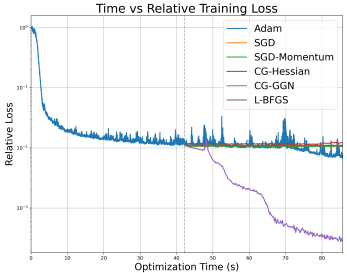


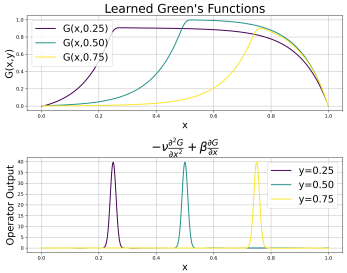
Convection dominated problems are hard, and Green's function learning is no different.

Example (Convection-dominated problem from Hao et al., [8])

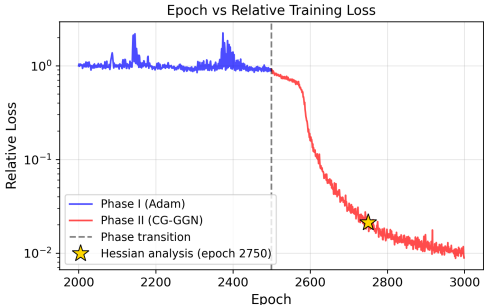
Find $G(x, y)$ such that $\mathcal{L}G = \delta(x - y)$ where $\mathcal{L}u := -0.1u'' + 1.0u', \quad u(0) = u(1) = 0$

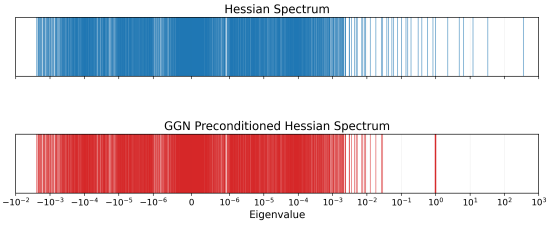






Preconditioning empirically clusters the eigenvalues for SciML's Hessian.





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- There are other machine learning frameworks such as LLMs, which have different goals for generalization.
- We aim to have a parameter *a priori* that informs the generalization in terms of a regret bound.

Questions?

Thank You!

Read the Paper!

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