Learning Nonlinear and Deep Representations from High-Dim Data

Nonconvex Optimization of Low-Dimensional Models

#### Sam Buchanan, Yi Ma, Qing Qu, Atlas Wang John Wright, Yuqian Zhang, Zhihui Zhu

June 7, 2023



→ < ∃ →</p>

Nonconvex Optimization

#### Outline

#### Introduction & Motivation of Nonconvex Optimization Motivating Examples Nonlinearality, Nonconvexity, and Symmetry

Symmetry & Geometry for Nonconvex Problems in Practice Problems with Rotational Symmetry Problems with Discrete Symmetry

(日) (四) (문) (문) (문)

3 Efficient Nonconvex Optimization Objectives of Nonconvex Optimization

#### Example: Low-rank Matrix Completion

We observe:

$$oldsymbol{Y} oldsymbol{Y} = \mathcal{P}_\Omega egin{bmatrix} oldsymbol{X} \ \mathsf{Complete\ ratings} \end{bmatrix}.$$





#### Matrix completion

via bilinear low-rank factorization

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

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

#### Example: Dictionary for Image Representation

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

 $I_{\text{noisy}} = A \times x + z.$  (1)



イロト 不得下 イヨト イヨト 二日

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

 $\begin{array}{l} Y = A \quad X.\\ \text{data} \quad \text{dictionary sparse} \end{array}$ (2)

- 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?)

#### Convex and Nonconvex Optimization



イロト イヨト イヨト イヨト

#### **Dictionary Learning**



Recovered solutions always obtain the same objective value.

× /		_		
VIIO	120		har	n or
1 u u	an	_	i ai	18.
				•

Image: A match a ma

#### Benign Nonconvex Optimization Landscape





#### **General Case**

#### **Structured Case**

Image: A matching of the second se

### Example: Sparse Blind Deconvolution

#### Sparse Blind Deconvolution:

the convolutional motif or sparse activation signal are unknown:

$$Y_{\text{data}} = A_{\text{motif}} * X_{\text{sparse}}$$
(3)

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



Kornel An

Observation



Natural Image



#### Sparse Blind Deconvolution



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

		_		
Vuo	112.0	_ /	221	<b>1</b> 00
1 u u	Iall	~	nai	ıĸ

• • • • • • • • • • • •

#### Convolutional Dictionary learning

$$egin{array}{lll} egin{array}{c} egin{arra$$



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

### Challenges of Nonconvex Optimization – Pessimistic Views

Consider the problem of minimizing a general nonlinear function:

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

In the worst case, even finding a *local* minimizer can be NP-hard<sup>1</sup>.

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  $\nabla^2 \varphi(\bar{z}) \succeq 0$ .



Spurious local minimizers

Flat saddle points

<sup>&</sup>lt;sup>1</sup>Some NP-complete problems in quadratic and nonlinear programming, K.G Murty and S. N. Kabadi, 1987

# 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  $\varphi$  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:

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

# 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  $\Gamma$ .

dictionary learning

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

for any signed permutation  $\Pi$ .

blind deconvolution

$$y = a_0 * x_0 = S_{\tau}[a_0] * S_{-\tau}[x_0]$$

for any signed shift  $\tau$ .

### 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  $z \in \mathbb{R}^n$ ,  $\mathfrak{g} \in \mathbb{G}$ ,  $\varphi(\mathfrak{g} \circ z) = \varphi(z)$ .

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



(日) (四) (日) (日) (日)

**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.

#### Nonlinearality, Nonconvexity, and 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



#### Outline

 Introduction & Motivation of Nonconvex Optimization Motivating Examples Nonlinearality, Nonconvexity, and Symmetry

2 Symmetry & Geometry for Nonconvex Problems in Practice Problems with Rotational Symmetry Problems with Discrete Symmetry

(日) (四) (문) (문) (문)

3 Efficient Nonconvex Optimization Objectives of Nonconvex Optimization

#### Problems with Rotational Symmetry



< □ > < 同 > < 回 > < 回 > < 回 >

#### Low rank matrix recovery Goal: Given $Y = \mathcal{A}(X)$ , recover low rank matrix $X = U_0V_0$



• Convex Formulation

$$\min_{oldsymbol{X} \in \mathbb{R}^{m imes n}} \hspace{0.1 in} \left\|oldsymbol{X}
ight\|_{\star} \hspace{0.1 in} ext{s.t.} \hspace{0.1 in} oldsymbol{Y} = \mathcal{A}(oldsymbol{X})$$

• Nonconvex Formulation

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

く 何 ト く ヨ ト く ヨ ト

#### 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  $\Gamma \in \mathbb{R}^{r \times r}$ .



#### 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  $\Gamma \in \mathbb{R}^{r \times r}$ .



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

Simplifications:

- $Y = \mathcal{A}(X) = X$
- $oldsymbol{X} = oldsymbol{U}_0^T$  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:

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

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

Critical points have zero gradient

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

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

$$= \boldsymbol{0}$$

therefore critical points must be one of the following

• 
$$\boldsymbol{u} = \pm \boldsymbol{u}_0$$

• u = 0

• • = • •

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

with the second order derivative

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

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

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  $oldsymbol{u}=\pmoldsymbol{u}_0$  and  $oldsymbol{u}oldsymbol{u}^T=oldsymbol{X}$ 

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

Maximizer u = 0

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

• • = • • = •

### Low Rank Matrix Recovery

Symmetric low rank matrix

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

General low rank matrix recover



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

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

#### Problems with Discrete Symmetry

### Problems with Discrete Symmetry



#### **Dictionary Learning**

Goal: Given dataset  $\boldsymbol{Y}$ , find the optimal dictionary  $\boldsymbol{A}$  that renders the sparsest coefficient  $\boldsymbol{X}$ 

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

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

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

Inherent Symmetry:

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

for any signed permutation matrix  $\boldsymbol{\Gamma}.$ 



#### Orthogonal Dictionary Learning

 Input: matrix Y which is the product of an orthogonal matrix A<sub>0</sub> (called a dictionary) and a sparse matrix X<sub>0</sub>:

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

Optimization Formulation

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

• Given the optimization constraint,  $oldsymbol{X}$  is uniquely defined in terms of  $oldsymbol{A}$ 

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

• Equivalent formulation

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

4

### Orthogonal Dictionary Learning

Instead of aiming to solve the entire matrix  $oldsymbol{A} = [oldsymbol{a}_1, \dots, oldsymbol{a}_n]$  at once via

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

A simpler model problem solves for the columns  $a_i$  one at a time

$$\min_{\boldsymbol{a}} \| \|_{2} = 1$$
  $\| \boldsymbol{a}^{*} \boldsymbol{Y} \|_{1}$ .

Stationary Points:

- $oldsymbol{a}=\pmoldsymbol{a}_i$ , then the Hessian is positive definite
- $m{a} = \sum_{i \in I} \pm rac{1}{\sqrt{|I|}} m{a}_i$ , there exist negative curvatures alone  $m{a}_i (i \in I)$

(日)

#### 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:

$$oldsymbol{y} = oldsymbol{a}_0 * oldsymbol{x}_0 = lpha s_l [oldsymbol{a}_0] * rac{1}{lpha} s_{-l} [oldsymbol{x}_0]$$

for any shift l and nonzero scaling.

The practical optimization problem can be written as

$$\min_{\|\boldsymbol{a}\|_F^2=1, \boldsymbol{x}} \quad rac{1}{2} \left\| \boldsymbol{y} - \boldsymbol{a} * \boldsymbol{x} 
ight\|_F^2 + \lambda \left\| \boldsymbol{x} 
ight\|_1.$$





#### **Objective Function – Near One Shift**



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

Objective function is **strongly convex** near a shift  $s_{\ell}[a_0]$  of the ground truth.

#### Objective Function – Linear Span of Two Shifts



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

#### Objective Function – Linear Span of Two Shifts



**Local minimizers** are near signed shifts  $\pm s_{\ell}[a_0]$ . **Negative curvature** between two shifts  $s_{\ell_1}[a_0]$ ,  $s_{\ell_2}[a_0]$ .

#### **Objective Function – Multiple Shifts**



Objective  $\varphi_{\rho}$  over the linear span  $S_{\ell_1,\ell_2,\ell_3} = \{\sum_{i=1}^3 \alpha_{\ell_i} s_{\ell_i} [a_0]\}$ Local minimizers are near signed shifts  $\pm s_{\ell_i} [a_0]$ .

### Symmetry and Nonconvexity

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



#### Outline

 Introduction & Motivation of Nonconvex Optimization Motivating Examples Nonlinearality, Nonconvexity, and Symmetry

2 Symmetry & Geometry for Nonconvex Problems in Practice Problems with Rotational Symmetry Problems with Discrete Symmetry

・ロト ・御ト ・ヨト ・ヨト 三田

3 Efficient Nonconvex Optimization Objectives of Nonconvex Optimization

### Nonconvex Optimization

Consider the problem of minimizing a general nonconvex function:

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

In the worst case, even finding a *local* minimizer can be NP-hard<sup>2</sup>.

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



<sup>2</sup>Some NP-complete problems in quadratic and nonlinear programming, K.G Murty and S. N. Kabadi, 1987  $(\square \rightarrow ( \bigcirc ) ( \odot ) ( \bigcirc ) ( \bigcirc ) ( \bigcirc ) ( \bigcirc ) ( \odot ) ( \bigcirc ) ( \bigcirc ) ( \odot ) ( \bigcirc ) ( \odot ) ( \odot$ 

### 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:

- **()** convergence to some critical point  $x_{\star}$  such that:  $\nabla f(x_{\star}) = 0$ ;
- **2** the critical point  $x_{\star}$  is second-order stationary:  $\nabla^2 f(x_{\star}) \succeq \mathbf{0}$ .

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



3 35 / 40

### "Any Reasonable Algorithm" Works

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



### "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





#### 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]. Randomly initialized gradient descent .... Obtains a minimizer almost surely [Lee et. al. '16]. Efficient for matrix completion, dictionary learning, ... not efficient in general.

### 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

### 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.

#### Gradient Descent Works for DL and Related Problems





Q

 $W^s(\alpha)$ 

- ( E

#### Gradient Descent Works for DL and Related Problems





**Dispersive structure**: Negative curvature  $\perp$  stable manifolds.

W.h.p. in random initialization  $q^{(0)} \sim \operatorname{uni}(\mathbb{S}^{n-1})$ , convergence to a neighborhood of a minimizer in polynomial iterations. [Gilboa,  $\mathbb{R}$  or

Yuqian Zhang

Nonconvex Optimization

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?