Learning Nonlinear and Deep Representations from High-Dim Data

Nonconvex Optimization of Low-Dimensional Models

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Outline

1 Introduction & Motivation of Nonconvex [Optimization](#page-1-0) [Motivating](#page-2-0) Examples [Nonlinearality,](#page-10-0) Nonconvexity, and Symmetry

2 Symmetry & Geometry for [Nonconvex](#page-16-0) Problems in Practice Problems with [Rotational](#page-17-0) Symmetry Problems with Discrete [Symmetry](#page-26-0)

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3 Efficient Nonconvex [Optimization](#page-37-0) Objectives of Nonconvex [Optimization](#page-38-0)

Example: Low-rank Matrix Completion

We observe:

$$
\mathbf{Y}_{\text{Observed ratings}} = \mathcal{P}_{\Omega} \begin{bmatrix} \mathbf{X} \\ \mathbf{Complete ratings} \end{bmatrix}.
$$

Observed (Incomplete) Ratings Y

Matrix completion

via bilinear low-rank factorization

$$
\min_{\boldsymbol{U},\boldsymbol{V}}f(\boldsymbol{U},\boldsymbol{V})=\sum_{(i,j)\in\Omega}[(\boldsymbol{U}\boldsymbol{V}^*)_{i,j}-\boldsymbol{Y}_{i,j}]^2+\underbrace{\frac{\lambda}{2}\|\boldsymbol{U}\|_F^2+\frac{\lambda}{2}\|\boldsymbol{V}\|_F^2}_{\text{reg}(\boldsymbol{U},\boldsymbol{V})}.
$$

$$
\|\bm{M}\|_{*} = \min_{\bm{M} = \bm{U}\bm{V}^{*}} \tfrac{\lambda}{2} \|\bm{U}\|_{F}^{2} + \tfrac{\lambda}{2} \|\bm{V}\|_{F}^{2}
$$

Example: Dictionary for Image Representation

Image processing (e.g. denoising or super-resolution) against a known sparsifying dictionary:

 $I_{\mathsf{noisy}} \;=\; \begin{array}{c c c c c c c c c} A & \times & x & + & z. \ \text{dictionary} & \text{sparse} & \text{noise} \end{array} \; (1)$

Dictionary learning: the motifs or atoms of the dictionary are unknown:

 $Y = A X$ *.* (2)
data dictionary sparse

- Band-limited signals: $A = F$, the Fourier transform;
- Piecewise smooth signals: $A = W$, the wavelet transforms;
- *•* Natural images *A* =? (How to learn *A* from the data *Y* ?)

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Convex and Nonconvex Optimization

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Dictionary Learning

Recovered solutions always obtain the same objective value.

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Benign Nonconvex Optimization Landscape

General Case **Structured Case**

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Example: Sparse Blind Deconvolution

Sparse Blind Deconvolution:

the convolutional motif or sparse activation signal are unknown:

> $Y = A * X$. (3) data motif

- *•* Scientific signals: activation signals are sparse
- *•* Image deblurring: natural images are sparse in the gradient domain

Observation Kernel A0 Natural Image

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Yugian Zhang Nonconvex [Optimization](#page-0-0) June 7, 2023 7 / 40

Sparse Blind Deconvolution

Recovered solutions are near signed shift-truncations of the ground truth.

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Convolutional Dictionary learning

$$
\mathop {\sum }\limits_{\rm data} = \sum_i \mathop {A_i}\limits_{\rm *} * \mathop {X_i}\limits_{\rm sparse}
$$

Recovered solutions are near signed shift-truncations of the ground

Challenges of Nonconvex Optimization – Pessimistic Views

Consider the problem of minimizing a general nonlinear function:

$$
\min_{\boldsymbol{z}} \varphi(\boldsymbol{z}), \quad \boldsymbol{z} \in C. \qquad (4)
$$

In the worst case, even finding a *local* minimizer can be NP-hard¹.

Hence typically people seek to work with relatively benign functions with benign guarantees:

- **1** convergence to some critical point \bar{z} such that $\nabla \varphi(\bar{z}) = 0$;
- 2 or convergence to some local minimizer $\nabla^2 \varphi(\bar{z}) \succeq 0$.

 1 Some NP-complete problems in quadratic and nonlinear programming, K.G Murty and S. N. Kabadi, 1987 (ロ) (_何) (ヨ) (ヨ Ω

Opportunities – Optimistic Views

However, nonconvex problems that arise from natural physical, geometrical, or statistical origins typically have nice structures. in terms of symmetries!

The function φ is invariant under certain group action:

• for low rank matrix recovery, invariant under a continuous rotation:

$$
\varphi((\boldsymbol{U}\boldsymbol{\Gamma},\boldsymbol{V}\boldsymbol{\Gamma}^{-1}))=\varphi((\boldsymbol{U},\boldsymbol{V})),\quad\forall\text{ invertible }\boldsymbol{\Gamma}.
$$

• for dictionary learning, invariant under signed permutations:

$$
\varphi((\boldsymbol{A},\boldsymbol{X}))=\varphi((\boldsymbol{A}\boldsymbol{\Pi},\boldsymbol{\Pi}^*\boldsymbol{X})),\quad \forall \boldsymbol{\Pi}\in \mathsf{SP}(n).
$$

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Nonlinearity and Symmetry

Intrinsic ambiguity against the uniqueness of the solution

• low rank matrix recovery

$$
\boldsymbol{X} = \boldsymbol{U}_0 \boldsymbol{V}_0^T = \boldsymbol{U}_0 \boldsymbol{\Gamma} \boldsymbol{\Gamma}^{-1} \boldsymbol{V}_0^T
$$

for any invertible Γ .

• dictionary learning

$$
\boldsymbol{Y}=\boldsymbol{A}_0\boldsymbol{X}_0=\boldsymbol{A}_0\boldsymbol{\Pi}\boldsymbol{\Pi}^*\boldsymbol{X}_0
$$

for any signed permutation Π .

• blind deconvolution

$$
\boldsymbol{y} = \boldsymbol{a}_0 * \boldsymbol{x}_0 = S_{\tau}[\boldsymbol{a}_0] * S_{-\tau}[\boldsymbol{x}_0]
$$

for any signed shift τ .

Optimization under Symmetry

Definition (Symmetric Function)

Let \mathbb{G} be a group acting on \mathbb{R}^n . A function $\varphi : \mathbb{R}^n \to \mathbb{R}^{n'}$ is \mathbb{G} -symmetric if for all $z \in \mathbb{R}^n$, $\mathfrak{a} \in \mathbb{G}$, $\varphi(\mathfrak{a} \circ z) = \varphi(z)$.

Most symmetric objective functions that arise in structured signal recovery do not have spurious local minimizers or flat saddles.

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Slogan 1: the (only!) local minimizers are symmetric versions of the ground truth.

Slogan 2: any local critical point has negative curvature in directions that break symmetry.

Basic Calculus

Critical points or stationary points: gradient vanishes

- convex function: critical point = minimizer
- *•* nonconvex function: not all critical points are minimizers

Basic Calculus

Critical points with non-singular hessian

- *•* minimizer: hessian is positive definite
- saddle points: hessian has both positive and negative eigenvalues
- *•* maximizer: hessian is negative definite

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3 Efficient Nonconvex [Optimization](#page-37-0) Objectives of Nonconvex [Optimization](#page-38-0)

Problems with Rotational Symmetry

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Low rank matrix recovery

Goal: Given $Y = A(X)$, recover low rank matrix $X = U_0 V_0$

• Convex Formulation

$$
\min_{\boldsymbol{X} \in \mathbb{R}^{m \times n}} \quad \|\boldsymbol{X}\|_{\star} \quad \text{s.t.} \quad \boldsymbol{Y} = \mathcal{A}(\boldsymbol{X})
$$

• Nonconvex Formulation

$$
\min_{\boldsymbol{U} \in \mathbb{R}^{m \times r}, \boldsymbol{V} \in \mathbb{R}^{n \times r}} \quad \left\| \boldsymbol{Y} - \mathcal{A}(\boldsymbol{U} \boldsymbol{V}^T) \right\|_F^2 + \mathsf{reg}(\boldsymbol{U}, \boldsymbol{V})
$$

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Low Rank Matrix Recovery

$$
\min_{\boldsymbol{U},\boldsymbol{V}} \quad \frac{1}{2} \left\| \boldsymbol{Y} - \mathcal{A}(\boldsymbol{U}\boldsymbol{V}^T) \right\|_F^2 + \mathsf{reg}(\boldsymbol{U},\boldsymbol{V})
$$

Inherent Symmetry:

$$
\boldsymbol{X} = \boldsymbol{U}_0 \boldsymbol{V}_0^T = \boldsymbol{U}_0 \boldsymbol{\Gamma} \boldsymbol{\Gamma}^{-1} \boldsymbol{V}_0^T
$$

for any invertible $\mathbf{\Gamma} \in \mathbb{R}^{r \times r}$.

Low Rank Matrix Recovery

$$
\min_{\boldsymbol{U},\boldsymbol{V}} \quad \frac{1}{2} \left\| \boldsymbol{Y} - \mathcal{A}(\boldsymbol{U}\boldsymbol{V}^T) \right\|_F^2 + \mathsf{reg}(\boldsymbol{U},\boldsymbol{V})
$$

Inherent Symmetry:

$$
\boldsymbol{X} = \boldsymbol{U}_0 \boldsymbol{V}_0^T = \boldsymbol{U}_0 \boldsymbol{\Gamma} \boldsymbol{\Gamma}^{-1} \boldsymbol{V}_0^T
$$

for any invertible $\mathbf{\Gamma} \in \mathbb{R}^{r \times r}$.

- \bullet Are $\left(\boldsymbol{U_0\Gamma},\boldsymbol{V_0\Gamma^{-1}}\right)$ the only local solutions?
- Does there exist any flat stationary point?

Simplifications:

- $Y = \mathcal{A}(X) = X$
- $\bm{X} = \bm{U_0} \bm{U_0^T}$ is symmetric and rank-1

$$
\boldsymbol{X}=\boldsymbol{u}_0\boldsymbol{u}_0^T=(-\boldsymbol{u}_0)(-\boldsymbol{u}_0^T)
$$

the rotational symmetry is reduced to sign symmetry.

Nonconvex formulation:

$$
\min_{\mathbf{u}} \quad \phi(\mathbf{u}) \doteq \frac{1}{4} \| \mathbf{X} - \mathbf{u}\mathbf{u}^T \|_F^2 + \underbrace{\lambda \| \mathbf{u} \|_2^2}_{const}
$$

 QQQ

$$
\min_{\boldsymbol{u}} \quad \phi(\boldsymbol{u}) \doteq \frac{1}{4} \left\| \boldsymbol{X} - \boldsymbol{u} \boldsymbol{u}^T \right\|_F^2
$$

Critical points have zero gradient

$$
\nabla \phi = (\boldsymbol{u}\boldsymbol{u}^T - \boldsymbol{X})\boldsymbol{u}
$$

$$
= ||\boldsymbol{u}||_2^2 \boldsymbol{u} - \boldsymbol{X}\boldsymbol{u}
$$

$$
= 0
$$

therefore critical points must be one of the following

$$
\bullet\;\; u=\pm u_0
$$

 $\bullet u=0$

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$$
\min_{\boldsymbol{u}} \quad \phi(\boldsymbol{u}) \doteq \frac{1}{4} \left\| \boldsymbol{X} - \boldsymbol{u} \boldsymbol{u}^T \right\|_F^2
$$

with the second order derivative

$$
\nabla^2 \phi = 2 \boldsymbol{u} \boldsymbol{u}^T + ||\boldsymbol{u}||_2^2 \boldsymbol{I} - \boldsymbol{X}.
$$

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$$
\min_{\boldsymbol{u}} \quad \phi(\boldsymbol{u}) \doteq \frac{1}{4} \left\| \boldsymbol{X} - \boldsymbol{u} \boldsymbol{u}^T \right\|_F^2
$$

with the second order derivative

$$
\nabla^2 \phi = 2 \boldsymbol{u} \boldsymbol{u}^T + ||\boldsymbol{u}||_2^2 \boldsymbol{I} - \boldsymbol{X}.
$$

Then the stationary points can be grouped as

• Local minimizer $u = \pm u_0$ and $uu^T = X$

$$
\nabla^2 \phi = \boldsymbol{u} \boldsymbol{u}^T + ||\boldsymbol{u}||_2^2 \boldsymbol{I}.
$$

• Maximizer $u = 0$

$$
\nabla^2 \phi = -\boldsymbol{X}.
$$

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Low Rank Matrix Recovery

Symmetric low rank matrix

$$
\min_{\mathbf{U}} \quad \phi(\mathbf{u}) \doteq \frac{1}{4} ||\mathbf{X} - \mathbf{U}\mathbf{U}^T||^2_F.
$$

General low rank matrix recover

$$
\min_{\mathbf{U},\mathbf{V}} \quad \phi(\mathbf{u}) \doteq \frac{1}{2} \| \mathbf{X} - \mathbf{U}\mathbf{V}^T \|_F^2 + \lambda \| \mathbf{U} \|_F^2 + \lambda \| \mathbf{V} \|_F^2.
$$

Local minimizers: are ground truth U_0 and V_0 up to rotation; Negative curvature: *between multiple local minimizers.*

Problems with Discrete Symmetry

Yugian Zhang Nonconvex [Optimization](#page-0-0) June 7, 2023 23 / 40

Dictionary Learning

Goal: Given dataset *Y* , find the optimal dictionary *A* that renders the sparsest coefficient *X*

$$
\min_{\mathbf{A},\mathbf{X}} \quad \|\mathbf{X}\|_1 \quad \text{s.t.} \quad \mathbf{Y} = \mathbf{A}\mathbf{X}.
$$

In presence of noise, the optimization problem can be rewritten as

$$
\min_{\mathbf{A},\mathbf{X}} \quad \frac{1}{2} \left\| \mathbf{Y} - \mathbf{A}\mathbf{X} \right\|_F^2 + \lambda \left\| \mathbf{X} \right\|_1.
$$

Inherent Symmetry:

$$
\boldsymbol{Y}=\boldsymbol{A}_0\boldsymbol{\Gamma}\boldsymbol{\Gamma}^*\boldsymbol{X}_0,
$$

for any signed permutation matrix Γ .

Orthogonal Dictionary Learning

• Input: matrix \boldsymbol{Y} which is the product of an orthogonal matrix \boldsymbol{A}_0 (called a dictionary) and a sparse matrix X_0 :

$$
\boldsymbol{Y} = \boldsymbol{A}_0 \boldsymbol{X}_0, \quad \boldsymbol{A}_0 \boldsymbol{A}_0^* = \boldsymbol{I}, \boldsymbol{X}_0 \text{ sparse.}
$$

• Optimization Formulation

$$
\min_{\mathbf{A},\mathbf{X}} \quad \|\mathbf{X}\|_1 \quad \text{s.t.} \quad \mathbf{Y} = \mathbf{A}\mathbf{X}, \quad \mathbf{A}\mathbf{A}^* = \mathbf{I}.
$$

• Given the optimization constraint, *X* is uniquely defined in terms of *A*

$$
X=A^*AX=A^*Y.
$$

• Equivalent formulation

$$
\min_{\boldsymbol{A}\in\mathcal{O}(n)}\quad\left\|\boldsymbol{A}^{*}\boldsymbol{Y}\right\|_{1}.
$$

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Orthogonal Dictionary Learning

Instead of aiming to solve the entire matrix $A = [a_1, \ldots, a_n]$ at once via

$$
\min_{\boldsymbol{A}\in\mathcal{O}(n)}\quad\|\boldsymbol{A}^*\boldsymbol{Y}\|_1\,.
$$

A simpler model problem solves for the columns *aⁱ* one at a time

$$
\min_{\|\boldsymbol{a}\|_2=1} \quad \|\boldsymbol{a}^*\boldsymbol{Y}\|_1\,.
$$

Stationary Points:

- $\boldsymbol{a} = \pm \boldsymbol{a}_i$, then the Hessian is positive definite
- $\boldsymbol{a} = \sum_{i \in I} \pm \frac{1}{\sqrt{2}}$ $\frac{1}{|I|}a_i$, there exist negative curvatures alone $a_i (i \in I)$

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Orthogonal Dictionary Learning — Geometry

Local minimizers are ground truth a_i or $-a_i$. Negative curvature between multiple local minimizers.

Short-and-Sparse Blind Deconvolution

Goal: Given convolutional data *y*, find the short signal *a* and the sparse signal *x* such that $y = a * x$.

Inherent Symmetry:

$$
\boldsymbol{y} = \boldsymbol{a}_0 * \boldsymbol{x}_0 = \alpha s_l[\boldsymbol{a}_0] * \frac{1}{\alpha} s_{-l}[\boldsymbol{x}_0]
$$

for any shift *l* and nonzero scaling.

The practical optimization problem can be written as

$$
\min_{\|a\|_F^2=1,\bm{x}} \quad \tfrac{1}{2} \left\| \bm{y} - \bm{a} * \bm{x} \right\|_F^2 + \lambda \left\| \bm{x} \right\|_1.
$$

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Objective Function – Near One Shift

$$
\mathbb{S}^{p-1}\cap\{\boldsymbol{a}\in\mathbb{S}^{p-1}\mid\|\boldsymbol{a}-s_{\ell}[\boldsymbol{a}_0]\|_2\leq r\}
$$

Objective function is **strongly convex** near a shift $s_\ell[\boldsymbol{a}_0]$ of the ground truth.

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Objective Function – Linear Span of Two Shifts

Subspace $\mathcal{S}_{\{\ell_1,\ell_2\}} = \{\alpha_{\ell_1} s_{\ell_1}[a_0] + \alpha_{\ell_2} s_{\ell_2}[a_0] \mid \alpha_{\ell_1}, \alpha_{\ell_2} \in \mathbb{R}\}.$

Objective Function – Linear Span of Two Shifts

Local minimizers are near signed shifts $\pm s_{\ell}[\boldsymbol{a}_0]$. **Negative curvature** between two shifts $s_{\ell_1}[\boldsymbol{a}_0], s_{\ell_2}[\boldsymbol{a}_0]$.

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Objective Function – Multiple Shifts

 $\text{Objective} \ \varphi_{\rho} \text{ over the linear span } \mathcal{S}_{\ell_1,\ell_2,\ell_3} = \{\sum_{i=1}^3 \alpha_{\ell_i} s_{\ell_i}[\bm{a}_0]\}$ **Local minimizers** are near signed shifts $\pm s_{\ell_i}[\boldsymbol{a}_0]$.

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Symmetry and Nonconvexity

- the (only!) local minimizers are symmetric versions of the ground truth.
- *•* there is negative curvature in directions that break symmetry.

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1 Introduction & Motivation of Nonconvex [Optimization](#page-1-0) [Motivating](#page-2-0) Examples [Nonlinearality,](#page-10-0) Nonconvexity, and Symmetry

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3 Efficient Nonconvex [Optimization](#page-37-0) Objectives of Nonconvex [Optimization](#page-38-0)

Nonconvex Optimization

Consider the problem of minimizing a general nonconvex function:

$$
\min_{\bm{x}} f(\bm{x}), \quad \bm{x} \in \mathsf{C}.\tag{5}
$$

In the worst case, even finding a *local* minimizer can be NP-hard2.

Nonconvex problems that arise from natural physical, geometrical, or statistical origins typically have nice structures, in terms of symmetries!

 2 Some NP-complete problems in quadratic and nonlinear programming, K.G Murty and S. N. Kabadi, 1987 (ロ) (_何) (ヨ) (ヨ Ω

Yuqian Zhang Nonconvex [Optimization](#page-0-0) Number 2023 34 / 40

Objectives

Hence typically people seek to work with relatively benign (gradient/Hessian Lipschitz continuous) functions:

$$
\forall \boldsymbol{x}, \boldsymbol{y} \quad \|\nabla f(\boldsymbol{y}) - \nabla f(\boldsymbol{x})\|_2 \le L_1 \|\boldsymbol{y} - \boldsymbol{x}\|_2 \tag{6}
$$

with benign objectives:

1 convergence to some critical point x_* such that: $\nabla f(x_*) = 0$;

2 the critical point x_{\star} is second-order stationary: $\nabla^2 f(x_{\star}) \succeq 0$.

Example: a function φ with symmetry only has regular critical points, while general *f* could have irregular second-order stationary points:

"Any Reasonable Algorithm" Works

Key issue: using negative curvature $\lambda_{\min}(\text{Hess } f) < 0$ to escape saddles.

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"Any Reasonable Algorithm" Works

Efficient (polynomial time) methods:

Trust region method, analyses in [Sun, Qu, W., '17] Curvilinear search, [Goldfarb, Mu, W., Zhou, '16] Noisy (stochastic) gradient descent, [Jin et. al. '17].

"Any Reasonable Algorithm" Works

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Worst Case vs. Naturally Occurring Strict Saddle Functions

Worst Case

[Du, Jin, Lee, Jordan, Poczos, Singh '17] Concentration around stable manifold

Naturally Occuring

DL, Other sparsification problems Dispersion away from stable manifold

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Worst Case vs. Naturally Occurring Strict Saddle Functions

- *•* Red: "slow region" of small gradient around a saddle point.
- *•* Green: stable manifold associated with the saddle point.
- *•* Black: points that flow to the slow region.
- Left: global negative curvature normal to the stable manifold
- *•* Right: positive curvature normal to the stable manifold randomly initialized gradient descent is more likely to encounter the slow region.

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Gradient Descent Works for DL and Related Problems

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Gradient Descent Works for DL and Related Problems

Dispersive structure: Negative curvature ⊥ stable manifolds.

W.h.p. in random initialization $q^{(0)} \sim \text{uni}(\mathbb{S}^{n-1})$, convergence to a neighborhood of a minimizer in polynomial i[te](#page-45-0)r[at](#page-47-0)[i](#page-44-0)[o](#page-45-0)[n](#page-46-0)[s](#page-47-0)[.](#page-37-0) [\[](#page-38-0)[Gi](#page-47-0)[lb](#page-36-0)[oa,](#page-47-0) Ω

Buchanan, W. '18] Yuqian Zhang Nonconvex [Optimization](#page-0-0) June 7, 2023 39 / 40

Conclusion and Coming Attractions

For Nonconvex, Sparse and Low-rank problems

- *•* Benign Geometry:
	- *•* The only local minimizers are symmetric copies of the ground truth
	- *•* There exist negative curvatures breaking symmetry
- *•* Efficient Algorithms:
	- *•* gradient descent algorithms always suffice
	- *•* proximal, projection, acceleration steps can be transferred over

Thank You! Questions?

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