

What Makes a Good Preconditioner for Data Science?

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Stochastic gradient descent is the workhorse of ML training optimizers.

Example

I want to minimize some loss, but the dataset is so large, the gradient computation takes forever!

What do I do?



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Definition (Preconditioned Stochastic Gradient Descent)

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

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

where $g(\mathbf{w}_k, \boldsymbol{\xi}_k) = \nabla_{\mathbf{w}} F_k(\mathbf{w})$ 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, Kingma and Ba, 2017 [1])

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

$$\mathbf{M}_{\text{Adam}} = \text{diag}(\sqrt{\mathbf{s}_k} + \epsilon),$$

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Example (Full or mini-batch Hessian)

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

$$\mathbf{H}_{\mathcal{B}}(\mathbf{w}) = \nabla^2 \mathcal{L}_{\mathcal{B}}(\mathbf{w}).$$



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Example (Fisher Information Matrix (FIM))

Using the FIM as a preconditioner corresponds to natural gradient descent [Amari, 1998].

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

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Classical Convergence Results for SGD

Theorem (Convergence of SGD, Robbins and Monro, 1951 [3])

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

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

Theorem (Strongly Convex Objective, Fixed Stepsize (Thm 4.6, Bottou, Curtis, and Nocedal, 2018 [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 $\bar{\alpha}$ satisfy

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

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)

$$\mathbb{V}_{\xi_k}[g(\mathbf{w}_k, \xi_k), \|\cdot\|_{\mathbf{M}^{-1}}] := \mathbb{E}_{\xi_k}[\|g(\mathbf{w}_k, \xi_k)\|_{\mathbf{M}^{-1}}^2] - \|\mathbb{E}_{\xi_k}[g(\mathbf{w}_k, \xi_k)]\|_{\mathbf{M}^{-1}}^2 = \text{tr}(\mathbf{M}^{-1}\Sigma(\mathbf{w})), \quad (3)$$

where $\Sigma(\mathbf{w}) := \text{Cov}(g(\mathbf{w}, \xi) \mid \mathbf{w})$. For late stage convergence

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

Preconditioning helps convex problems converge faster with a lower loss.

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

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

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



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Theorem

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

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



Polyak-Łojasiewicz functions are structured but nonconvex.

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

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

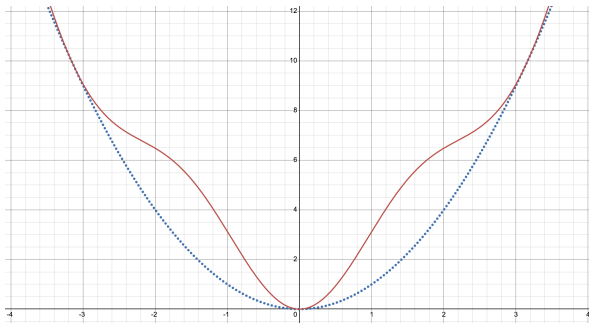


Figure 1: Comparing a convex function $F(x) = x^2$ with a $\mu = \frac{1}{40}$ – PL function $F(x) = x^2 + 3 \sin^2(x)$.



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

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

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

For a fixed step size $\alpha_k = \bar{\alpha}$,

- we have linear convergence (depending on $\uparrow \hat{\mu}_{\text{PL}}$)



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- and convergence up until a noise floor, which depends on a tradeoff between
 - $\downarrow \hat{L}/\hat{\mu}_{\text{PL}}$ and
 - $\downarrow K$.



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For a harmonic step size $\alpha_k \propto 1/k$



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For a harmonic step size $\alpha_k \propto 1/k$

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We stay in the basin w.h.p. depending on $1 - \mathcal{O}(\hat{L}K) - \sum_k \delta_k$, 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:

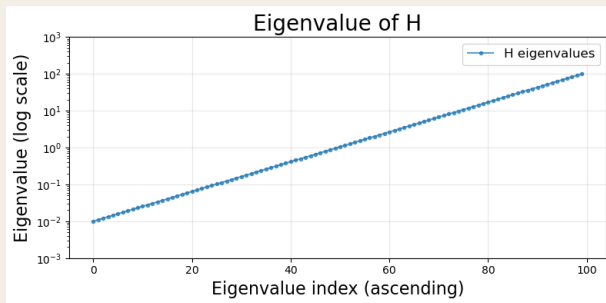
$$F(\mathbf{w}) = \frac{1}{2}(\mathbf{w} - \mathbf{w}_*)^\top \mathbf{H}(\mathbf{w} - \mathbf{w}_*),$$

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

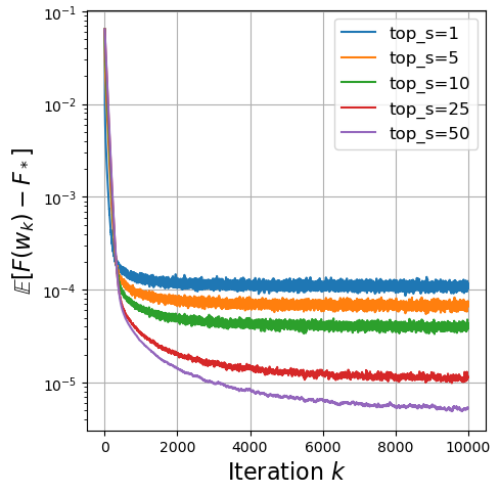
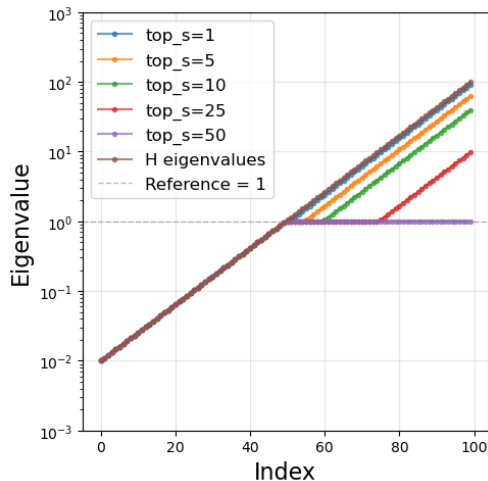
We add stochastic noise, so

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

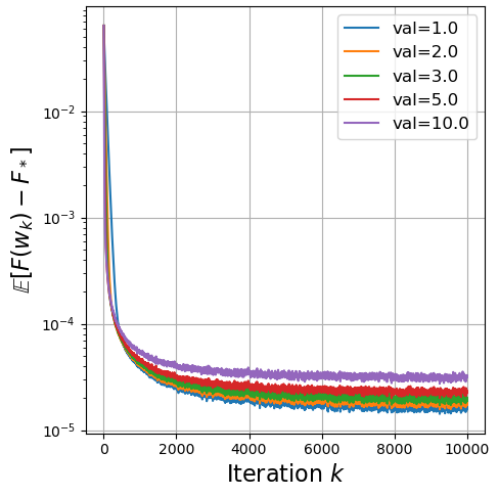
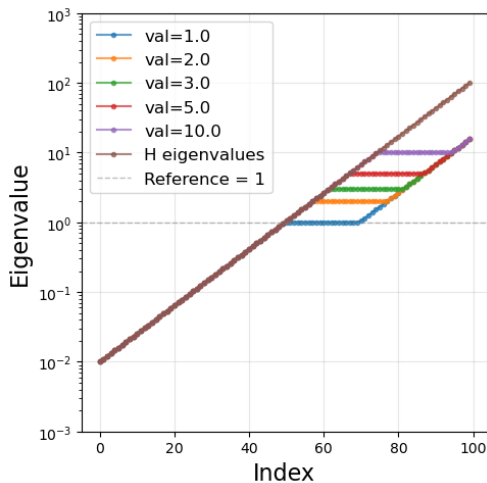
and run (preconditioned) SGD.



Deflation preconditioners lead to faster convergence and lower loss floor.



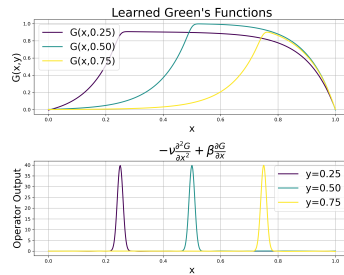
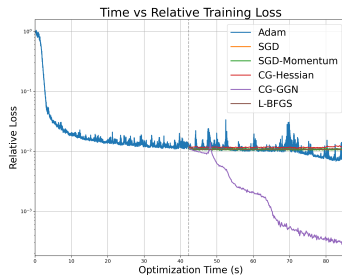
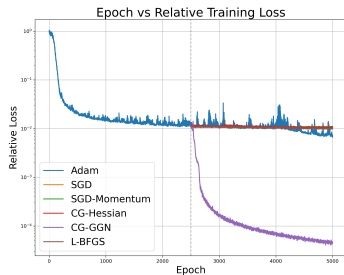
Generic deflation preconditioners demonstrate that a lower trace leads to a lower loss floor.



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

Example (Convection-dominated problem from Hao et al. 2024, [6])

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



Preconditioning empirically clusters the eigenvalues for SciML's Hessian.

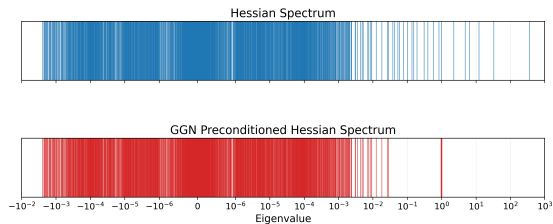
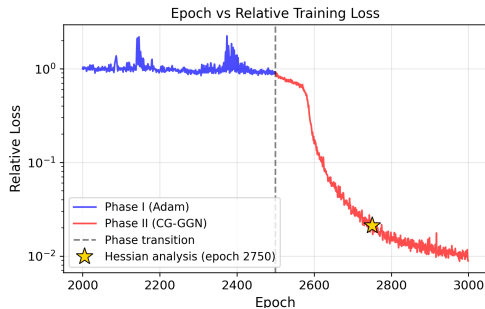


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Studying the Geometry of the (preconditioned) Loss Landscape

Example (Nonlinear Least Squares)

Given data points $(x_i, y_i), i = 1, \dots, m \in \mathbb{R}^n$ let $\mathbf{r}_i(\mathbf{w}) := f(x_i, \mathbf{w}) - y_i$ be the loss of a nonlinear least squares problem. The Hessian is

$$\mathbf{H} := \mathbf{J}(\mathbf{w})\mathbf{J}(\mathbf{w})^\top + \text{small residuals}$$

where $\mathbf{J}$ is the Jacobian of $\mathbf{r}$,

Remark

As $n \rightarrow \infty$, we (Pennington and Bahri, 2017 [7]) could view the Hessian as

$$\mathbf{H} := \mathbf{H}_0 + \mathbf{H}_1 = \frac{1}{T}\mathbf{X}\mathbf{X}^\top + \frac{1}{2}\left(\mathbf{W} + \mathbf{W}^\top\right), \quad \text{where } \mathbf{X}, \mathbf{W} \sim \mathcal{N}(0, 1)$$



How do we precondition this Loss Surface?

Let $\mathbf{X} \in \mathbb{R}^{d \times T}$ and $\mathbf{Y} \in \mathbb{R}^{d \times S}$ be free, standard Gaussian matrices, and define

$$\mathbf{H}_0 = \frac{1}{T} \mathbf{X} \mathbf{X}^\top, \quad \mathbf{M} = \frac{1}{S} \mathbf{Y} \mathbf{Y}^\top, \quad d/T \rightarrow q \in (0, 1), \quad d/S \rightarrow \psi \in (0, 1).$$

Theorem (Spectrum for Sample Covariance Preconditioning, S. *et al.*, '26b, [8])

Let

$$\overline{\mathbf{H}}_0 = (1 - \psi) \mathbf{M}^{-1/2} \mathbf{H}_0 \mathbf{M}^{-1/2}, \quad p = \frac{\psi}{1 - \psi}.$$

Then the empirical spectral distribution of $\overline{\mathbf{H}}_0$ converges almost surely to a compact law with support

$$[\lambda_-, \lambda_+], \quad \lambda_{\pm} = 1 + q + 2p \pm 2\sqrt{(1+p)(q+p)}. \quad (6)$$

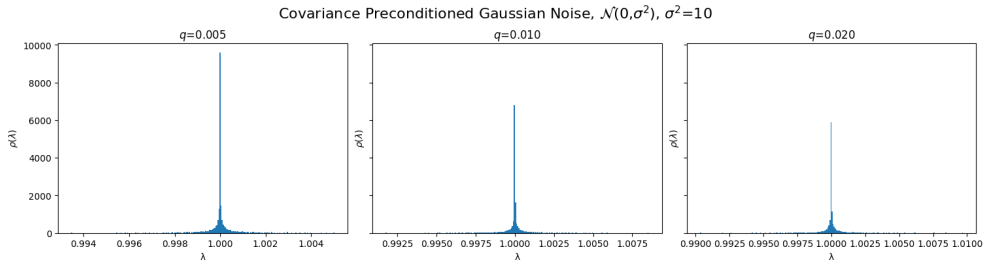


How does preconditioning affect the noise?

Given this model $\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_1$, the goal is to precondition the bulk $\mathbf{H}_0$ without amplifying the noise $\mathbf{H}_1$.

$$\mathbf{M}^{-1/2} (\mathbf{H}_0 + \mathbf{H}_1) \mathbf{M}^{-1/2} \approx \mathbf{\Pi} + \mathbf{M}_0^{-1/2} \mathbf{H}_1 \mathbf{M}_0^{-1/2}$$

where $\mathbf{\Pi}$ is a projector matrix.



Full covariance inversion can widen the preconditioned spectrum

Let

$$\mathbf{M} = \frac{1}{S} \mathbf{Y} \mathbf{Y}^\top, \quad d/S \rightarrow \psi \in (0, 1), \quad \mathbf{\Sigma} = \sigma_\xi^2 \mathbf{I},$$

Then

$$\frac{1}{d} \operatorname{tr}(\mathbf{M}^{-1} \mathbf{\Sigma}) \rightarrow \frac{\sigma_\xi^2}{1 - \psi}, \quad \lambda_{\max}(\mathbf{M}^{-1}) \rightarrow (1 - \sqrt{\psi})^{-2} \quad (7)$$

Remark

As $\psi \nearrow 1$, the upper edge grows. Thus uncontrolled full inversion can broaden the effective curvature bulk.



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Conclusion and Future Work

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A well-designed preconditioner $\mathbf{M}$
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does the following:

- ① enhancing local conditioning—decreasing $\hat{L}/\hat{c}$ ($\hat{L}/\hat{\mu}_{\text{PL}}$ for nonconvexity)
→ speeds up contraction,



Conclusion and Future Work

Conclusion:

A well-designed preconditioner M does the following:

- ① enhancing local conditioning—decreasing $\hat{L}/\hat{c}$ ($\hat{L}/\hat{\mu}_{\text{PL}}$ for nonconvexity)
→ speeds up contraction,
- ② reducing the preconditioned noise level K ,
lowering the effective noise floor,
- ③ permitting a larger basin radius r , which jointly improves basin stability,
- ④ responding robustly to Gaussian or heavy-tailed noise, and
- ⑤ targeting the recoverable signal spikes.

Future Work: Generalization of Preconditioners

- This work was based on late stage convergence for Scientific Machine Learning, where generalization is straightforward.
- There are other machine learning frameworks such as LLMs, which have different goals for generalization.



Questions?

Thank You!



Read the Paper!



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- [7] Jeffrey Pennington and Yasaman Bahri. “Geometry of Neural Network Loss Surfaces via Random Matrix Theory”. In: *Proceedings of the 34th International Conference on Machine Learning*. Ed. by Doina Precup and Yee Whye Teh. Vol. 70. Proceedings of Machine Learning Research. PMLR, 2017, pp. 2798–2806. URL: <https://proceedings.mlr.press/v70/pennington17a.html>.
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6 Additional Figures



Spectrum of RMT Ensembles

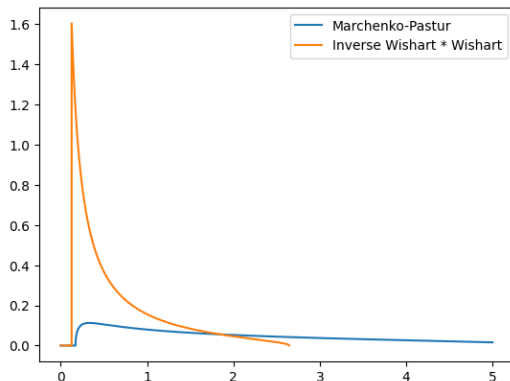


Figure 3: Comparing **Marchenko - Pastur** with $q = 2$ with **Inverse Wishart Preconditioning** with $q = 2, \psi = 0.5$