Nonconvex Low-Rank Matrix Estimation: Geometry, Robustness, and Acceleration

Yuejie Chi

### **Carnegie Mellon University**

SIAM Conference on Imaging Science July 9, 2020 Our research is supported by National Science Foundation, Office of Naval Research and Army Research Office.



### Sensing and imaging advances

New imaging/sensing modalities allow us to probe the nature in unprecedented manners.





microscopy

The large amount of data brings exciting opportunities that call for new tools that are scalable in computation and memory.

#### Low-rank matrices in imaging science

#### Why low-rank images?

- redundant representations of latent information;
- a small number of sources of interest;
- "lifting" of indirect correlation measurements.







radar imaging



# Beyond imaging science



recommendation systems



localization





community detection

bioinformatics

#### Low-rank matrix sensing



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



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





#### 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, ...



#### 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, ...

Poor scalability: operate in the ambient matrix space

$$\min_{oldsymbol{Z} \in \mathbb{R}^{n_1 imes n_2}} \operatorname{rank}(oldsymbol{Z}) \qquad ext{ s.t. } oldsymbol{y} pprox \mathcal{A}(oldsymbol{Z})$$







#### Nonconvex problems are hard (in theory)!



"...in fact, the great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity.

R. T. Rockafellar, in SIAM Review, 1993

# Nonconvex problems are hard (in theory)!



"...in fact, the great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity.

R. T. Rockafellar, in SIAM Review, 1993

#### Recent developments: provable nonconvex optimization



"Nonconvex Optimization Meets Low-Rank Matrix Factorization: An Overview," Chi, Lu, Chen TSP 2019 Phase retrieval: Netrapalli et al. '13, Candès, Li, Soltanolkotabi '14, Chen, Candès '15, Cai, Li, Ma '15, Zhang et al. '16, Wang et al. '16, Sun, Qu, Wright '16, Ma et al. '17, Chen et al. '18, Soltani, Hegde '18, Ruan and Duchi, '18, ...

Matrix sensing/completion: Keshavan et al. '09, Jain et al. '09, Hardt '13, Jain et al. '13, Sun, Luo '15, Chen, Wainwright '15, Tu et al. '15, Zheng, Lafferty '15, Bhojanapalli et al. 16, Ge, Lee, Ma '16, Jin et al. '16, Ma et al. '17, Chen and Li'17, Cai et al. '18, Li, Zhu, Tang, Wakin '18, Charisopoulos et al. '19, ...

Blind deconvolution/demixing: Li et al. '16, Lee et al. '16, Cambareri, Jacques' 16, Ling, Strohmer' 16, Huang, Hand' 16, Ma et al. '17, Zhang et al. '18, Li, Bresler' 18, Dong, Shi' 18, Shi, Chi' 19, Qu et al. '19...

**Dictionary learning:** Arora et al. '14, Sun et al. '15, Chatterji, Bartlett '17, Bai et al. '18, Gilboa et al. '18, Rambhatla et al. '19, Qu et al. '19,...

Robust principal component analysis: Netrapalli et al. '14, Yi et al. '16, Gu et al. '16, Ge et al. '17, Cherapanamjeri et al. '17, Vaswani et al. '18, Maunu et al. '19, ...

**Deep learning:** Zhong et al. '17, Bai, Mei, Montanari '17, Du et al. '17, Ge, Lee, Ma '17, Du et al. '18, Soltanolkotabi and Oymak, '18...

#### **Optimization geometry:**

When and why does simple gradient descent work well for low-rank matrix estimation?

#### **Robustness to adversarial outliers:**

Can we design provably robust gradient algorithms that are oblivious to the presence of outliers?

#### Acceleration for ill-conditioned matrix estimation:

Can we design provably fast gradient algorithms that are insensitive to the condition number of low-rank matrices?

# Geometry and implicit regularization in nonconvex low-rank matrix estimation



Yuxin Chen Princeton



Cong Ma Princeton



Kaizheng Wang Princeton



Yuanxin Li CMU

# Low-rank matrix completion: dealing with missing data



Given partial samples of a *low-rank* matrix  $M = X_{\star}X_{\star}^{\top} \in \mathbb{R}^{n \times n}$ in an index set  $\Omega$ , fill in missing entries.

$$\min_{oldsymbol{X} \in \mathbb{R}^{n imes r}} f(oldsymbol{X}) = rac{1}{2} \left\| \mathcal{P}_{\Omega}(oldsymbol{X}oldsymbol{X}^{ op} - oldsymbol{M}) 
ight\|_{\mathrm{F}}^2$$

#### What might the loss function look like?

Full observation = PCA: 
$$f(X) = \left\| X X^{\top} - M \right\|_{\mathrm{F}}^{2}$$
.

 $f\left(oldsymbol{X}
ight)$  restricted strongly convex and smooth

along descent direction V when X is close to  $X_{\star}$ .



# Parameter recovery via gradient descent (GD)

#### a two-step recovery strategy:



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

$$\boldsymbol{X}_0 = \mathsf{SVD}_r(\mathcal{P}_\Omega(\boldsymbol{M}))$$

• Gradient iterations:

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t - \eta \,\nabla f(\boldsymbol{X}_t)$$

for t = 0, 1, ...

# Parameter recovery via gradient descent (GD)

#### a two-step recovery strategy:



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

$$X_0 = \mathsf{SVD}_r(\mathcal{P}_\Omega(M))$$

• Gradient iterations:

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t - \eta \,\nabla f(\boldsymbol{X}_t)$$

for 
$$t = 0, 1, ...$$

#### Question: Does vanilla GD still work with partial observations?

### Which region has benign geometry?

**Finite-sample level (** $p \asymp \frac{\text{polylog}n}{n}$ **) :** assume every entry is observed i.i.d. with probability 0 .



# Which region has benign geometry?

**Finite-sample level (** $p \asymp \frac{\text{polylog}n}{n}$ **) :** assume every entry is observed i.i.d. with probability 0 .



Low-rank matrix completion is only well-defined for "incoherent" matrices whose energies are spread evenly across the entries.

# Which region has benign geometry?

**Finite-sample level (** $p \asymp \frac{\text{polylog}n}{n}$ **) :** assume every entry is observed i.i.d. with probability 0 .

 $f\left( \bm{X} \right) \mbox{ restricted strongly convex and smooth}$  along descent direction  $\bm{V}$  only when  $\bm{X}$  is incoherent:

 $\|oldsymbol{X}-oldsymbol{X}_{\star}\|_{2,\infty} \ll \|oldsymbol{X}_{\star}\|_{2,\infty}$ 





region of local strong convexity + smoothness

# Our findings: gradient descent is implicitly regularized



Gradient descent implicitly forces iterates to remain incoherent even without regularization

#### Theoretical guarantees - noise-free case

#### Theorem (Ma, Wang, Chi, Chen, FoCM 2020)

Suppose  $M = X_{\star}X_{\star}^{\top}$  is rank-r,  $\mu$ -incoherent and has a condition number  $\kappa = \sigma_{\max}(M)/\sigma_{\min}(M)$ . Vanilla GD (with spectral initialization) achieves

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

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

 $n^2 p \gtrsim n r^3 \mathsf{poly}(\mu, \kappa, \log n).$ 

#### Key idea: the iterates are implicitly regularized

#### Noisy matrix completion via vanilla GD



Near-optimal entry-wise error control:

$$\left\| \boldsymbol{X}_{t} \boldsymbol{X}_{t}^{\top} - \boldsymbol{M} \right\|_{\infty} \lesssim \left( \rho^{t} \mu r \sqrt{\frac{\log n}{np}} + \frac{\sigma}{\sigma_{\min}} \sqrt{\frac{n \log n}{p}} \right) \| \boldsymbol{M} \|_{\infty}$$

# The phenomenon is quite general

	Prior theory		Our theory	
	sample complexity	iteration complexity	sample complexity	iteration complexity
Phase retrieval	$n\log n$	$n\log\left(\frac{1}{\varepsilon}\right)$	$n\log n$	$\log n \log \left(\frac{1}{\varepsilon}\right)$
Quadratic sensing	$nr^6\log^2 n$	$n^4 r^2 \log\left(\frac{1}{\varepsilon}\right)$	$nr^4\log n$	$r^2 \log\left(\frac{1}{\varepsilon}\right)$
Matrix completion	n/a	n/a	$nr^3$ poly $\log n$	$\log\left(\frac{1}{\varepsilon}\right)$
Blind deconvolution	n/a	n/a	$K$ poly $\log m$	$\log\left(\frac{1}{\varepsilon}\right)$



#### Towards robustness to adversarial outliers



Yuanxin Li CMU



Yingbin Liang OSU



Huishuai Zhang MSRA

#### Outlier-corrupted low-rank matrix sensing



$$oldsymbol{y} = \mathcal{A}(oldsymbol{M}) + \underbrace{s}_{ ext{outliers}}, \quad \mathcal{A}(oldsymbol{M}) = \{\langle oldsymbol{A}_i, oldsymbol{M} 
angle\}_{i=1}^m$$

Arbitrary but sparse outliers:  $\|s\|_0 \le \alpha \cdot m$ , where  $0 \le \alpha < 1$  is fraction of outliers.

### Existing approaches fail

• Spectral initialization would fail:  $X_0 \leftarrow \mathsf{top}\text{-}r \mathsf{SVD}$  of



$$oldsymbol{Y} = rac{1}{m}\sum_{i=1}^m oldsymbol{y}_ioldsymbol{A}_i$$

• Gradient iterations would fail:

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t - \frac{\eta}{m} \sum_{i=1}^m \nabla \ell_i(\boldsymbol{y}_i; \boldsymbol{X}_t)$$

for 
$$t = 0, 1, ...$$

Even a single outlier can fail the algorithm!

#### Median-truncated gradient descent



Key idea: "median-truncation" discard samples *adaptively* based on how large sample gradients / values deviate from median

#### Median-truncated gradient descent



Key idea: "median-truncation" discard samples *adaptively* based on how large sample gradients / values deviate from median

• Robustify spectral initialization:  $X_0 \leftarrow \mathsf{top}\text{-}r$  SVD of

$$\boldsymbol{Y} = \frac{1}{m} \sum_{i:|y_i| \lesssim \text{median}(|y_i|)} y_i \boldsymbol{A}_i$$

#### Median-truncated gradient descent



Key idea: "median-truncation" discard samples *adaptively* based on how large sample gradients / values deviate from median

• Robustify spectral initialization:  $X_0 \leftarrow \mathsf{top}\text{-}r$  SVD of

$$m{Y} = rac{1}{m} \sum_{i:|y_i| \lesssim \mathsf{median}(|y_i|)} y_i m{A}_i$$

• Robustify gradient descent:

$$\boldsymbol{X}_{t+1} = \boldsymbol{X}_t - \frac{\eta}{m} \sum_{i: |r_t^i| \lesssim \text{median}(|r_t^i|)} \nabla \ell_i(y_i; \boldsymbol{X}_t), \quad t = 0, 1, \dots$$

where  $r_t^i := |y_i - \langle {oldsymbol A}_i, {oldsymbol X}_t 
angle|$  is the size of the gradient.

#### Theoretical guarantees

#### Theorem (Li, Chi, Zhang, and Liang, IMIAI 2020)

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

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

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

 $m\gtrsim nr^2\mathsf{poly}(\kappa,\log n);$ 

Robustness: and the fraction of outliers

 $\alpha \lesssim 1/\sqrt{r}.$ 

#### Theoretical guarantees

#### Theorem (Li, Chi, Zhang, and Liang, IMIAI 2020)

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

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

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

 $m \gtrsim nr^2 \mathsf{poly}(\kappa, \log n);$ 

• Robustness: and the fraction of outliers  $\alpha \leq 1/\sqrt{r}.$ 

Median-truncated GD adds robustness to GD obliviously.

#### Numerical example

#### Low-rank matrix sensing:

$$y_i = \langle \boldsymbol{A}_i, \boldsymbol{M} \rangle + s_i, \quad i = 1, \dots, m$$



# Median-truncated GD achieves similar performance as if performing GD on the clean data.

Li, Chi, Zhang and Liang, "Non-convex low-rank matrix recovery with arbitrary outliers via median-truncated gradient descent", Information and Inference: A Journal of the IMA, 2020.

### Accelerating ill-conditioned matrix estimation



Tian Tong CMU



Cong Ma Princeton

#### Convergence slows down for ill-conditioned matrices



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

— Can we accelerate the convergence to  $O(\log \frac{1}{\epsilon})$ ?

# A new algorithm: scaled gradient descent (ScaledGD)



- Spectral initialization.
- Scaled gradient iterations:

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

for t = 0, 1, ...

# A new algorithm: scaled gradient descent (ScaledGD)



- Spectral initialization.
- Scaled gradient iterations:

$$oldsymbol{X}_{t+1} = oldsymbol{X}_t - \eta \, 
abla f(oldsymbol{X}_t) \underbrace{(oldsymbol{X}_t^{ op} oldsymbol{X}_t)^{-1}}_{ ext{preconditioner}}$$

for t = 0, 1, ...

For the asymmetric case:

$$\begin{aligned} \boldsymbol{X}_{t+1} &= \boldsymbol{X}_t - \eta \, \nabla_{\boldsymbol{X}} f(\boldsymbol{X}_t, \boldsymbol{Y}_t) (\boldsymbol{Y}_t^\top \boldsymbol{Y}_t)^{-1} \\ \boldsymbol{Y}_{t+1} &= \boldsymbol{Y}_t - \eta \, \nabla_{\boldsymbol{Y}} f(\boldsymbol{X}_t, \boldsymbol{Y}_t) (\boldsymbol{X}_t^\top \boldsymbol{X}_t)^{-1} \end{aligned}$$

# A new algorithm: scaled gradient descent (ScaledGD)



- Spectral initialization.
- Scaled gradient iterations:

$$oldsymbol{X}_{t+1} = oldsymbol{X}_t - \eta \, 
abla f(oldsymbol{X}_t) \underbrace{(oldsymbol{X}_t^{ op} oldsymbol{X}_t)^{-1}}_{ ext{preconditioner}}$$

for t = 0, 1, ...

For the asymmetric case:

$$\begin{aligned} \boldsymbol{X}_{t+1} &= \boldsymbol{X}_t - \eta \, \nabla_{\boldsymbol{X}} f(\boldsymbol{X}_t, \boldsymbol{Y}_t) (\boldsymbol{Y}_t^\top \boldsymbol{Y}_t)^{-1} \\ \boldsymbol{Y}_{t+1} &= \boldsymbol{Y}_t - \eta \, \nabla_{\boldsymbol{Y}} f(\boldsymbol{X}_t, \boldsymbol{Y}_t) (\boldsymbol{X}_t^\top \boldsymbol{X}_t)^{-1} \end{aligned}$$

ScaledGD is a *preconditioned* gradient method.

#### ScaledGD for low-rank matrix completion



**Huge computational saving:** ScaledGD converges in an  $\kappa$ -independent manner with a minimal overhead!

#### Theoretical guarantees of ScaledGD

#### Theorem (Tong, Ma and Chi, 2020)

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

$$\| oldsymbol{X}_t oldsymbol{Y}_t^{ op} - oldsymbol{M} \|_{ ext{F}} \lesssim arepsilon \cdot \sigma_{\min}(oldsymbol{M})$$

- **Computational:** within  $O(\log \frac{1}{\epsilon})$  iterations;
- Statistical: the sample complexity satisfies

 $m\gtrsim nr^2\kappa^2.$ 

Acceleration for ill-conditioning: ScaledGD provably accelerates vanilla GD for low-rank matrix sensing.

# ScaledGD works more broadly



# ScaledGD is more efficient when the low-rank matrix is ill-conditioned.

Code available at https://github.com/Titan-Tong/ScaledGD

# Final remarks

# Bridging the theory-practice gap



#### Nonconvex low-rank matrix estimation:

- identification and exploitation of benign geometric properties;
- analyzing iterate trajectories beyond black-box optimization;
- simple variants of GD lead to robust and accelerated convergence.

# Future directions



#### Limitations of current framework:

- largely case-by-case: lengthy proofs, somewhat similar recipes;
- somewhat strong assumptions, e.g. Gaussian measurements, uniformly sampling...

#### References

Overview:

- Nonconvex Optimization Meets Low-Rank Matrix Factorization: An Overview, Y. Chi, Y. M. Lu and Y. Chen, *IEEE Trans. on Signal Processing*, 2019.
- 2. Harnessing Structures in Big Data via Guaranteed Low-Rank Matrix Estimation, Y. Chen and Y. Chi, *IEEE Signal Processing Magazine*, 2018.

#### Geometry and implicit regularization:

- Implicit Regularization for Nonconvex Statistical Estimation, C. Ma, K. Wang, Y. Chi and Y. Chen, Foundations of Computational Mathematics, 2020.
- Nonconvex Matrix Factorization from Rank-One Measurements, Y. Li, C. Ma, Y. Chen, and Y. Chi, AISTATS 2019.

Accelerating ill-conditioned low-rank matrix estimation:

1. Accelerating III-Conditioned Low-Rank Matrix Estimation via Scaled Gradient Descent, T. Tong, C. Ma, and Y. Chi, preprint, 2020.

Robustness to adversarial outliers:

- Non-convex low-rank matrix recovery with arbitrary outliers via median-truncated gradient descent, Y. Li, Y. Chi, H. Zhang and Y. Liang, *Information and Inference: A Journal of the IMA*, 2020.
- 2. Median-Truncated Nonconvex Approach for Phase Retrieval with Outliers, H. Zhang, Y. Chi and Y. Liang, *IEEE Trans. on Information Theory*, 2019.

# Thanks!



#### https://users.ece.cmu.edu/~yuejiec/