Taming Nonconvexity in Statistical and Reinforcement Learning



Yuxin Chen

Princeton University

Nonconvex problems are everywhere

Empirical risk minimization is usually nonconvex

 $\mathsf{minimize}_{\boldsymbol{x}} \quad f(\boldsymbol{x};\mathsf{data})$



Nonconvex optimization may be super scary



There may be bumps everywhere and exponentially many local optima e.g. 1-layer neural net (Auer, Herbster, Warmuth '96; Vu '98)

Nonconvex optimization may be super scary



But they are solved on a daily basis via simple algorithms like *(stochastic) gradient descent*

Towards demystifying nonconvex optimization



- Characterize optimization landscapes
- Exploit statistical tools to understand finite-sample behavior



nonconvex optimization

(high-dimensional) statistics

- 1. Nonconvex statistical learning
 - an efficient nonconvex algorithm for noisy tensor completion
- 2. Nonconvex reinforcement learning

— an expotential lower bound for policy gradient methods & an efficient remedy

1. Nonconvex optimization for tensor completion





Changxiao Cai Princeton

Gen Li Tsinghua



Yuejie Chi CMU

H. Vincent Poor Princeton

"Nonconvex low-rank tensor completion from noisy data," C. Cai, G. Li, H. Poor, Y. Chen, *Operations Research*, 2021+ "Subspace estimation from unbalanced and incomplete data matrices: $\ell_{2,\infty}$ statistical guarantees," C. Cai, G. Li, Y. Chi, H. Poor, Y. Chen, *Annals of Statistics*, 2021+

"Uncertainty quantification for nonconvex tensor completion," C. Cai, H. Poor, Y. Chen, ICML, 2020

Ubiquity of high-dimensional tensor data



Imperfect data acquisition



Key to enabling reliable reconstruction from incomplete data — exploiting **low CP-rank structure**



$$oldsymbol{T}^{\star} = \sum_{i=1}^r oldsymbol{u}_i^{\star} \otimes oldsymbol{u}_i^{\star} \otimes oldsymbol{u}_i^{\star}$$

Setup



• unknown rank-r tensor T^{\star} :

$$oldsymbol{T}^{\star} = \sum_{i=1}^r oldsymbol{u}_i^{\star} \otimes oldsymbol{u}_i^{\star} \otimes oldsymbol{u}_i^{\star} \in \mathbb{R}^{d imes d imes d}$$

Setup



- unknown rank-r tensor T^\star : $T^\star = \sum_{i=1}^r u_i^\star \otimes u_i^\star \otimes u_i^\star \in \mathbb{R}^{d \times d \times d}$
- incomplete & noisy observations over a random sampling set Ω :

$$T_{i,j,k} = T_{i,j,k}^{\star} + \text{noise}, \qquad (i,j,k) \in \Omega$$

Goal: recover $\{u_i^{\star}\}_{i=1}^r$ and T^{\star}

Statistical-computational gap (r = O(1))



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"I can't find an efficient algorithm, but neither can all these people."

Statistical-computational gap (r = O(1))



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Prior art



- Gandy, Recht, Yamada '11
- Liu, Musialski, Wonka, Ye'12
- Kressner, Steinlechner, Vandereycken '13
- Xu, Hao, Yin, Su'13
- Romera-Paredes, Pontil '13
- Jain, Oh '14
- Huang, Mu, Goldfarb, Wright '15
- Barak, Moitra '16
- Zhang, Aeron '16
- Yuan, Zhang '16
- Montanari, Sun'16
- Kasai, Mishra'16
- Potechin, Steurer '17
- Dong, Yuan, Zhang '17
- Xia, Yuan '19
- Zhang'19
- ...

Prior art (r = O(1))



	algorithm	sample size	comput. cost	recovery type (noiseless)
Yuan, Zhang '16	tensor nuclear norm	d	NP-hard	exact
Xia, Yuan '17	spectral method + GD on manifold	$d^{3/2}$	slow	exact
Montanari, Sun '18	spectral method	$d^{3/2}$	d^3	inexact
Barak, Moitra '16	sum-of-squares	$d^{3/2}$	slow (d^{15})	exact
Potechin et al. '17	sum-of-squares	$d^{3/2}$	slow (d^{10})	exact

Prior art (r = O(1))



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Yuan, Zhang '16 Xia, Yuan '17	tensor nuclear norm spectral method $+$	d $d^{3/2}$	NP-hard	exact
Montanari, Sun '18 Barak, Moitra '16 Potechin et al. '17	GD on manifold spectral method sum-of-squares sum-of-squares	$d^{3/2} \\ d^{3/2} \\ d^{3/2} \\ d^{3/2}$	d^3 slow (d^{15}) slow (d^{10})	inexact exact exact

	algorithm	ℓ_2 error (noisy)	ℓ_∞ error (noisy)
Xia, Yuan, Zhang '17 Barak, Moitra '16	spectral method + tensor power method sum-of-squares	suboptimal suboptimal	n/a n/a

Can we design an algorithm that is simultaneously sample-efficient, computationally fast, & minimax-optimal?

A nonconvex least squares formulation

$$\underset{\boldsymbol{U} = [\boldsymbol{u}_1, \cdots, \boldsymbol{u}_r] \,\in\, \mathbb{R}^{d \times r}}{\text{minimize}} f(\boldsymbol{U}) := \sum_{(i, j, k) \in \Omega} \left\{ \left(\sum_{s=1}^r \boldsymbol{u}_s^{\otimes 3} \right)_{i, j, k} - T_{i, j, k} \right\}^2$$

squared loss over observed entries

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squared loss over observed entries

- pros: statistically efficient if we can find global solutions
- cons: highly nonconvex \longrightarrow computationally challenging

Gradient descent (GD) with random initialization?

$$\underset{\boldsymbol{U} = [\boldsymbol{u}_1, \cdots, \boldsymbol{u}_r] \, \in \, \mathbb{R}^{d \times r}}{\text{minimize}} \, f(\boldsymbol{U}) := \sum_{(i, j, k) \in \Omega} \left\{ \left(\, \sum_{s=1}^r \boldsymbol{u}_s^{\otimes 3} \right)_{i, j, k} - T_{i, j, k} \right\}^2$$



- initialize U^0 randomly
- gradient descent: for $t = 0, 1, \cdots$,

$$\boldsymbol{U}^{t+1} = \boldsymbol{U}^t - \eta_t \nabla f(\boldsymbol{U}^t)$$

- succeeds for phase retrieval (Chen et al. '18)

Randomly initialized GD does NOT work unless sample size $>\ d^2$



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When sample size $\asymp d^{1.5}$:

 $\bullet \ \mathbb{E}[\mathsf{search}\,\mathsf{direction}] \text{ is desirable}$

A negative conjecture

Randomly initialized GD does NOT work unless sample size $>\ d^2$



When sample size $\asymp d^{1.5}$:

- $\bullet \ \mathbb{E}[\mathsf{search}\,\mathsf{direction}] \text{ is desirable}$
- issue: variance $\gtrsim \sqrt{d} \operatorname{mean}^2$

A negative conjecture

Randomly initialized GD does NOT work unless sample size $> d^2$



A negative conjecture

Randomly initialized GD does NOT work unless sample size $> d^2$



Our proposal: a two-stage nonconvex algorithm





1. initialization: U^0

- estimate span $\{u_i^\star\}$ via spectral method
- disentangle individual factors $\{u_i^{\star}\}$ from subspace estimate



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- disentangle individual factors $\{u_i^\star\}$ from subspace estimate
- **2. gradient descent:** for $t = 0, 1, \cdots$

$$\boldsymbol{U}^{t+1} = \boldsymbol{U}^t - \eta \nabla f(\boldsymbol{U}^t)$$



- 1. initialize within a local basin sufficiently close to global min (restricted) strongly convex
- 2. iterative refinement

A bit more details about initialization

Step 1.1: estimate span $\{u_i^{\star}\}_{1\leq i\leq r}$ \longrightarrow U_{sub}

- matricizition: A = unfold(T)
- estimate rank-r subspace of $\mathcal{P}_{\mathsf{off}\mathsf{-}\mathsf{diag}}(AA^{\top})$ (diagonal deletion)



A bit more details about initialization

Step 1.1: estimate span $\{u_i^{\star}\}_{1\leq i\leq r}$ \longrightarrow U_{sub}

- matricizition: $A = \mathsf{unfold}(T)$
- estimate rank-r subspace of $\mathcal{P}_{\mathsf{off}\mathsf{-}\mathsf{diag}}(AA^{\top})$ (diagonal deletion)



Step 1.2: retrieve tensor factors from subspace estimate

- generate a random vector g from U_{sub}
- compute leading eigenvector of $m{T}\otimesm{g}=\sum\langlem{u}_i^\star,m{g}
 anglem{u}_i^\starm{u}_i^{\star op}+$ noise
- repeat ...

find the $oldsymbol{u}_i^{\star}$ most aligned with $oldsymbol{g}$

Assumptions

$$oldsymbol{T}^{\star} = \sum_{i=1}^r oldsymbol{u}_i^{\star} \otimes oldsymbol{u}_i^{\star} \otimes oldsymbol{u}_i^{\star} \in \mathbb{R}^{d imes d imes d}$$

 \bullet random sampling: each entry is observed independently with prob. p

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- random noise: independent zero-mean sub-Gaussian noise with variance ${\cal O}(\sigma^2)$
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- $\bullet~{\rm random~sampling}:$ each entry is observed independently with prob. p
- random noise: independent zero-mean sub-Gaussian noise with variance ${\cal O}(\sigma^2)$
- ground truth: low-rank (r = O(1)), well-conditioned, incoherent ({u_i^{*}} are de-localized and not aligned)

There exists some constant $\rho < 1$ and some permutation matrix $\Pi \in \mathbb{R}^{r \times r}$ s.t. with high prob., the t-th iterate satisfies

$$\begin{split} \left\| \boldsymbol{U}^{t} \boldsymbol{\Pi} - \boldsymbol{U}^{\star} \right\|_{\mathrm{F}} &\lesssim \left(\rho^{t} + \sigma \sqrt{d/p} \right) \left\| \boldsymbol{U}^{\star} \right\|_{\mathrm{F}} \\ \left\| \boldsymbol{T}^{t} - \boldsymbol{T}^{\star} \right\|_{\mathrm{F}} &\lesssim \left(\rho^{t} + \sigma \sqrt{d/p} \right) \left\| \boldsymbol{T}^{\star} \right\|_{\mathrm{F}} \end{split}$$

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provided that sample size $\gtrsim d^{1.5} \mathrm{poly} \log(d)$

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 $\bullet~$ linear/geometric convergence $~~\longrightarrow~~$ linear-time algorithm

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• near-optimal sample complexity (among poly-time algorithms)

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provided that sample size $\gtrsim d^{1.5} \mathrm{poly} \log(d)$

• near-optimal statistical accuracy (both ℓ_2 and ℓ_∞)

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provided that sample size $\gtrsim d^{1.5} \mathrm{poly} \log(d)$

• no need of sample splitting

 \longrightarrow can handle complicated stat dependency across iterations



$$d = 100, r = 4, p = 0.1$$

Leave out a small amount of randomness and re-run the algorithm

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- Stein '72
- El Karoui, Bean, Bickel, Lim, Yu'13
- El Karoui '15
- Javanmard, Montanari '15
- Zhong, Boumal '17
- Lei, Bickel, El Karoui '17
- Sur, Chen, Candès '17
- Abbe, Fan, Wang, Zhong '17
- Chen, Fan, Ma, Wang '17
- Ma, Wang, Chi, Chen '17
- Chen, Chi, Fan, Ma'18
- Ding, Chen '18
- Dong, Shi'18
- Chen, Liu, Li'19
- Chen, Fan, Ma, Yan '19
- Pananjady, Wainwright '19
- Ling '20
- Chen, Fan, Ma, Yan '20
- Agarwal, Kakade, Yang '20
- Abbe, Fan, Wang '20
- Li, Wei, Chi, Gu, Chen '20

Foundations and Trends[®] in Machine Learning Spectral Methods for Data Science: A Statistical Perspective

Suggested Citation: Yuxin Chen, Yuejie Chi, Jianqing Fan and Cong Ma (2020), "Spectral Methods for Data Science: A Statistical Perspective", Foundations and Trends[®] in

4 Fine-grained analysis: ℓ_{∞} and $\ell_{2,\infty}$ perturbation theory 126 4.1 Leave-one-out-analysis: An illustrative example 127

For each $1 \le l \le d$, generate leave-one-out auxiliary iterates $\{U^{t,(l)}\}$ by replacing l^{th} slice with true values



For each $1 \le l \le d$, generate leave-one-out auxiliary iterates $\{U^{t,(l)}\}$ by replacing l^{th} slice with true values



- exploit partial statistical independence
- exploit leave-one-out stability
- enable optimal ℓ_∞ error control

Summary of Part 1



Summary of Part 1



2: Nonconvex optimization in reinforcement learning



"Softmax policy gradient methods can take exponential time to converge," G. Li, Y. Wei, Y. Chi, Y. Gu, Y. Chen, arxiv:2102.11270, 2021

"Fast global convergence of natural policy gradient methods with entropy regularization," S. Cen, C. Cheng, Y. Chen, Y. Wei, Y. Chi, under revision, *Operations Research*, 2020

Recent successes in reinforcement learning (RL)







Policy optimization: a major contributor to recent RL advances

RL challenges

In RL, an agent learns by interacting with an unknown environment



- enormous state and action space
- delayed rewards
- credit assignments
- nonconvexity everywhere

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How to enable scalable and guaranteed RL despite nonconvexity?

Backgrounds: policy optimization for MDPs





• S: state space • A: action space





- S: state space A: action space
- $r(s, a) \in [0, 1]$: immediate reward





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- $\pi(\cdot|s)$: policy (or action selection rule)





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- $\pi(\cdot|s)$: policy (or action selection rule)
- $P(\cdot|s,a)$: transition probabilities

Value function of policy π



cumulative discounted reward: $V^{\pi}(s) := \mathbb{E} \left| \sum_{t=0}^{\infty} \gamma^{t} r_{t} \right| s_{0} = s \left| s \in \mathcal{S} \right|$

• expectation is over randomness of MDP & policy π

Value function of policy π



cumulative discounted reward: $V^{\pi}(s) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^{t} r_{t} \mid s_{0} = s\right], s \in \mathcal{S}$

- expectation is over randomness of MDP & policy π
- $\gamma \in [0,1)$: discount factor
 - take $\gamma \rightarrow 1$ to approximate long-horizon MDPs
 - effective horizon: $\frac{1}{1-\gamma}$

Optimal policy and optimal value



- goal: find optimal policy π^* that maximizes value functions
- optimal value function: $V^{\star}(s) := \max_{\pi} V^{\pi}(s)$ for all $s \in \mathcal{S}$

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How to accomplish it via nonconvex optimization algorithms?

Given state distribution $s\sim\rho$ (e.g. uniform)

$$\max_{\pi} V^{\pi}(\rho) \coloneqq \mathop{\mathbb{E}}_{s \sim \rho} \left[V^{\pi}(s) \right]$$











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- (Mei et al. '20) Softmax PG converges to global opt in

 $O(\frac{1}{\varepsilon})$ iterations

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However, "asymptotic convergence" might mean "taking forever"
Theorem 2 (Li, Wei, Chi, Chen '21)

There exists an MDP s.t. it takes softmax PG at least

 $rac{1}{\eta} |\mathcal{S}|^{1.5^{\Theta(rac{1}{1-\gamma})}}$ iterations

to achieve $\|V^{(t)} - V^{\star}\|_{\infty} \leq 1/2$ (even with infinite samples)

 Softmax PG method can take exponential time to converge (in problems w/ large state space & long effective horizon)!

MDP construction for our lower bound



MDP construction for our lower bound



Key design ingredients: for $3 \le s \le H \asymp \frac{1}{1-\gamma}$,

- *a*₁ is optimal action delayed rewards
- $\pi^{(t)}(a_1|s)$ keeps decreasing until $\pi^{(t)}(a_1|s-2) \approx 1$







observation: convergence time for state s grows geometrically as $s \uparrow$



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convergence-time
$$(s) \gtrsim (\text{convergence-time}(s-2))^{1.5}$$

Booster 1: entropy regularization

accelerate convergence by regularizing objective function

$$V_{\tau}^{\pi}(s_0) \coloneqq \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t (r_t - \tau \log \pi(a_t | s_t)) \, \Big| \, s_0\right]$$

Booster 1: entropy regularization

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- τ : regularization parameter
- d_s^{π} : certain marginal distribution

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- τ : regularization parameter
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entropy-regularized value maximization

maximize_{$$\theta$$} $V_{\tau}^{\pi_{\theta}}(\rho) := \mathbb{E}_{s \sim \rho} [V_{\tau}^{\pi_{\theta}}(s)]$

Theorem 3 (Li, Wei, Chi, Chen '21)

There is an MDP s.t. it takes entropy-regularized softmax PG at least

$$\min\left\{\exp\left(\Theta\left(\frac{1}{\varepsilon}\right)\right), \ \frac{1}{\eta} \left|\mathcal{S}\right|^{2^{\Theta\left(\frac{1}{1-\gamma}\right)}}\right\} \text{ iterations}$$

to achieve $\|V^{(t)} - V^{\star}\|_{\infty} \leq \varepsilon$ (even with infinite samples)

• Softmax PG method with entropy regularization can still take exponential time to converge!

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- Softmax PG method with entropy regularization can still take exponential time to converge!
- (Mei et al. '20) entropy-regularized softmax PG converges in

 $c(|\mathcal{S}|, |\mathcal{A}|, \frac{1}{1-\gamma}, \cdots) O(\frac{1}{\varepsilon})$ iterations

Booster 2: natural policy gradient (NPG)

precondition gradients to improve search directions ...



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NPG method (Kakade '02)

$$\theta^{(t+1)} = \theta^{(t)} + \eta(\mathcal{F}^{\theta}_{\rho})^{\dagger} \nabla_{\theta} V^{(t)}_{\tau}(\rho), \qquad t = 0, 1, \cdots$$
$$\mathcal{F}^{\theta}_{\rho} := \mathbb{E}\left[\left(\nabla_{\theta} \log \pi_{\theta}(a|s) \right) \left(\nabla_{\theta} \log \pi_{\theta}(a|s) \right)^{\top} \right]: \text{ Fisher info}$$

Entropy-regularized natural gradient helps!

A toy bandit example: 3 arms with rewards 1, 0.9 and 0.1





How to characterize the efficiency of entropy-regularized NPG in tabular settings?

Linear convergence with exact gradients



exact access to gradients:

Theorem 4 (Cen, Cheng, Chen, Wei, Chi '20) If $\eta \leq (1 - \gamma)/\tau$ and $\tau \leq \frac{(1 - \gamma)\varepsilon}{4 \log |\mathcal{A}|}$, entropy-regularized NPG achieves $\|V^{\star} - V^{(t+1)}\|_{\infty} \leq C_1 \gamma (1 - \eta \tau)^t + \varepsilon/2, \quad t = 0, 1, \cdots$ number of iterations needed to reach $\|V^{\star} - V^{(t)}\|_{\infty} \leq \varepsilon$:

• general learning rates ($0 < \eta < \frac{1-\gamma}{\tau}$):

$$\frac{1}{\eta\tau}\log\left(\frac{2C_1\gamma}{\varepsilon}\right)$$

• optimal choice $(\eta = \frac{1-\gamma}{\tau})$:

$$\frac{1}{1-\gamma}\log\left(\frac{2C_1\gamma}{\varepsilon}\right)$$

number of iterations needed to reach $\|V^{\star} - V^{(t)}\|_{\infty} \leq \varepsilon$:

• general learning rates ($0 < \eta < \frac{1-\gamma}{\tau}$):

$$\frac{1}{\eta\tau}\log\left(\frac{2C_1\gamma}{\varepsilon}\right)$$

• optimal choice $(\eta = \frac{1-\gamma}{\tau})$:

$$\frac{1}{1-\gamma}\log\left(\frac{2C_1\gamma}{\varepsilon}\right)$$

Nearly dimension-free global linear convergence!

Regularized NPG vs. unregularized NPG

regularized NPG

unregularized NPG $\tau = 0$



Regularized NPG vs. unregularized NPG

regularized NPG unregularized NPG $\tau = 0.001$ $\tau = 0$ 10^{2} - 10^{2} n = 0.01n = 0.01= 0.1 $\eta = 0.1$ 10^{0} 10^{0} n = 1 10^{-2} 10^{-2} $\left\|Q_{\tau}^{\star}-Q_{\tau}^{(t)}\right\|_{\infty}$ $||Q^* - Q^{(t)}||_{\infty}$ 10^{-4} 10^{-4} 10^{-6} 10^{-6} 10^{-8} 10^{-8} 10^{-10} 10^{-10} 10^{-12} 10^{-12} 1000 2000 3000 4000 5000 1000 2000 3000 4000 5000 0 #iterations #iterations linear rate: $\frac{1}{n\tau} \log\left(\frac{1}{\varepsilon}\right)$ sublinear rate: $\frac{1}{\min\{n,(1-\gamma)^2\}\varepsilon}$ (Agarwal et al. '19) Ours

Entropy regularization enables faster convergence!



- Softmax policy gradient can take exponential time to converge
- Entropy regularization & natural gradients help!

Concluding remarks

