Global Optimality in Structured Matrix Factorization

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High-Dimensional Data

- · In many areas, we deal with high-dimensional data
 - Signal processing
 - Speech processing
 - Computer vision
 - Medical imaging
 - Medical robotics
 - Bioinformatics







The Language of Surgery



Modeling the skills of human expert surgeons to train a new generation of students. [more]



Low Rank Modeling

- Models involving factorization are ubiquitous
 - PCA
 - Nonnegative Matrix Factorization
 - Dictionary Learning
 - Matrix Completion
 - Robust PCA

Face clustering and classification



Affine structure from motion





Convex Formulations of Matrix Factorization

- Nuclear Norm Matrix Approximation $\min_{X} \frac{1}{2} \|Y - X\|_{F}^{2} + \lambda \|X\|_{*} = \sum \sigma_{i}(X)$
- Robust Principal Component Analysis $\min_{X} \|Y - X\|_1 + \lambda \|X\|_*$







Non-Convex Formul. of Matrix Factorization

Principal Component Analysis

$$\min_{U,V} \|Y - UV^{\top}\|_F^2 \quad \text{s.t.} \quad U^{\top}U = I$$

Nonnegative Matrix Factorization

$$\min_{U,V} \|Y - UV^{\top}\|_{F}^{2} \quad \text{s.t.} \quad U \ge 0, V \ge 0$$

Sparse Dictionary Learning

 $\min_{U,V} \|Y - UV^{\top}\|_F^2 \quad \text{s.t.} \quad \|U_i\|_2 \le 1, \|V_i\|_0 \le r$



Typical Low-Rank Formulations

- Convex formulations $\min_{X} \ell(Y, X) + \lambda \Theta(X)$
 - X
 - Robust PCA
 - Matrix completion
- Convex
- Large problem size
- Unstructured factors

• Factorized formulations $\min_{U,V} \ell(Y, UV^{\top}) + \lambda \Theta(U, V)$



- Nonnegative matrix factorization
- Dictionary learning
- Non-Convex
- Small problem size
- Structured factors



Why Do We Need Structured Factors?

• Given a low-rank video $Y \in \mathbb{R}^{p \times t}$ $\min \|Y - X\|_1 + \lambda \|X\|_*$





(a) Original frames

(b) Low-rank \hat{L}

(c) Sparse \hat{S}

 $\min_{U,V} \ell(Y, UV^{\top}) + \lambda \Theta(U, V)$

- U: spatial basis
 - Low total-variation
 - Non-negative

- V: temporal basis
 - Sparse on particular basis set
 - Non-negative

[1] Candes, Li, Ma, Wright. Robust Principal Component Analysis? Journal of the ACM, 2011.



Why Do We Need Structured Factors?

- Nonnegative matrix factorization $\min_{U,V} \|Y UV^{\top}\|_F^2 \quad \text{s.t.} \quad U \ge 0, V \ge 0$
- Sparse dictionary learning

 $\min_{U,V} \|Y - UV^{\top}\|_F^2 \quad \text{s.t.} \quad \|U_i\|_2 \le 1, \|V_i\|_0 \le r$

Challenges to state-of-the-art methods

- Need to pick size of U and V a priori
- Alternate between U and V, without guarantees of convergence to a global minimum



Why do We Care About Convexity?



• A local minimizer of a convex problem is a global minimizer.

http://support.sas.com/documentation/cdl/en/ormpug/63352/HTML/default/viewer.htm#ormpug_optgp_sect001.htm



Why is Non Convexity a Problem?





Contributions

$$\min_{U,V} \ell(Y, UV^{\top}) + \lambda \Theta(U, V)$$

• Assumptions:

- $\ell(Y,X)$: convex and once differentiable in X
- Θ : sum of positively homogeneous functions of degree 2

$$f(\alpha X^1, \dots, \alpha X^K) = \alpha^p f(X^1, \dots, X^K) \quad \forall \alpha \ge 0$$

- Theorem 1: A local minimizer (U,V) such that for some i $U_i = V_i = 0$ is a global minimizer
- **Theorem 2:** If the size of the factors is large enough, local descent can reach a global minimizer from any initialization



Contributions

$$\min_{U,V} \ell(Y, UV^{\top}) + \lambda \Theta(U, V)$$

Assumptions:

- $\ell(Y,X)$: convex and once differentiable in X
- Θ : sum of positively homogeneous functions of degree 2

$$f(\alpha X^1, \dots, \alpha X^K) = \alpha^p f(X^1, \dots, X^K) \quad \forall \alpha \ge 0$$

• Theorem 2:





Tackling Non-Convexity: Nuclear Norm Case

• Convex problem $\min_{X} \ell(Y, X) + \lambda \|X\|_{*}$ Factorized problem $\min_{U,V} \ell(Y, UV^{\top}) + \lambda \Theta(U, V)$

Variational form of the nuclear norm

$$||X||_* = \min_{U,V} \left[\sum_{i=1}^r |U_i|_2 |V_i|_2 \right]$$
 s.t. $UV^\top =$

- Theorem: Assume loss ℓ is convex and once differentiable in X. A local minimizer of the factorized problem such that for some i $U_i = V_i = 0$ is a global minimizer of both problems
- Intuition: regularizer Θ "comes from a convex function"



X

Tackling Non-Convexity: Nuclear Norm Case

• Convex problem $\min_{X} \ell(Y, X) + \lambda \|X\|_{*}$ Factorized problem $\min_{U,V} \ell(Y, UV^{\top}) + \lambda \Theta(U, V)$





• Theorem: Assume loss ℓ is convex and once differentiable in X. A local minimizer of the factorized problem such that for some i $U_i = V_i = 0$ is a global minimizer of both problems



Tackling Non-Convexity: Tensor Norm Case

- A natural generalization is the projective tensor norm [1,2] $\|X\|_{u,v} = \min_{U,V} \sum_{i=1}^{r} \|U_i\|_u \|V_i\|_v \quad \text{s.t.} \quad UV^{\top} = X$
- Theorem 1 [3,4]: A local minimizer of the factorized problem $\min_{U,V} \ell(Y, UV^{\top}) + \lambda \sum_{i=1}^r \|U_i\|_u \|V_i\|_v$

such that for some i $U_i = V_i = 0$, is a global minimizer of both the factorized problem and of the convex problem

$$\min_{X} \ell(Y, X) + \lambda \|X\|_{u, v}$$

[1] Bach, Mairal, Ponce, Convex sparse matrix factorizations, arXiv 2008.

[2] Bach. Convex relaxations of structured matrix factorizations, arXiv 2013.

[3] Haeffele, Young, Vidal. Structured Low-Rank Matrix Factorization: Optimality, Algorithm, and Applications to Image Processing, ICML '14

[4] Haeffele, Vidal. Global Optimality in Tensor Factorization, Deep Learning and Beyond, arXiv '15



Tackling Non-Convexity: Tensor Norm Case

• Theorem 2: If the number of columns is large enough, local descent can reach a global minimizer from any initialization



• Meta-Algorithm:

- If not at a local minima, perform local descent to reach a local minima
- If optimality condition is satisfied, then local minima is global
- If condition fails, choose descent direction (u,v), and set

$$r \leftarrow r+1 \quad U \leftarrow \begin{bmatrix} U & u \end{bmatrix} \quad V \leftarrow \begin{bmatrix} V & v \end{bmatrix}$$



Optimization

$$\min_{U,V} \ell(Y, UV^{\top}) + \lambda \sum_{i=1}^{r} \|U_i\|_u \|V_i\|_v$$

- Convex in U given V and vice versa
- Alternating proximal gradient descent
 - Calculate gradient of smooth term
 - Compute proximal operator
 - Acceleration via extrapolation
- Advantages
 - Easy to implement
 - Highly parallelizable
 - Guaranteed convergence to Nash equilibrium (may not be local min)



Example: Nonnegative Matrix Factorization

Original formulation

 $\min_{U,V} \|Y - UV^{\top}\|_F^2 \quad \text{s.t.} \quad U \ge 0, V \ge 0$

New factorized formulation

$$\min_{U,V} \|Y - UV^{\top}\|_F^2 + \lambda \sum_i |U_i|_2 |V_i|_2 \quad \text{s.t.} \quad U, V \ge 0$$

Note: regularization limits the number of columns in (U,V)



Example: Sparse Dictionary Learning

Original formulation

 $\min_{U,V} \|Y - UV^{\top}\|_F^2 \quad \text{s.t.} \quad \|U_i\|_2 \le 1, \|V_i\|_0 \le r$

New factorized formulation

$$\min_{U,V} \|Y - UV^{\top}\|_F^2 + \lambda \sum_i |U_i|_2 (|V_i|_2 + \gamma |V_i|_1)$$



Non Example: Robust PCA

• Original formulation [1]

 $\min_{X,E} \|E\|_1 + \lambda \|X\|_* \quad \text{s.t.} \quad Y = X + E$

• Equivalent formulation

$$\min_{X} \|Y - X\|_1 + \lambda \|X\|_*$$

• New factorized formulation

$$\min_{U,V} \|Y - UV^{\top}\|_1 + \lambda \sum_i |U_i|_2 |V_i|_2$$

• Not an example because loss is not differentiable

[1] Candes, Li, Ma, Wright. Robust Principal Component Analysis? Journal of the ACM, 2011.



Neural Calcium Image Segmentation

Find neuronal shapes and spike trains in calcium imaging



In Vivo Results (Small Area)

$$\min_{U,V} \|Y - \Phi(UV^{\top})\|_{F}^{2} + \lambda \sum_{i=1}^{r} \|U_{i}\|_{u} \|V_{i}\|_{v} \\
\| \cdot \|_{u} = \| \cdot \|_{2} + \| \cdot \|_{1} + \| \cdot \|_{TV} \\
\| \cdot \|_{v} = \| \cdot \|_{2} + \| \cdot \|_{1}$$
60 microns

Raw Data



+ Low Rank

+Total Variation



In Vivo Results

- PCA
 - Sensitive to noise
 - Hard to interpret

Mean Fluorescence

Feature obtained by PCA





- Proposed method
 - Found 46/48 manually identified active regions
 - Features are easy to interpret
 - Minimal postprocessing for segmentation

Example Image Frames

Features by Our Method





Neural Calcium Image Segmentation





- $Y \in \mathbb{R}^{p \times t}$: hyperspectral image of a certain area at multiple (t>100) wavelengths of light
- Different regions in space correspond to different materials
 - rank(Y) = number of materials
- U: spatial features
 - Low total-variation
 - Non-negative
- V: spectral features
 Non-negative



$\min_{U,V} \ell(Y, UV^{\top}) + \lambda \Theta(U, V)$

MAGING

[1] Candes, Li, Ma, Wright. Robust Principal Component Analysis? Journal of the ACM, 2011.

• Prior method: NucTV (Golbabaee et al., 2012)

$$\min_{X} \|X\|_{*} + \lambda \sum_{i=1}^{\circ} \|X_{i}\|_{TV} \quad \text{s.t.} \quad \|Y - \Phi(X)\|_{F}^{2} \le \epsilon$$

- 180 Wavelengths
- 256 x 256 Images
- Computation per Iteration
 - SVT of whole image volume
 - 180 TV Proximal Operators
 - Projection onto Constraint Set





• Our method

$$\min_{U,V} \|Y - \Phi(UV^{\top})\|_F^2 + \lambda \sum_{i=1} \|U_i\|_u \|V_i\|_v$$

- (U,V) have 15 columns
- Problem size reduced by 91.6%
- Computation per Iteration
 - Calculate gradient
 - 15 TV Proximal Operators
- Random Initializations





$$\frac{\|X_{true} - UV^{\top}\|_F}{\|X_{true}\|_F}$$





Conclussions

- Structured Low Rank Matrix Factorization
 - Structure on the factors captured by the Projective Tensor Norm
 - Efficient optimization for Large Scale Problems

• Local minima of the non-convex factorized form are global minima of both the convex and non-convex forms

- Advantages in Applications
 - Neural calcium image segmentation
 - Compressed recovery of hyperspectral images



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More Information,

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Thank You!

