Hunting the Hessian: Randomized Methods

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Joint work with
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Outline

Preconditioning

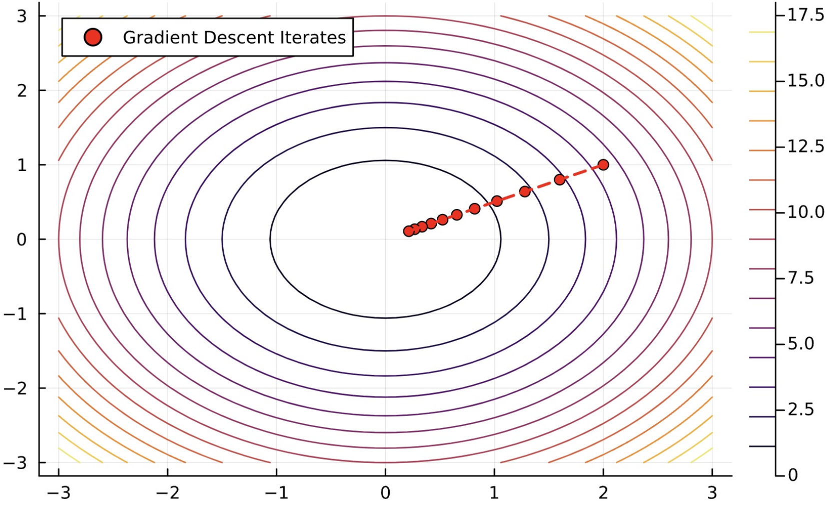
Nyström preconditioning

NysADMM

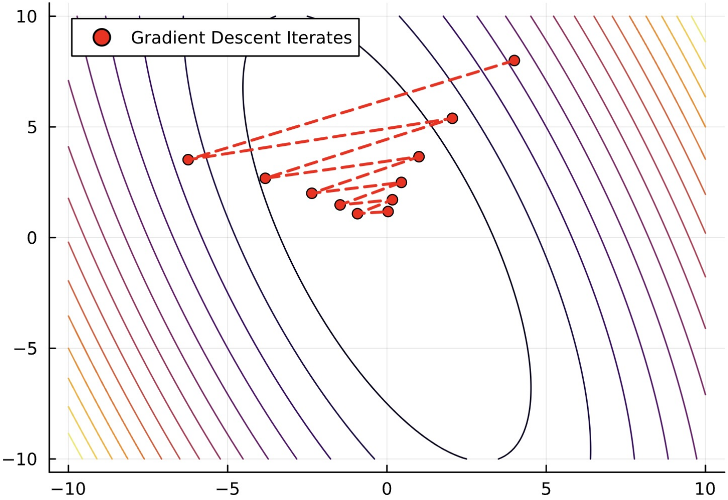
Optimization for deep learning

PINNs

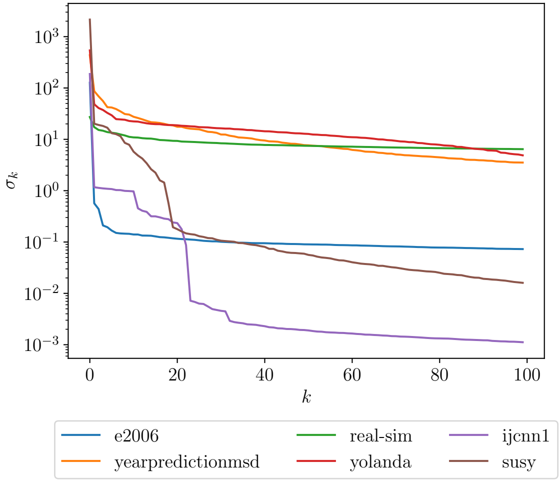
Gradient methods converge quickly on well-conditioned data



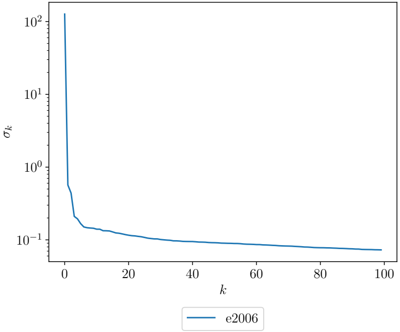
Gradient methods converge slowly on ill-conditioned data

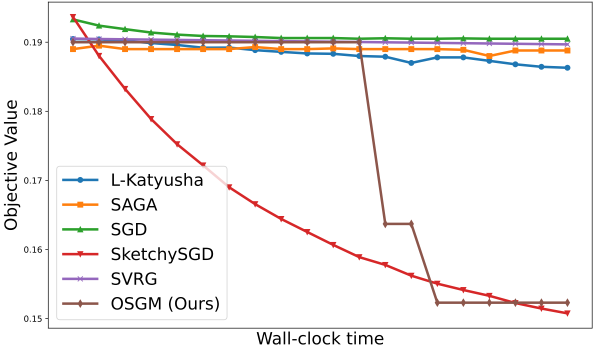


Ill-conditioning is common in ML data...



. . . and it makes optimization slower!





Recap: convergence analysis for gradient descent

$$\text{minimize} \quad f(x)$$

recall: we say (twice-differentiable) f is μ-strongly convex and L-smooth if

$$\mu I \preceq \nabla^2 f(x) \preceq LI$$

recall: if f is μ-strongly convex and L-smooth, gradient descent converges linearly

$$f(x^{K+1}) - p^\star \leq \frac{Lc^K}{2} \|x^1 - x^\star\|^2,$$

where $c = (\frac{\kappa-1}{\kappa+1})^2$, $\kappa = \frac{L}{\mu} \geq 1$ is condition number

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idea: can we minimize another function with $\kappa \approx 1$ whose solution will tell us the minimizer of f?

Preconditioning

for invertible D, the two problems

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a gradient step on $f(Dz)$ with step-size $t > 0$ is

$$\begin{aligned} z^+ &= z - tD^T \nabla f(Dz) \\ Dz^+ &= Dz - tDD^T \nabla f(Dz) \\ x^+ &= x - tDD^T \nabla f(x) \end{aligned}$$

this iteration is *preconditioned gradient descent* (PGD) with preconditioner $P = DD^T$.

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Preconditioning a linear system

Preconditioning a linear system. for any $P \succ 0$,

$$Ax = b \quad \Longleftrightarrow \quad \begin{aligned} P^{-1/2}Ax &= P^{-1/2}b \\ P^{-1/2}AP^{-1/2}z &= P^{-1/2}b \end{aligned}$$

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- preconditioning works well when $\kappa(P^{-1/2}AP^{-1/2}) \ll \kappa(A)$

Low rank approximation via eigenvalues

given $A \in \mathbf{S}_+^p$ (symmetric positive definite), find the best rank-s approximation:

- compute the eigenvalue decomposition $\triangleright O(p^3)$ flops

$$A = \sum_{i=1}^{p} \lambda_i u_i u_i^T = U \Lambda U^T$$

with $\lambda_1 \geq \cdots \geq \lambda_p$, $\Lambda = \mathbf{diag}(\lambda_1, \ldots, \lambda_p)$, $u_i^T u_j = \delta_{ij}$.

- truncate to top s eigenvector/value pairs:

$$\hat{A} = \sum_{i=1}^{s} \lambda_i u_i u_i^T = U_s \Lambda_s U_s^T$$

where Λ_s and U_s are truncated versions of Λ and U.

Efficient eigs via randomized NLA

given $A \in \mathbf{S}_+^p$, find a good rank-s approximation:

- draw random Gaussian matrix $\Omega \in \mathbb{R}^{p \times s}$
- compute randomized linear sketch $Y = A\Omega$.

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$$\hat{A}_{\text{nys}} = (A\Omega)(\Omega^T A\Omega)^\dagger (A\Omega)^T = Y(\Omega^T Y)^\dagger Y^T.$$

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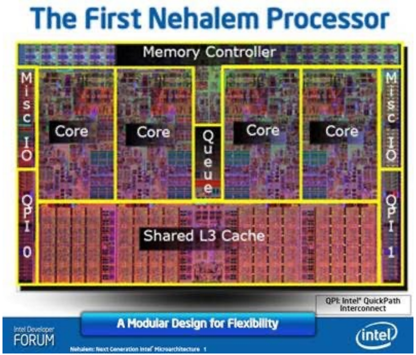
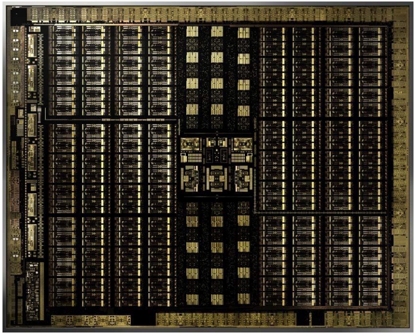
properties:

- total computation: s matvecs + $O(ps^2)$
- total storage: $O(ps)$
- $\hat{A}_{\text{nys}}$ is spd, $\textbf{rank}(\hat{A}_{\text{nys}}) \leq s$, and $\hat{A}_{\text{nys}} \preceq A$
- requires only matvecs with A, streaming ok.

Speed depends on hardware



CPU: complex, sequential tasks



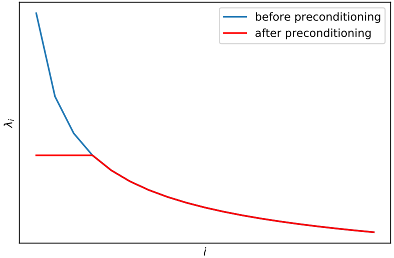
GPU: simple, parallel tasks

- traditional matrix decompositions: hopelessly serial (e.g., Gaussian elimination)
- randNLA: naturally parallel (mostly matvecs)

An optimal low-rank preconditioner

- suppose $\lfloor A \rfloor_s = V_s \Lambda_s V_s^T$ is a best rank-s apx to $A \in \mathbf{S}_+^p$.
- the best preconditioner (e.g., for PCG) using this information is

$$P_\star = \frac{1}{\lambda_{s+1}} V_s(\Lambda_s)V_s^T + (I - V_s V_s^T)$$



Nyström preconditioner

Given a rank-s Nyström approximation

$$\hat{A}_{\text{nys}} = V \hat{\Lambda} V^T \qquad \approx \qquad A \in \mathbf{S}_+^p,$$

the *Nyström preconditioner* for $(A + \mu I)x = b$ is

$$P_{\text{nys}} = \frac{1}{\hat{\lambda}_s + \mu} V(\hat{\Lambda} + \mu I)V^T + (I - VV^T)$$

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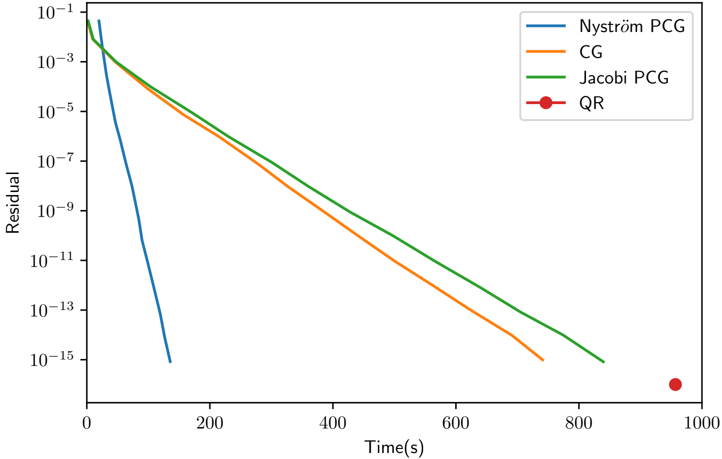
inverse can be applied in $O(ps)$:

$$P^{-1} = (\hat{\lambda}_s + \mu)V(\hat{\Lambda} + \mu I)^{-1}V^T + (I - VV^T)$$

Nyström preconditioner is fast!



Random features regression on YearMSD dataset $(463,715 \times 15,000)$. Regularization $\mu = 10^{-5}$; sketch size $s = 500$.

Low rank approximation for faster optimization

randNLA allows approximate inverse of p$\times$p matrix A in $\mathcal{O}(p)$ time
$\implies$ can improve conditioning for many optimization problems.

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2. NysADMM for composite optimization minimize $f(Ax) + g(x)$, e.g.,
   - lasso
   - regularized logistic regression
   - support vector machine

   randNLA beats SOTA solver for all these problems!

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   randNLA beats SOTA solver for all these problems!
3. approximate Newton methods for deep learning and stochastic optimization
   low rank approximation for Newton system improves
   - robustness (vs first-order methods) and
   - speed (vs other quasi-Newton methods)

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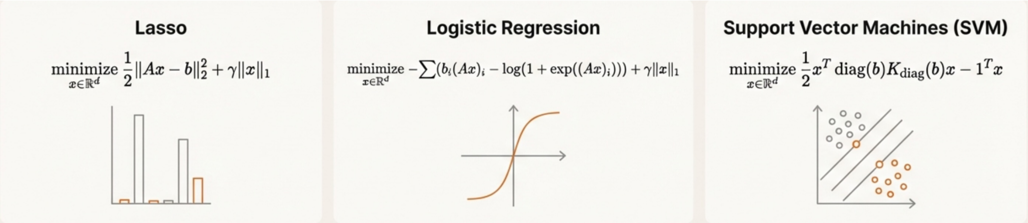
Composite optimization

$$\text{minimize} \quad \ell(Ax) + r(x)$$

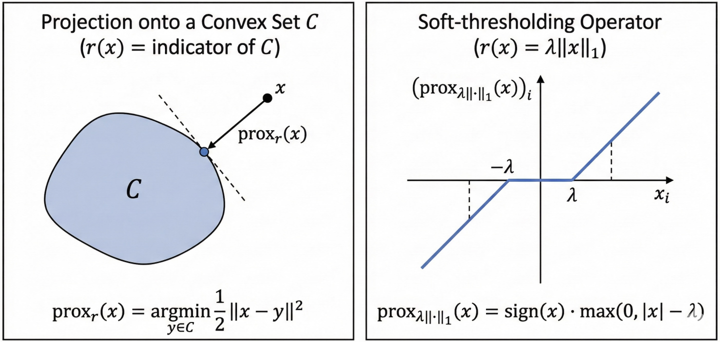
- $A : \mathbf{R}^p \to \mathbf{R}^m$ linear
- $\ell : \mathbf{R}^m \to \mathbf{R}$ smooth
- $r : \mathbf{R}^p \to \mathbf{R}$ *proxable*



Proximal operators

$r : \mathbf{R}^p \to \mathbf{R}$ is called *proxable* if it is easy to compute the *proximal operator*

$$\mathbf{prox}_r(x) := \operatorname*{argmin}_y r(y) + \frac{1}{2}\|x - y\|^2$$



Alternating Directions Method of Multipliers

Algorithm ADMM

Input: loss function $\ell \circ A$, regularization r, stepsize ρ,
initial z^0, $u^0 = 0$
for $k = 0, 1, \ldots$ **do**
    $x^{k+1} = \text{argmin}_x \{\ell(Ax) + \frac{\rho}{2}\|x - z^k + u^k\|_2^2\}$
    $z^{k+1} = \text{argmin}_z \{r(z) + \frac{\rho}{2}\|x^{k+1} - z + u^k\|_2^2\}$
    $u^{k+1} = u^k + x^{k+1} - z^{k+1}$
return $x_\star$ (nearly) minimizing $\ell(Ax) + r(x)$

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problem: x-min involves the (large) data: not easy to solve!

solution: NysADMM [Zhao, Frangella, and Udell (2022)]

- *approximate* x-min with linear system
- solve (to moderate tolerance) with Nyström PCG

Quadratic approximation

if ℓ is twice diffable, approximate obj near prev iterate x^k

$$\ell(Ax) \approx \ell(Ax^k) + (x - x^k)^T A^T \nabla \ell(Ax^k) + \frac{1}{2}(x - x^k)^T A^T H_\ell(Ax^k) A(x - x^k)$$

where H_ℓ is the Hessian of ℓ.

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where H_ℓ is the Hessian of ℓ.

with this approximation, x-min becomes linear system: find x so

$$(A^T H_\ell(Ax^k)A + \rho I)x = r^k$$

where $r^k = \rho z^k - \rho u^k + A^T H_\ell(Ax^k)Ax^k - A^T \nabla \ell(Ax^k)$

NysADMM algorithm

Algorithm NysADMM

input loss function $\ell \circ A$, regularization r, stepsize ρ, positive summable sequence $\{\varepsilon^k\}_{k=0}^{\infty}$, initial z^0, $u^0 = 0$

for $k = 0, 1, \ldots$ **do**

  compute $r^k = \rho z^k - \rho u^k + A^T H_\ell(Ax^k)Ax^k - A^T \nabla \ell(Ax^k)$

  use Nyström PCG to find ε^k-apx solution x^{k+1} to

$$(A^T H_\ell(Ax^k)A + \rho I)x^{k+1} = r^k$$

  $z^{k+1} = \text{argmin}_z\{r(z) + \frac{\rho}{2}\|x^{k+1} - z + u^k\|_2^2\}$

  $u^{k+1} = u^k + x^{k+1} - z^{k+1}$

return $x_\star$ (nearly) minimizing $\ell(Ax) + r(x)$

The competition

lasso:

- SSNAL, a Newton augmented Lagrangian method [X. Li, Sun, and Toh (2018)]
- mfIPM, a matrix-free interior point method [Fountoulakis, Gondzio, and Zhlobich (2014)]
- glmnet, a coordinate-descent method [Friedman, Hastie, and Tibshirani (2010)]

logistic regression:

- SAGA, a stochastic average gradient method [Defazio, Bach, and Lacoste-Julien (2014)]

SVM:

- LIBSVM, a sequential minimal optimization (pairwise coordinate descent) method [Chang and Lin (2011)]

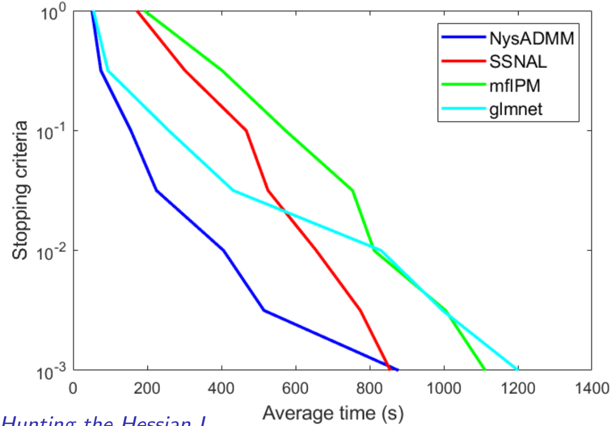
Numerical experiments: settings

- pick datasets with $n > 10,000$ or $d > 10,000$ from LIBSVM, UCI, and OpenML.
- use random feature map to generate more features
- use same stopping criterion and parameter settings as the standard solver for each problem class
- constant sketch size $s = 30$

Lasso results

stl10 dataset. stop iteration when

$$\frac{\|x - \mathrm{prox}_{\gamma\|\cdot\|_1}(x - A^T(Ax - b))\|}{1 + \|x\| + \|Ax - b\|} \leq \epsilon.$$



Lasso results

Task	Time for $\epsilon = 10^{-1}$ (s)			
	NysADMM	mfIPM	SSNAL	glmnet
STL-10	**165**	573	467	278
CIFAR-10-rf	**251**	655	692	391
smallNorb-rf	**219**	552	515	293
E2006.train	**313**	875	903	554
sector	**235**	678	608	396
realsim-rf	**193**	–	765	292
rcv1-rf	**226**	563	595	273
cod-rna-rf	**208**	976	865	324

ℓ_1-regularized logistic regression results

Table: Results for ℓ_1-regularized logistic regression experiment.

Task	NysADMM time (s)	SAGA (sklearn) time (s)
STL-10	**3012**	6083
CIFAR-10-rf	**7884**	21256
p53-rf	**528**	2116
connect-4-rf	**866**	4781
smallnorb-rf	**1808**	6381
rcv1-rf	**1237**	3988
con-rna-rf	**7528**	21513

Support vector machine results

NysADMM is $\geq 5\times$ faster, although code is pure python!

Table: Results of SVM experiment.

Task	NysADMM time (s)	LIBSVM time (s)
STL-10	**208**	11573
CIFAR-10	**1636**	8563
p53-rf	**291**	919
connect-4-rf	**7073**	42762
realsim-rf	**17045**	52397
rcv1-rf	**564**	32848
cod-rna-rf	**4942**	36791

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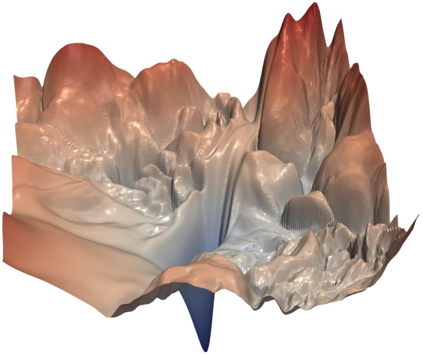
Optimization landscape

best methods for optimization depend on the landscape

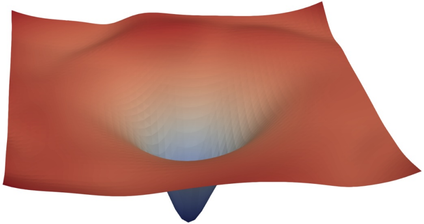
- local minima?
- saddle points?
- ill-conditioning?

what landscapes should we expect in modern problems (eg, deep learning)?

Architectural choices govern optimization landscape



(a) without skip connections



(b) with skip connections

Figure 1: The loss surfaces of ResNet-56 with/without skip connections. The proposed filter normalization scheme is used to enable comparisons of sharpness/flatness between the two figures.

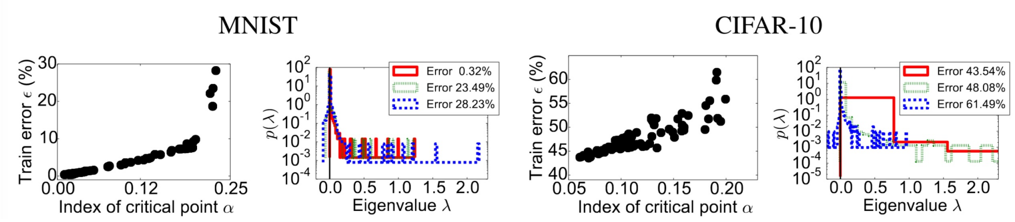
Source: H. Li, Xu, Taylor, et al., 2018

Saddle points vs local minima in deep learning

- **index** of critical point is

  $$\# \text{ negative Hessian eigenvalues} = \text{directions of negative curvature}$$

- observation: all local minima are (nearly) global minima
- but there are plenty of saddles! or just degenerate local minima?
  - "negative" eigenvalues are all nearly 0



Source: MLP experiments from Dauphin, Pascanu, Gulcehre, et al., 2014; for a modern take, see Sun, Li, Liang, et al., 2020.

Landscape-aware optimization

agenda:

1. **local minima.** ignore them: they are rarely a problem in modern architectures
    - or try random restarts / judicious initialization ...

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2. **saddles.**
   - seek and follow directions of negative curvature? [Royer, O'Neill, and Wright (2020)]
   - nah, ignore them: associated eigenvalues are small [Alain, Roux, and Manzagol (2019) and Rathore, Lei, Frangella, et al. (2024)]

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but how to query and use the $p \times p$ Hessian of $f : \mathbf{R}^p \to \mathbf{R}$?

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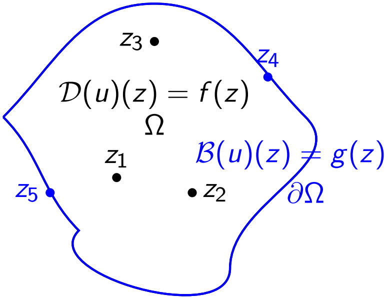
Physics-Informed Neural Networks (PINNs)

goal: solve PDE to find solution $u : \Omega \to \mathbf{R}$

$$\mathcal{D}(u)(z) = f(z), \quad z \in \Omega$$
$$\mathcal{B}(u)(z) = g(z), \quad z \in \partial\Omega,$$

where $\mathcal{D}$ is a differential operator, f is a forcing function, $\mathcal{B}$ is initial condition/boundary condition operator, and g is boundary function.

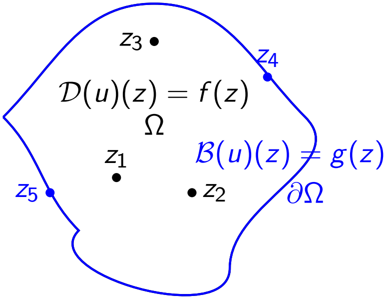


Physics-Informed Neural Networks (PINNs)

goal: solve PDE to find solution $u : \Omega \to \mathbf{R}$

$$\mathcal{D}(u)(z) = f(z), \quad z \in \Omega$$
$$\mathcal{B}(u)(z) = g(z), \quad z \in \partial\Omega,$$

where $\mathcal{D}$ is a differential operator, f is a forcing function, $\mathcal{B}$ is initial condition/boundary condition operator, and g is boundary function.



PINNs train a neural network $u_\theta(z)$ to approximate the PDE solution by minimizing a loss function that includes both data and physics-based terms

$$\frac{1}{N_{\mathrm{r}}} \sum_{i=1}^{N_{\mathrm{r}}} \|\mathcal{D}(u_\theta(z_i)) - f(z_i)\|^2 + \frac{1}{N_{\mathcal{B}}} \sum_{i=1}^{N_{\mathcal{B}}} \|\mathcal{B}(u_\theta(z_i)) - g(z_i)\|^2$$

PINNs suffer from under-optimization

- After training, gradient norm is typically on the order 10^{-2} or 10^{-3}
- L-BFGS stops early because PyTorch detects instability in the preconditioner
- Our proposal: fine-tune with NysNewton-CG (NNCG), i.e.,
  use Newton's method and solve linear system with NyströmPCG

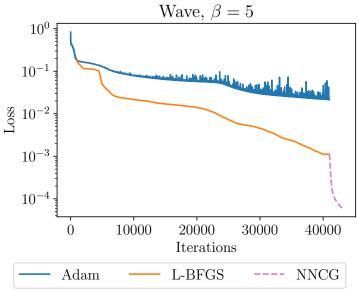


Figure: Even after running L-BFGS, the loss can be improved.

Source: [Rathore, Lei, Frangella, et al. (2024)]

We can access $\nabla^2 f(w)$ with automatic differentiation!

automatic differentiation (AD) on $f : \mathbf{R}^p \to \mathbf{R}$ can compute gradients $\nabla f(w)$ and Hessian-vector products (hvp) $(\nabla^2 f(w))v$ in $O(p)$ time!

1. compute gradient with automatic differentiation (AD) $g(w) = \nabla f(w)$
2. define Hessian vector product with vector v

$$(\nabla^2 f(w))v = \nabla(g(w) \cdot v)$$

   and compute using AD on $g(w) \cdot v$ (Pearlmutter's trick)
3. cost: two passes of AD $\approx 4\times$ cost of function evaluation (usually, $O(p)$)

Newton-CG: a matvec-only nearly-second-order optimizer

Newton-CG: repeat

- approximate f locally as a quadratic with $A = \nabla^2 f(x_0)$

$$f(x) \approx f(x_0) + \nabla f(x_0)^T (x - x_0) + \frac{1}{2}(x - x_0)^T A(x - x_0).$$

- (optionally) find a good preconditioner for A
- solve linear system $Ax = Ax_0 - \nabla f(x_0)$ with PCG.

algorithm only uses gradient evaluations and matrix-vector products with A
$\implies$ compatible with AD

Source: [Rathore, Lei, Frangella, et al. (2024)]

Preconditioners can improve conditioning

plot spectral density of PINN Hessian for different PDEs

- blue: original function
- orange: after preconditioning

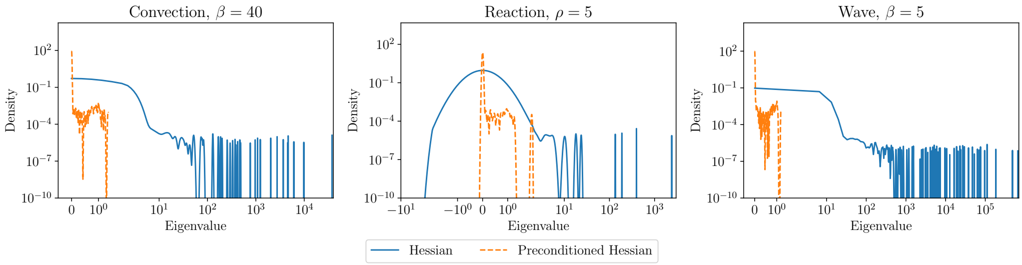
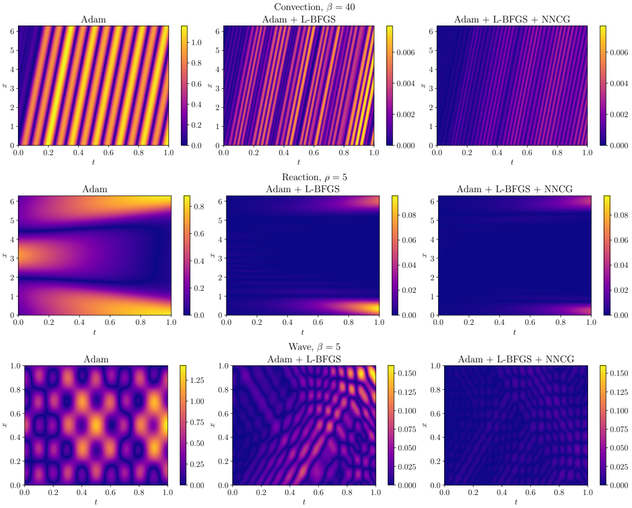


Figure: The total loss is ill-conditioned for all three PDEs. [Rathore, Lei, Frangella, et al. (2024)]

Source: Approximate spectral density with kernel smoothing + stochastic trace estimation + Gaussian quadrature + Lanczos [Ubaru, Chen, and Saad (2017) and Yao, Gholami, Keutzer, and Mahoney (2020)]

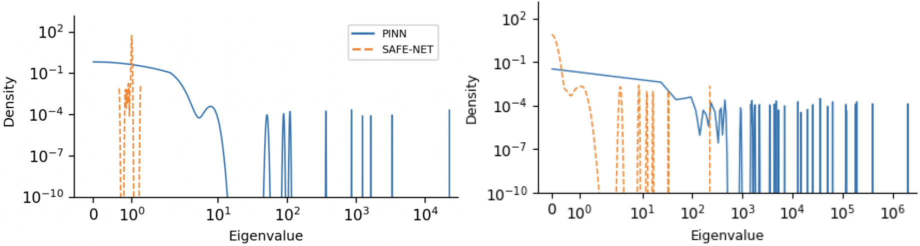
Preconditioned optimizers improve fits



Architectural choices can improve conditioning

plot spectral density of PINN Hessian for wave PDEs

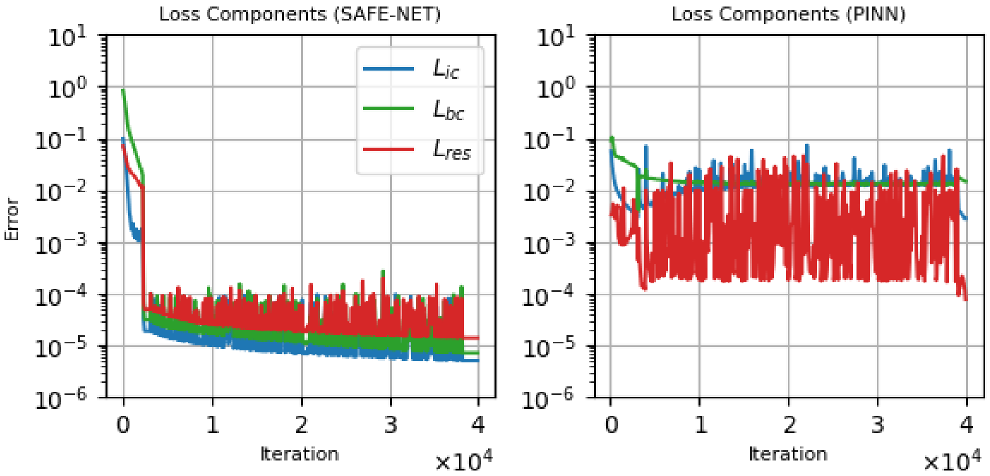
- blue: standard MLP architecture
- orange: with SAFE-NET architecture (single layer with fourier features)



(a) Early into Training (b) End of Training

Figure: Spectral density for the wave PDE using SAFE-NET and PINN at the early stages of training and at the end of training.

Well-conditioned architectures improve fits



(a) Wave

rlaopt: Randomized Linear Algebra for Scalable Optimization

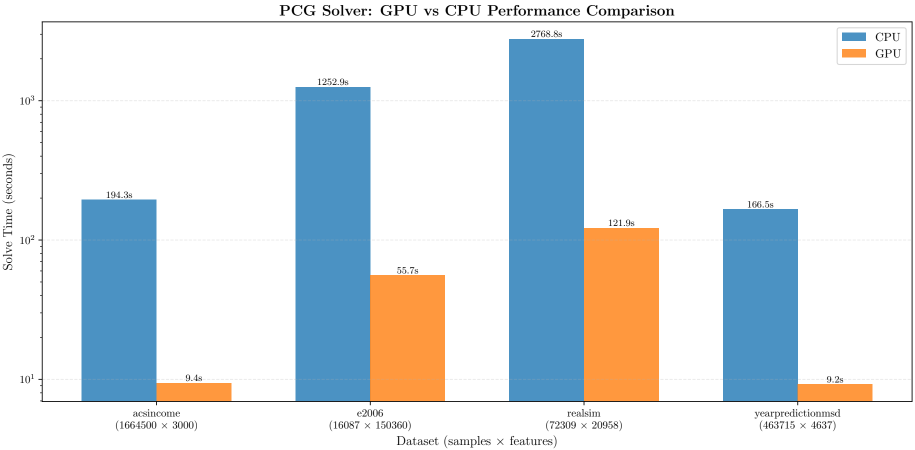
problems:

- solve linear systems $Ax = b$ faster
- composite optimization: minimize $f(Ax) + g(x)$
- stochastic optimization: minimize $\sum_{i=1}^{n} f_i(x)$

algorithms:

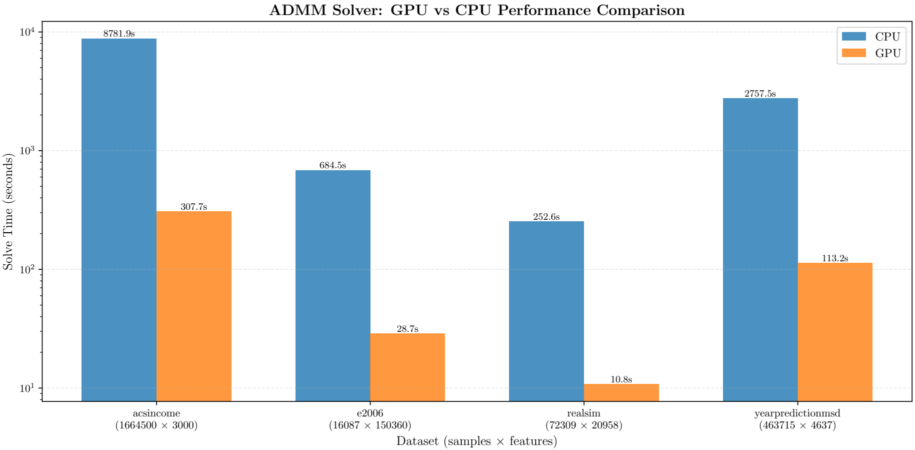
- Nyström PCG for solving linear systems
- Nyström ADMM for composite optimization
- PROMISE: low-rank stochastic optimization
- SAPPHIRE: stochastic proximal gradient method

rlaopt delivers 20× speedups solving dense linear system



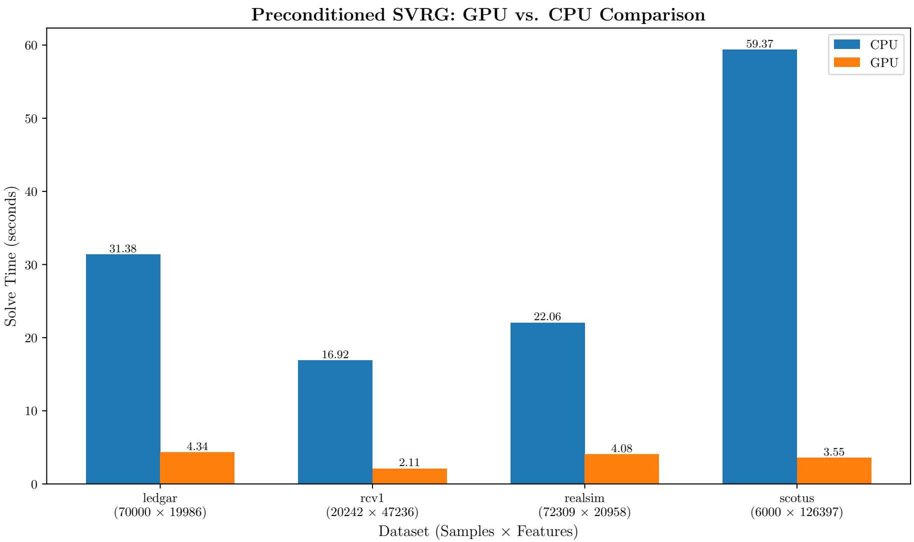
ridge regression solved with PCG + Nyström preconditioner

rlaopt delivers 25× speedups solving elastic net



elastic net with a box constraint solved with NysADMM

rlaopt delivers 8× speedups solving logistic regression



Conclusion

does your optimization suffer from ill-conditioning?

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  - randomized Nyström approximation
  - autodiff from Hessian-vector products

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  - randomized Nyström approximation
  - autodiff from Hessian-vector products
- randomized preconditioners can speed up
  - composite optimization (e.g.NysADMM)
  - deep learning (e.g.NysNewton-CG)
  - stochastic optimization (e.g.SketchySGD, PROMISE, SAPPHIRE)

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  - randomized Nyström approximation
  - autodiff from Hessian-vector products
- randomized preconditioners can speed up
  - composite optimization (e.g.NysADMM)
  - deep learning (e.g.NysNewton-CG)
  - stochastic optimization (e.g.SketchySGD, PROMISE, SAPPHIRE)
- (tomorrow) online scaled gradient method
  - provably competes with the best offline methods
  - flexible framework can improve many optimization algorithms

Where can I learn more?

- randomized Nyström approximation to a psd matrix: https://arxiv.org/abs/1706.05736 NeurIPS 2017
- Nyström PCG to solve $Ax = b$: https://arxiv.org/abs/2110.02820 SIMAX 2023
- NysADMM for composite optimization minimize $\ell(x) + r(x)$:
  - algorithm (NysADMM): https://arxiv.org/abs/2202.11599
  - convergence (GeNI-ADMM): https://arxiv.org/abs/2302.03863
  - solver (GeNIOS): https://github.com/tjdiamandis/GeNIOS.jl
- almost-second-order stochastic optimization:
  - SketchySGD (improves SGD): https://arxiv.org/abs/2211.08597 SIMODS 2024
  - PROMISE (improves SVRG etc.): https://arxiv.org/abs/2309.02014 JMLR 2024
  - NNCG for PINNs: https://arxiv.org/abs/2402.01868 ICML 2024
  - SAFE-NET for PINNs: http://arxiv.org/abs/2502.07209
- PyTorch implementation of all these methods: rlaopt https:www.github.com/udellgroup/rlaopt