The Power of Preconditioning in Overparameterized Low-Rank Matrix Sensing

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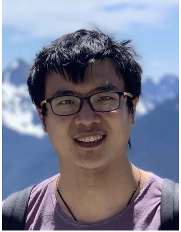
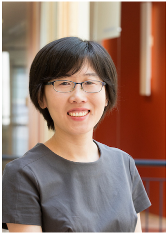
Department of Statistics, UChicago

Quantitative Methods Seminar, Purdue University, Dec. 2023

Xingyu Xu
CMU

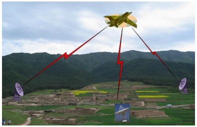


Yandi Shen
UChicago → CMU

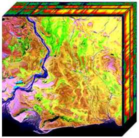


Yuejie Chi
CMU

Low-rank matrices in data science

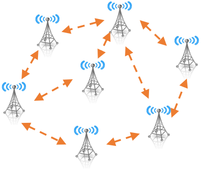


radar imaging

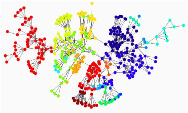


hyperspectral imaging

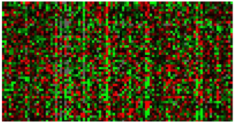
recommendation systems



localization



community detection



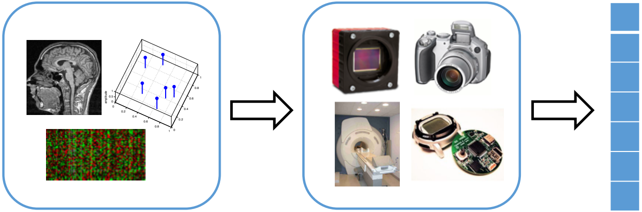
bioinformatics

Low-rank matrix recovery

$\boldsymbol{M} \in \mathbb{R}^{n_1 \times n_2}$
$\mathrm{rank}(\boldsymbol{M}) = r$

$\mathcal{A}(\cdot)$
linear map

$\boldsymbol{y} \in \mathbb{R}^m$



$$\boldsymbol{y} = \mathcal{A}(\boldsymbol{M})$$

Goal: recover $\boldsymbol{M}$ in the sample-starved regime

$$\underbrace{(n_1 + n_2)r}_{\text{degrees of freedom}} \quad \lesssim \quad \underbrace{m}_{\text{no. ofmeasurements}} \quad \ll \quad \underbrace{n_1 n_2}_{\text{ambient dimension}}$$

Convex relaxation via nuclear norm minimization

$$\min_{\boldsymbol{Z}\in\mathbb{R}^{n_1\times n_2}} \quad \mathsf{rank}(\boldsymbol{Z}) \qquad \text{s.t.} \qquad \boldsymbol{y}\approx\mathcal{A}(\boldsymbol{Z})$$

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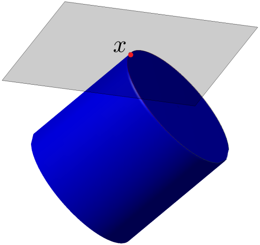
$$\Big\Downarrow \text{cvx surrogate}$$

$$\min_{\boldsymbol{Z}\in\mathbb{R}^{n_1\times n_2}} \quad \|\boldsymbol{Z}\|_* \qquad \text{s.t.} \quad \boldsymbol{y}\approx\mathcal{A}(\boldsymbol{Z})$$

where $\|\cdot\|_*$ is the nuclear norm



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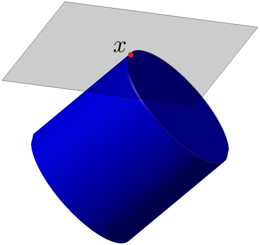

Significant developments in the last decade:

Fazel '02, Recht, Parrilo, Fazel '10, Candès, Recht '09, Candès, Tao '10, Cai et al. '10, Gross '10, Negahban, Wainwright '11, Sanghavi et al. '13, Chen, Chi '14, ...

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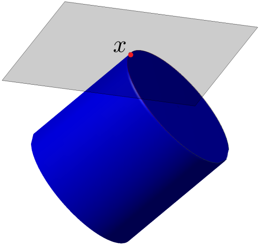

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Poor scalability: operate in the *ambient* matrix space

Low-rank matrix factorization

$$\min_{\mathrm{rank}(\boldsymbol{Z})=r} \quad \frac{1}{2}\left\|\boldsymbol{y}-\mathcal{A}(\boldsymbol{Z})\right\|_2^2$$

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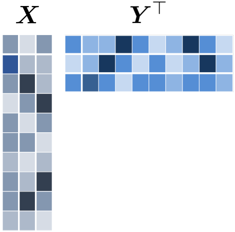
$$\Downarrow$$

$\boldsymbol{Z} =$



$$\min_{\boldsymbol{X}\in\mathbb{R}^{n_1\times r},\boldsymbol{Y}\in\mathbb{R}^{n_2\times r}} \quad f(\boldsymbol{X},\boldsymbol{Y}) = \frac{1}{2}\left\|\boldsymbol{y}-\mathcal{A}(\boldsymbol{X}\boldsymbol{Y}^\top)\right\|_2^2$$

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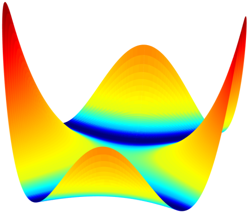

$\Downarrow$

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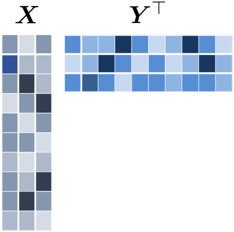

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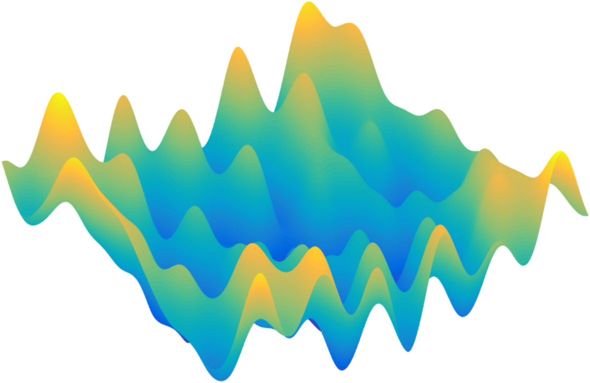
Nonconvex problems are hard (in theory)



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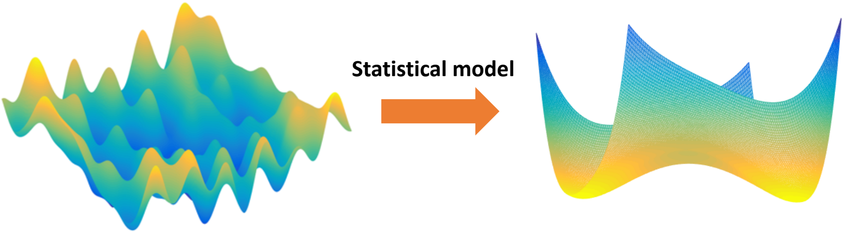
Statistics meets optimization

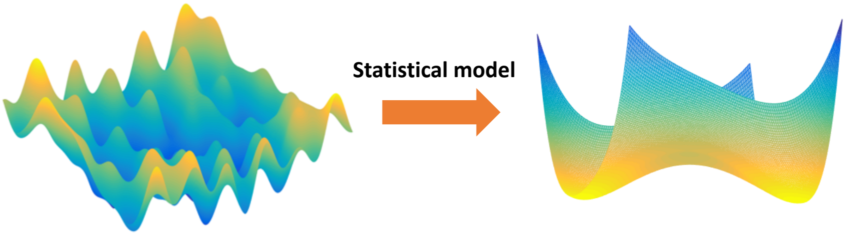


Statistical model

worst case

average case

Statistics meets optimization



Statistical model

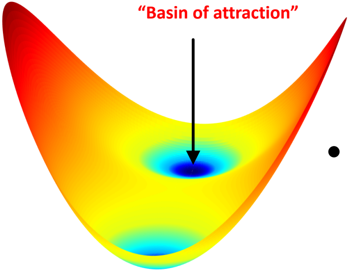
worst case

average case

Simple algorithms can be efficient for nonconvex problems

Matrix sensing: GD with balancing regularization

$$\min_{\boldsymbol{X},\boldsymbol{Y}} \quad f_{\mathrm{reg}}(\boldsymbol{X},\boldsymbol{Y}) = \frac{1}{2}\left\|\boldsymbol{y} - \mathcal{A}(\boldsymbol{X}\boldsymbol{Y}^\top)\right\|_2^2 + \frac{1}{8}\left\|\boldsymbol{X}^\top\boldsymbol{X} - \boldsymbol{Y}^\top\boldsymbol{Y}\right\|_{\mathrm{F}}^2$$



- **Spectral initialization:** find an initial point in the "basin of attraction"

$$(\boldsymbol{X}_0, \boldsymbol{Y}_0) \leftarrow \mathsf{SVD}_r(\mathcal{A}^*(\boldsymbol{y}))$$

- **Gradient iterations:** for $t = 0, 1, \dots,$

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t - \eta \nabla_{\boldsymbol{X}} f_{\mathrm{reg}}(\boldsymbol{X}_t, \boldsymbol{Y}_t)$$
$$\boldsymbol{Y}_{t+1} = \boldsymbol{Y}_t - \eta \nabla_{\boldsymbol{Y}} f_{\mathrm{reg}}(\boldsymbol{X}_t, \boldsymbol{Y}_t)$$

Prior theory for vanilla GD

Condition number $\kappa = \frac{\sigma_{\max}(\boldsymbol{M})}{\sigma_{\min}(\boldsymbol{M})}$

Theorem 1 (Tu et al., ICML 2016)

For low-rank matrix sensing with i.i.d. Gaussian design, vanilla GD (with spectral initialization) achieves

$$\|\boldsymbol{X}_t \boldsymbol{Y}_t^\top - \boldsymbol{M}\|_{\mathrm{F}} \leq \varepsilon \cdot \sigma_{\min}(\boldsymbol{M})$$

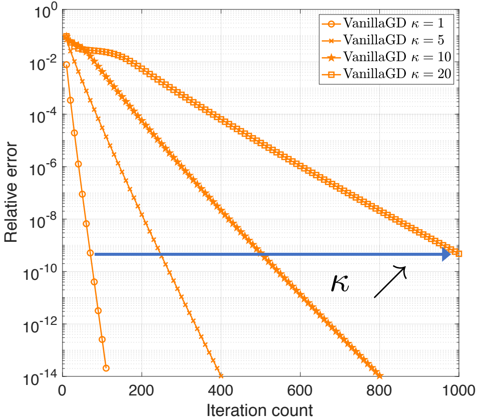
- ***Computational:*** *within* $O(\kappa \log \frac{1}{\varepsilon})$ *iterations;*
- ***Statistical:*** *as long as the sample size satisfies*

$$m \gtrsim (n_1 + n_2) r^2 \kappa^2$$

Similar results hold for many other low-rank problems

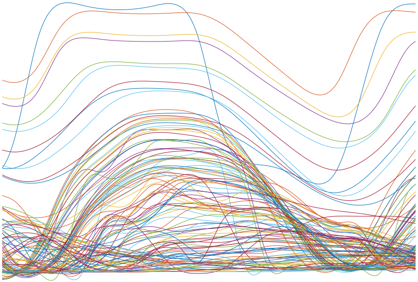
GD slows down for ill-conditioned matrices

Condition number $\kappa = \frac{\sigma_{\max}(\boldsymbol{M})}{\sigma_{\min}(\boldsymbol{M})}$

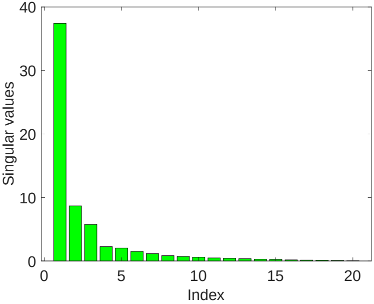


Vanilla GD converges in $O\big(\kappa \log \frac{1}{\varepsilon}\big)$ iterations

Condition number can be large



chlorine concentration levels
120 junctions, 180 time slots



power-law spectrum

Data source: `www.epa.gov/water-research/epanet`

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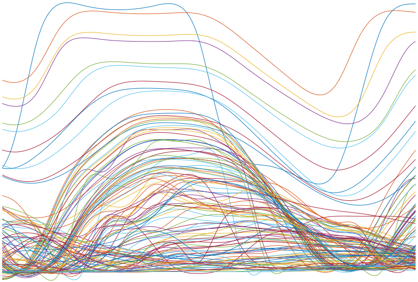

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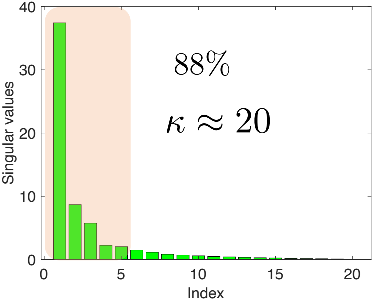
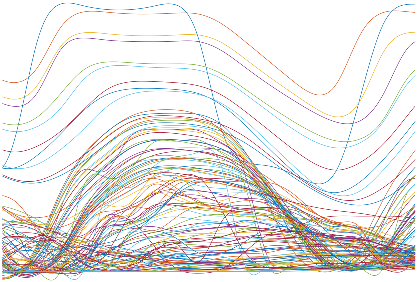


rank-5 approximation

Data source: `www.epa.gov/water-research/epanet`

Condition number can be large



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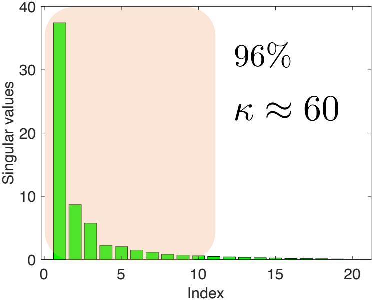

rank-10 approximation

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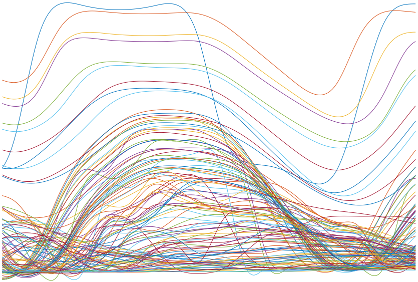

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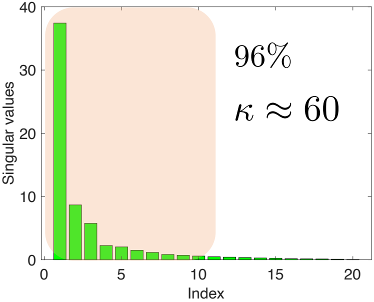


rank-10 approximation

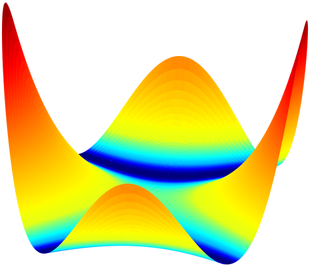
Can we accelerate the convergence rate of GD to $O(\log \frac{1}{\varepsilon})$?

Data source: `www.epa.gov/water-research/epanet`

A recipe: scaled gradient descent (ScaledGD)

—joint work with Tian Tong, and Yuejie Chi

$f(\boldsymbol{X},\boldsymbol{Y}) = \|\boldsymbol{y} - \mathcal{A}(\boldsymbol{X}\boldsymbol{Y}^\top)\|_2^2$



- **Spectral initialization:** find an initial point in the “basin of attraction”
- **Scaled gradient iterations:** for $t = 0, 1, \ldots,$

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t - \eta \nabla_{\boldsymbol{X}} f(\boldsymbol{X}_t, \boldsymbol{Y}_t) \underbrace{(\boldsymbol{Y}_t^\top \boldsymbol{Y}_t)^{-1}}_{\texttt{preconditioner}}$$

$$\boldsymbol{Y}_{t+1} = \boldsymbol{Y}_t - \eta \nabla_{\boldsymbol{Y}} f(\boldsymbol{X}_t, \boldsymbol{Y}_t) \underbrace{(\boldsymbol{X}_t^\top \boldsymbol{X}_t)^{-1}}_{\texttt{preconditioner}}$$

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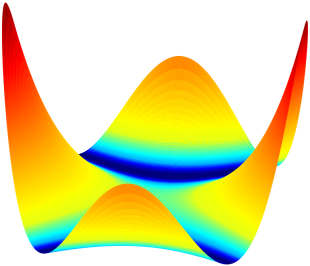

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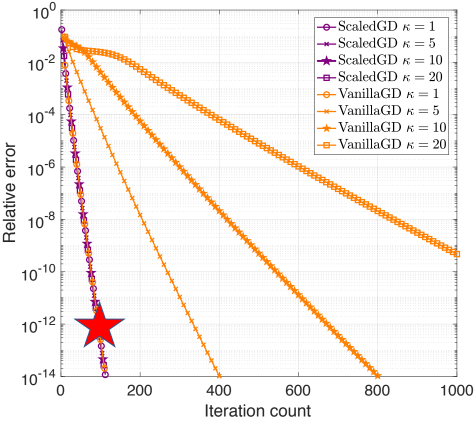
ScaledGD is a *preconditioned* gradient method
without balancing regularization

ScaledGD for low-rank matrix completion



Huge computational saving: ScaledGD converges in a κ-independent manner with minimal overhead

A closer look at ScaledGD

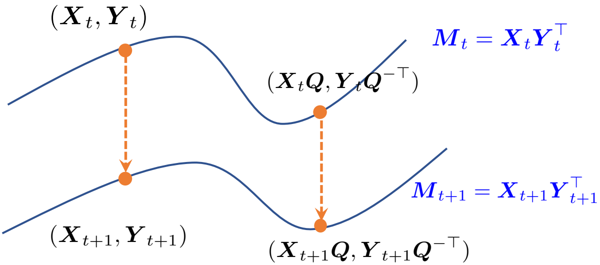
Connection to quasi-Newton method :

Define $\boldsymbol{F}_t = [\boldsymbol{X}_t^\top, \boldsymbol{Y}_t^\top]^\top \in \mathbb{R}^{(n_1+n_2)\times r}$. One can write update rule as

$$
\begin{aligned}
&\mathrm{vec}(\boldsymbol{F}_{t+1}) \\
&= \mathrm{vec}(\boldsymbol{F}_t) - \eta \underbrace{\begin{bmatrix} (\boldsymbol{Y}_t^\top \boldsymbol{Y}_t) \otimes \boldsymbol{I}_{n_1} & \boldsymbol{0} \\ \boldsymbol{0} & (\boldsymbol{X}_t^\top \boldsymbol{X}_t) \otimes \boldsymbol{I}_{n_2} \end{bmatrix}^{-1}}_{=: \boldsymbol{H}_t^{-1}} \mathrm{vec}(\nabla_{\boldsymbol{F}} \mathcal{L}(\boldsymbol{F}_t))
\end{aligned}
$$

A closer look at ScaledGD

Invariance to invertible transforms:


$(\boldsymbol{X}_t, \boldsymbol{Y}_t)$
$\boldsymbol{M}_t = \boldsymbol{X}_t \boldsymbol{Y}_t^\top$
$(\boldsymbol{X}_t \boldsymbol{Q}, \boldsymbol{Y}_t \boldsymbol{Q}^{-\top})$
$\boldsymbol{M}_{t+1} = \boldsymbol{X}_{t+1} \boldsymbol{Y}_{t+1}^\top$
$(\boldsymbol{X}_{t+1}, \boldsymbol{Y}_{t+1})$
$(\boldsymbol{X}_{t+1} \boldsymbol{Q}, \boldsymbol{Y}_{t+1} \boldsymbol{Q}^{-\top})$

— not true for GD

Theoretical guarantees of ScaledGD

Theorem 2 (Tong, Ma and Chi, JMLR 2021)

For low-rank matrix sensing with i.i.d. Gaussian design, ScaledGD with spectral initialization achieves

$$\|\boldsymbol{X}_t \boldsymbol{Y}_t^\top - \boldsymbol{M}\|_{\mathrm{F}} \lesssim \varepsilon \cdot \sigma_{\min}(\boldsymbol{M})$$

- ***Computational:*** *within* $O\big(\log \frac{1}{\varepsilon}\big)$ *iterations*
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$$m \gtrsim (n_1 + n_2) r^2 \kappa^2$$

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- ***Statistical:*** *the sample complexity satisfies*

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Strict improvement over Tu et al.: ScaledGD provably accelerates vanilla GD with the same sample complexity

Key ingredient in analysis

Scaled distance metric:

$$\mathsf{dist}^2\left(\begin{bmatrix}\boldsymbol{X}_t\\ \boldsymbol{Y}_t\end{bmatrix},\begin{bmatrix}\boldsymbol{X}\\ \boldsymbol{Y}\end{bmatrix}\right)=\inf_{\boldsymbol{Q}\in\mathrm{GL}(r)}\left\|(\boldsymbol{X}_t\boldsymbol{Q}-\boldsymbol{X})\boldsymbol{\Sigma}^{1/2}\right\|_{\mathrm{F}}^2+\left\|(\boldsymbol{Y}_t\boldsymbol{Q}^{-\top}-\boldsymbol{Y})\boldsymbol{\Sigma}^{1/2}\right\|_{\mathrm{F}}^2$$

where $\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}$ is SVD of $\boldsymbol{M}$, $\boldsymbol{X}=\boldsymbol{U}\boldsymbol{\Sigma}^{1/2}$, $\boldsymbol{U}=\boldsymbol{V}\boldsymbol{\Sigma}^{1/2}$

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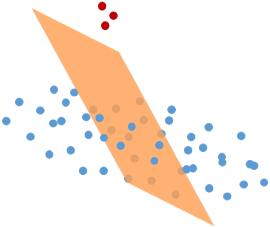
where $\boldsymbol{U\Sigma V}$ is SVD of $\boldsymbol{M}$, $\boldsymbol{X} = \boldsymbol{U\Sigma}^{1/2}$, $\boldsymbol{U} = \boldsymbol{V\Sigma}^{1/2}$

- Account for ambiguity arising from invertible transforms
- Fidelity to reconstruction loss: locally, we have

$$\mathsf{dist}^2\left(\begin{bmatrix}\boldsymbol{X}_t\\ \boldsymbol{Y}_t\end{bmatrix}, \begin{bmatrix}\boldsymbol{X}\\ \boldsymbol{Y}\end{bmatrix}\right) \asymp \|\boldsymbol{X}_t\boldsymbol{Y}_t^\top - \boldsymbol{M}\|_{\mathrm{F}}^2$$

ScaledGD works more broadly



$$\begin{bmatrix} \checkmark & ? & ? & ? & \checkmark \\ ? & ? & \checkmark & \checkmark & ? \\ \checkmark & ? & ? & \checkmark & ? \\ ? & ? & \checkmark & ? & ? \\ \checkmark & ? & ? & ? & ? \\ ? & \checkmark & ? & ? & \checkmark \end{bmatrix}$$

	Robust PCA		**Matrix completion**	
Algorithms	corruption fraction	iteration complexity	sample complexity	iteration complexity
GD	$\frac{1}{\mu r^{3/2}\kappa^{3/2}\vee\mu r\kappa^2}$	$\kappa\log\frac{1}{\varepsilon}$	$(\mu\vee\log n)\mu n r^2\kappa^2$	$\kappa\log\frac{1}{\varepsilon}$
ScaledGD	$\frac{1}{\mu r^{3/2}\kappa}$	$\log\frac{1}{\varepsilon}$	$(\mu\kappa^2\vee\log n)\mu n r^2\kappa^2$	$\log\frac{1}{\varepsilon}$

Huge computational saving at comparable sample complexities

What if we do not know the exact rank?

So far we have assumed the exact rank is given.... what if we do not know the exact rank?

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Misspecification by overparameterization:

$$\boldsymbol{M} = \boldsymbol{X}\boldsymbol{X}^\top, \qquad \boldsymbol{X} \in \mathbb{R}^{n \times \tilde{r}}, \qquad \tilde{r} > r$$

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ScaledGD:

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t - \eta \nabla_{\boldsymbol{X}} f(\boldsymbol{X}_t) \underbrace{(\boldsymbol{X}_t^\top \boldsymbol{X}_t)^{-1}}_{\texttt{preconditioner}}$$

analysis break down and might be unstable...

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ScaledGD(λ):

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t - \eta\,\nabla_{\boldsymbol{X}} f(\boldsymbol{X}_t)\underbrace{(\boldsymbol{X}_t^\top \boldsymbol{X}_t + \lambda \boldsymbol{I})^{-1}}_{\texttt{preconditioner}}$$

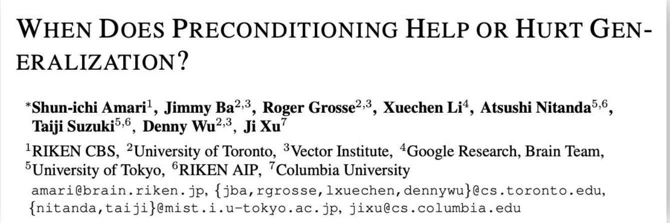
add regularization to stablize the preconditioner

Does preconditioning hurt generalization?

- Infinitely many global minima, not all generalize
- Can we still guarantee generalization?

optimization

generalization



WHEN DOES PRECONDITIONING HELP OR HURT GENERALIZATION?

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Theoretical guarantees

Theorem 3 (Xu, Shen, Chi, Ma, ICML 2023)

For low-rank matrix sensing with i.i.d. Gaussian design, overparameterized ScaledGD(λ) *with* $\lambda \asymp \sigma_{\min}(\boldsymbol{M})$, $\eta \asymp 1$, *and a sufficiently small random initialization achieves*

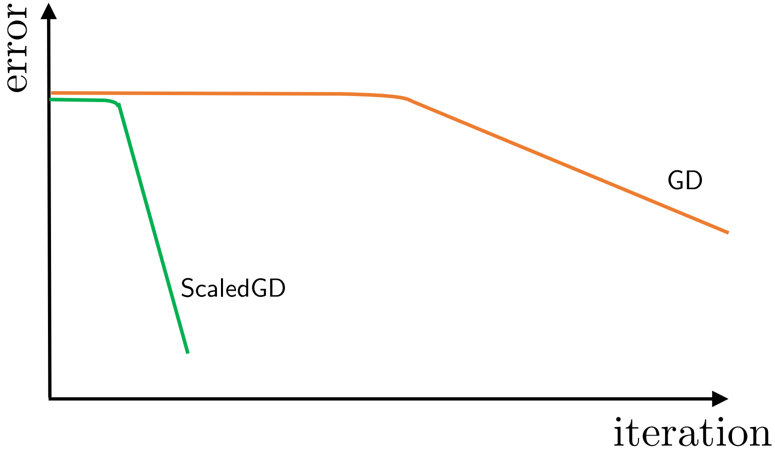
$$\|\boldsymbol{X}_t\boldsymbol{X}_t^\top - \boldsymbol{M}\|_{\mathrm{F}} \lesssim \varepsilon \cdot \sigma_{\min}(\boldsymbol{M})$$

- ***Computational:*** *within* $O\big(\log\kappa\log(\kappa n) + \log\frac{1}{\varepsilon}\big)$ *iterations;*
- ***Statistical:*** *the sample complexity satisfies*

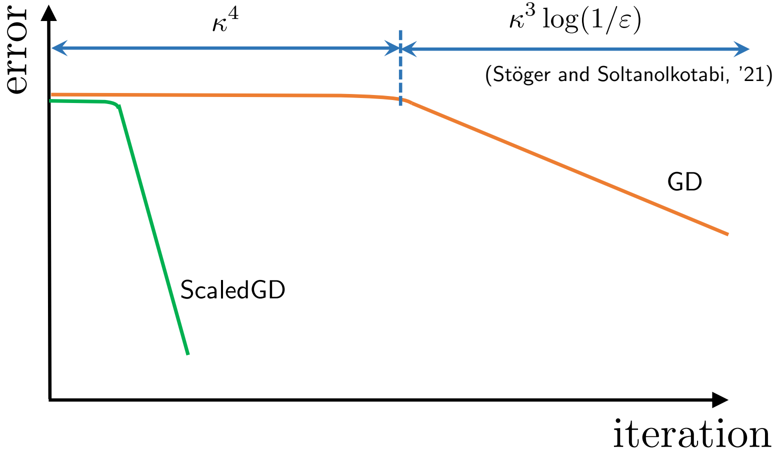
$$m \gtrsim nr^2\mathsf{poly}(\kappa)$$

- Our analysis also enables exact convergence under random initialization with correct rank specification

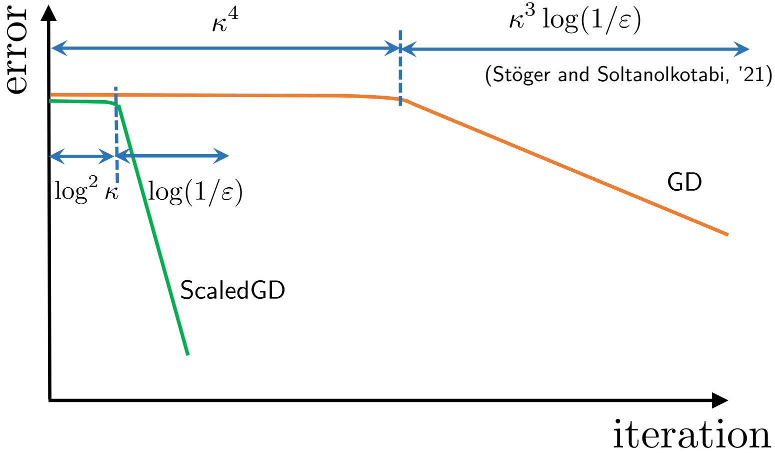
Comparison with overparameterized GD



Comparison with overparameterized GD



Comparison with overparameterized GD



ScaledGD picks up the signal component much faster than GD even from small random initialization

Comparisons with prior art

Comparison with Zhang, Fattahi, and Zhang '21

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t - \eta \nabla_{\boldsymbol{X}} f(\boldsymbol{X}_t) \underbrace{(\boldsymbol{X}_t^\top \boldsymbol{X}_t + \lambda_t \boldsymbol{I})^{-1}}_{\texttt{preconditioner}}$$

where $\lambda_t = \|\mathcal{A}(\boldsymbol{X}_t \boldsymbol{X}_t^\top - \boldsymbol{M})\|$

- Local analysis: require spectral initialization
- Large sample complexity: sample complexity is $n\tilde{r}^2 \operatorname{poly}(\kappa)$, depending on the overparameterized rank $\tilde{r}$ instead of the true rank r

Robustness to noise

Consider the noisy setting

$$y_i = \langle A_i, \boldsymbol{M} \rangle + \xi_i, \quad \text{where} \quad \xi_i \sim \mathcal{N}(0, \sigma^2)$$

Theorem 4 (Xu, Shen, Chi, Ma, '23)

For low-rank matrix sensing with i.i.d. Gaussian design, overparameterized ScaledGD(λ) with the same configuration as before achieves

$$\|\boldsymbol{X}_t \boldsymbol{X}_t^\top - \boldsymbol{M}\|_{\mathrm{F}} \lesssim \kappa^2 \sigma \sqrt{nr}$$

ScaledGD(λ) is nearly optimal

ScaledGD(λ) achieves

$$\|\boldsymbol{X}_t \boldsymbol{X}_t^\top - \boldsymbol{M}\|_{\mathrm{F}} \lesssim \kappa^2 \sigma \sqrt{nr}$$

- ScaledGD(λ) is minimax optimal (up to κ^2) for recovering rank-r matrices, cf. Candès and Plan '09
- Both the rate and sample size requirement improve over prior art (e.g., Zhuo et al., '21, Zhang et al., '23) as ours depend on true rank r

A little analysis

Phase I: approximating power method

Recall update rule of ScaledGD(λ)

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t - \eta\mathcal{A}^*\mathcal{A}(\boldsymbol{X}_t\boldsymbol{X}_t^\top - \boldsymbol{M})\boldsymbol{X}_t(\boldsymbol{X}_t^\top\boldsymbol{X}_t + \lambda\boldsymbol{I})^{-1}$$

Since initialization is small, i.e., $\boldsymbol{X}_t \approx \boldsymbol{0}$, we have

$$\begin{aligned}\boldsymbol{X}_{t+1} &\approx \boldsymbol{X}_t + \eta\mathcal{A}^*\mathcal{A}(\boldsymbol{M})\boldsymbol{X}_t\lambda^{-1} \\ &= \underbrace{\left(\boldsymbol{I} + \frac{\eta}{\lambda}\mathcal{A}^*\mathcal{A}(\boldsymbol{M})\right)\boldsymbol{X}_t}_{\text{power method iterates}}\end{aligned}$$

Phase I: approximating power method

Indeed, we show that

$$\boldsymbol{X}_t \approx \left(I + \frac{\eta}{\lambda}\mathcal{A}^*\mathcal{A}(\boldsymbol{M})\right)^t \boldsymbol{X}_0, \qquad \text{when } t \lesssim \tfrac{1}{\eta}$$

Consequently, ScaledGD(λ) has three nice properties after phase I

- subspace misalignment is small
- signal strength is mildly large
- overparameterization error remains small

Phase II: exponential amplification of the signal

In phase II, equipped with the three properties, signal is exponentially amplified in the sense that

$$\sigma_{\min}(\boldsymbol{\Sigma}^{-1/2}\boldsymbol{U}^\top\boldsymbol{X}_t) \quad \text{grows at rate } 1+\eta$$

until a constant level

$$\boldsymbol{U}^\top\boldsymbol{X}_t\boldsymbol{X}_t^\top\boldsymbol{U} \succeq 0.1\boldsymbol{\Sigma}$$

Scaled signal strength $\sigma_{\min}(\boldsymbol{\Sigma}^{-1/2}\boldsymbol{U}^\top\boldsymbol{X}_t)$ is the key

Phase II: comparison with GD

Note that signal is amplified in a scale-independent way

$$\begin{aligned} &\sigma_{\min}(\boldsymbol{\Sigma}^{-1/2}\boldsymbol{U}^\top \boldsymbol{X}_t) && \text{grows with rate } 1+\eta \\ \Longrightarrow\ &\sigma_i^2(\boldsymbol{U}^\top \boldsymbol{X}_t)/\sigma_i(\boldsymbol{M}) && \text{grows uniformly with rate } 1+\eta \end{aligned}$$

In contrast, for GD the growth of different singular values are different:

$$\sigma_i^2(\boldsymbol{U}^\top \boldsymbol{X}_t^{\mathsf{GD}}) \text{ grows with rate } 1+\eta\sigma_i(\boldsymbol{M}),$$

Phase II: comparison with GD

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$$

In contrast, for GD the growth of different singular values are different:

$$\sigma_i^2(\boldsymbol{U}^\top\boldsymbol{X}_t^{\mathsf{GD}}) \text{ grows with rate } 1+\eta\sigma_i(\boldsymbol{M}),$$

Issue: GD requires $\eta\sigma_{\max}(\boldsymbol{M}) \lesssim 1$ to stay in control, but then the growth rate for $\sigma_r^2(\boldsymbol{U}^\top\boldsymbol{X}_t^{\mathsf{GD}})$ would only be $1+O(\kappa^{-1})$

Phase III: local convergence

Recall update rule of ScaledGD(λ)

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t - \eta \mathcal{A}^* \mathcal{A}(\boldsymbol{X}_t \boldsymbol{X}_t^\top - \boldsymbol{M}) \boldsymbol{X}_t (\boldsymbol{X}_t^\top \boldsymbol{X}_t + \lambda \boldsymbol{I})^{-1}$$

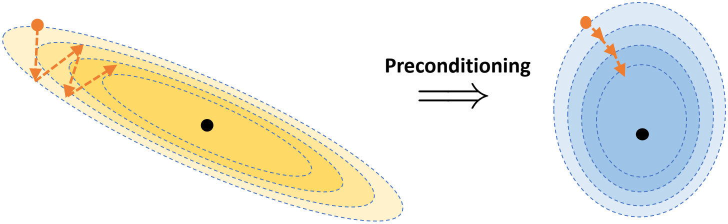
When signal is at constant level, $\boldsymbol{X}_t^\top \boldsymbol{X}_t$ dominates $\lambda \boldsymbol{I}$, which yields

$$\boldsymbol{X}_{t+1} \approx \boldsymbol{X}_t - \eta \mathcal{A}^* \mathcal{A}(\boldsymbol{X}_t \boldsymbol{X}_t^\top - \boldsymbol{M}) \boldsymbol{X}_t (\boldsymbol{X}_t^\top \boldsymbol{X}_t)^{-1}$$

ScaledGD(λ) is similar to ScaledGD locally

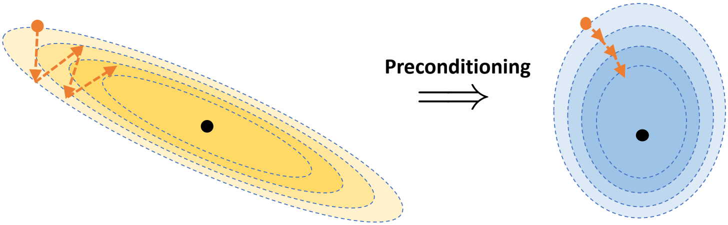
Concluding remarks

Preconditioning helps!



Preconditioning can dramatically increase the computational efficiency of vanilla gradient methods without hurting statistical efficiency

Preconditioning helps!



Preconditioning can dramatically increase the computational efficiency of vanilla gradient methods without hurting statistical efficiency

Future directions:

- streaming/stochastic variants of ScaledGD
- generalizing the idea of ScaledGD to other learning problems

Papers:

"The power of preconditioning in overparameterized low-rank matrix sensing," X. Xu, Y. Shen, Y. Chi, and C. Ma, ICML 2023

"Accelerating ill-conditioned low-rank matrix estimation via scaled gradient descent," T. Tong, C. Ma, and Y. Chi, JMLR 2021