Projected Power Method: An Efficient Algorithm for Discrete Assignment

Yuxin Chen



Department of Electrical Engineering, Princeton University Joint work with Emmanuel Candes, David Tse, Govinda Kamath, Changho Suh, Tao Zhang

Nonconvex problems are everywhere

Maximum likelihood is usually nonconvex

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- low-rank matrix completion
- graph clustering
- dictionary learning
- graph matching
- ...



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)

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Solving discrete problems is hard

Finding maximum cut in a graph is



Solving discrete problems is hard



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

Fig credit: coding horror

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Convex relaxation

Can relax into convex problems by

• finding convex surrogates (e.g. compressed sensing, matrix completion)

Convex relaxation

Can relax into convex problems by

- finding convex surrogates (e.g. compressed sensing, matrix completion)
- lifting the problem into higher dimensions (e.g. Max-Cut, phase retrieval)



Goemans, Williamson '95



 $\mathsf{maximize}_{\boldsymbol{x}} \qquad \boldsymbol{x}^\top \boldsymbol{W} \boldsymbol{x}$

subj. to $x_i^2 = 1, \quad i = 1, \dots, n$

Goemans, Williamson '95



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Problem: explosion in dimensions $(\mathbb{R}^n \to \mathbb{R}^{n \times n})$

How about solving nonconvex problems directly without lifting?

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This talk: an efficient paradigm for discrete problems

- n unknown variables: x_1, \cdots, x_n
- m possible states: $x_i \in \{1, 2, \cdots, m\}$



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• Measurements: pairwise differences

$$y_{i,j} \stackrel{\text{ind.}}{=} x_i - x_j + \underbrace{\eta_{i,j}}_{\text{noise}} \mod m, \quad i \neq j$$



 $x_i - x_j \mod m$

Bandeira, Charikar, Singer, Zhu '13; Chen, Guibas, Huang '14

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$$y_{i,j} \stackrel{\text{ind}}{=} \begin{cases} x_i - x_j \mod m & \text{with prob. } \pi_0 \\ \text{Uniform } (m) & \text{else} \end{cases}$$

• π_0 : non-corruption rate

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• Goal: recover $\{x_i\}$ (up to global offset)

Bandeira, Charikar, Singer, Zhu '13; Chen, Guibas, Huang '14

Motivation: community recovery

Community structures are common in many social networks



Fig. credit: The Future Buzz



Fig. credit: S. Papadopoulos

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Community recovery: partition users into several clusters based on their friendships / similarities





• phase info x_i for each SNP: (1) $x_i = 0$: maternally inherited (2) $x_i = 1$: paternally inherited



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Phasing: retrieve phase info (haplotype) of all SNPs from paired reads

Jointly align a collection of images/shapes of the same physical object

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• x_i : angle of rotation associated with each shape



Step 1: compute pairwise estimates of relative angles of rotations $\{x_i - x_j\}$



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Step 2: aggregate these pairwise information for joint alignment



Many other related applications ...

- Structure from motion in computer vision
- Cryo-EM in structural biology
- Water-fat separation in MRI
- ...

Maximum likelihood estimates (MLE)

$$\begin{split} \mathsf{maximize}_{\{x_i\}} & \sum_{i,j} \ell\left(x_i, x_j; y_{i,j}\right) \\ \mathsf{subj. to} & x_i \in \{1, \cdots, m\}\,, \quad 1 \leq i \leq n \end{split}$$

• Log-likelihood function ℓ may be complicated

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- \bullet Log-likelihood function ℓ may be complicated
- Discrete input space
- Looks daunting

Alternative representation of discrete variables

Discrete variables \rightarrow orthogonal vectors in higher-dimensional space


Pairwise sample $y_{i,j} \rightarrow \text{encode } \ell(x_i, x_j)$ by $L_{i,j} \in \mathbb{R}^{m \times m}$

$$[\boldsymbol{L}_{i,j}]_{\alpha,\beta} = \ell(x_i = \alpha, x_j = \beta)$$

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• e.g. random corruption model

$$y_{i,j} = \begin{cases} x_i - x_j, & \text{w.p. } \pi_0 \\ \text{Unif}(m), & \text{else} \end{cases} \quad \Rightarrow \quad \ell(x_i, x_j) = \begin{cases} \log(\pi_0 + \frac{1 - \pi_0}{m}), & \text{if } x_i - x_j = y_{i,j} \\ \log(\frac{1 - \pi_0}{m}), & \text{else} \end{cases}$$

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This enables quadratic representation

$$\ell(x_i, x_j) = \boldsymbol{x}_i^\top \boldsymbol{L}_{i,j} \boldsymbol{x}_j$$



MLE is equivalent to a binary quadratic program



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This is essentially nonconvex constrained PCA

How to solve nonconvex constrained PCA?



Power method:

for
$$t = 1, 2, \cdots$$

 $\boldsymbol{z}^{(t)} = \boldsymbol{L} \boldsymbol{z}^{(t-1)}$
 $\boldsymbol{z}^{(t)} \leftarrow \text{normalize} (\boldsymbol{z}^{(t)})$

How to solve nonconvex constrained PCA?



Constrained PCA	
\max_{x} imize _x	$\boldsymbol{x}^\top \boldsymbol{L} \boldsymbol{x}$
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Projected power method:

for
$$t = 1, 2, \cdots$$

 $\boldsymbol{z}^{(t)} = \boldsymbol{L} \boldsymbol{z}^{(t-1)}$
 $\boldsymbol{z}^{(t)} \leftarrow \operatorname{Project}_{\Delta^n} (\mu \boldsymbol{z}^{(t)})$

• μ : scaling factor

Projection onto standard simplex

$$\begin{array}{ll} \mathsf{maximize}_{\boldsymbol{x}=\{\boldsymbol{x}_i\}} \quad \boldsymbol{x}^\top \boldsymbol{L} \boldsymbol{x} & \mathsf{s.t.} \; \boldsymbol{x}_i \in \{\boldsymbol{e}_1, \cdots, \boldsymbol{e}_m\} \\ \\ \boldsymbol{z}^{(t)} \; = \; \boldsymbol{L} \boldsymbol{z}^{(t-1)} \\ \boldsymbol{z}^{(t)} \; \leftarrow \; \mathsf{Project}_{\Delta^n} \; \left(\mu \boldsymbol{z}^{(t)} \right) \end{array}$$

Projection onto standard simplex

$$\begin{array}{l} \Delta^n \text{ is convex hull of feasibility set,} \\ \text{i.e. } \left\{ \boldsymbol{z} = [\boldsymbol{z}_i]_{1 \leq i \leq n} \ \mid \ \forall i : \ \boldsymbol{1}^\top \boldsymbol{z}_i = 1; \ \boldsymbol{z}_i \geq \boldsymbol{0} \end{array} \right\} \end{array}$$



Initialization?



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Spectral initialization

1. $\hat{L} \leftarrow \mathsf{rank}\text{-}m$ approximation of L

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Spectral initialization

- 1. $\hat{L} \leftarrow \mathsf{rank}\text{-}m$ approximation of L
- 2. $\boldsymbol{z}^{(0)} \leftarrow \operatorname{Project}_{\Delta^n}(\mu \hat{\boldsymbol{z}})$, where $\hat{\boldsymbol{z}}$ is a random column of $\hat{\boldsymbol{L}}$

Summary of projected power method (PPM)



- 1. Spectral initialization
- 2. For $t = 1, 2, \cdots$

$$oldsymbol{z}^{(t)} \hspace{0.1in} \leftarrow \hspace{0.1in} \mathsf{Project}_{\Delta^n}\left(\mu oldsymbol{L}oldsymbol{z}^{(t-1)}
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Random corruption model





Random corruption model



Theorem (C. & Candès '16) Fix m > 0 and set $\mu \gtrsim 1/\sigma_2(L)$. With high prob., PPM recovers the truth exactly within $O(\log n)$ iterations if

• signal-to-noise ratio (SNR) not too small: π_0

$$> 2\sqrt{\frac{\log n}{mn}}$$

Implications

Theorem (C. & Candès '16) \cdots PPM succeeds within $O(\log n)$ iterations if non-corruption rate $\pi_0 > 2\sqrt{\frac{\log n}{mn}}$

• PPM succeeds even when most (i.e. $1 - O(\sqrt{\frac{\log n}{n}})$) entries are corrupted

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- PPM succeeds even when most (i.e. $1 O(\sqrt{\frac{\log n}{n}})$) entries are corrupted
- Nearly linear time algorithm
- Works for any initialization obeying $\|\boldsymbol{z}^{(0)} \boldsymbol{x}\| < 0.5 \|\boldsymbol{x}\|$

Empirical misclassification rate



Misclassification rate when n and π_0 vary $(\mu = 10/\sigma_2(\boldsymbol{L}))$

$$y_{i,j} = x_i - x_j + \eta_{i,j} \mod m, \quad \text{where } \eta_{i,j} \stackrel{\text{i.i.d.}}{\sim} P_0$$

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Distributions of $y_{i,j}$ under different hypotheses



Theorem (C. & Candès '16) Fix m > 0 and set $\mu \gtrsim 1/\sigma_2(L)$. Under mild conditions, PPM succeeds within $O(\log n)$ iterations with high prob., provided that

$$\mathsf{KL}_{\min} := \min_{1 \le l < m} \mathsf{KL}(P_0 \parallel P_l) > \frac{4 \log n}{n}$$

Empirical misclassification rate

 $\begin{array}{ll} \text{Modified Gaussian noise model:} \\ \mathbb{P}\left\{\eta_{i,j}=z\right\} \; \propto \; \exp\left(-\frac{z^2}{2\sigma^2}\right), \quad |z| \leq \frac{m-1}{2} \end{array}$



PPM is information-theoretically optimal



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Theorem (Chen-Candès'16) Fix m > 0. No method achieves exact recovery if

$$\mathsf{KL}_{\min} < \frac{4\log n}{n}$$

Large-m case: random corruption model

$$y_{i,j} = \begin{cases} x_i - x_j, & \text{with prob. } \pi_0 \\ \text{Unif}(m), & \text{else} \end{cases}$$

Theorem (C. & Candès '16) Suppose $\log n \leq m \leq poly(n)$. PPM succeeds if

$$\pi_0 \gtrsim \frac{1}{\sqrt{n}}$$

Singer'09; Wang & Singer'12; Bandeira et al'14; Boumal'16; Liu et al'16, Perry et al'16 ...

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– Succeeds even if a dominant fraction $1-O(1/\sqrt{n})$ of inputs are corrupted

Singer'09; Wang & Singer'12; Bandeira et al'14; Boumal'16; Liu et al'16, Perry et al'16 ...

Joint shape alignment: Chair dataset from ShapeNet¹



20 representative 3D shapes (out of 50)

¹We add extra noise to each point of the shapes to make it more challenging.

Joint shape alignment: Chair dataset from ShapeNet¹



20 representative 3D shapes (out of 50)



pairwise cost $-\ell_{i,j}(x_i, x_j)$: avg nearest-neighbor squared distance

¹We add extra noise to each point of the shapes to make it more challenging.

Joint shape alignment: Chair dataset from ShapeNet¹



¹We add extra noise to each point of the shapes to make it more challenging.
Joint shape alignment: angular estimation errors²



	projected power method	semidefinite relaxation
Runtime	2.4 sec	895.6 sec

 $^{^2\}mbox{We}$ add extra noise to each point of the shapes to make it more challenging.

Joint graph matching: CMU House dataset



111 images of a toy house

Joint graph matching: CMU House dataset



111 images of a toy house



input matches

3 representative images

Joint graph matching: CMU House dataset



111 images of a toy house



input matches

optimized matches

3 representative images

Dixon imaging in body MRI

Zhang et al., Magn. Reson. Med., 2016

2 phasor candidates for field inhomogeneity at each voxel

candidate 1



candidate 2

Dixon imaging in body MRI

Zhang et al., Magn. Reson. Med., 2016

2 phasor candidates for field inhomogeneity at each voxel



Dixon imaging in body MRI

Zhang et al., Magn. Reson. Med., 2016

Representative cases of water signal recovery



commercial software



projected power method

Another important issue: missing data + sample locality

Nodes often have locality

Most prior work: (almost) equally likely to sample between any pair of nodes

- Condon et al., Jalali et al., Chen et al., Abbe et al., Mossel et al., Hajek et al., Chin et al...



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More realistically: samples come mainly (or exclusively) from nearby nodes





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In new technologies like 10x-Genomics: (1) $n\sim 10^5$ SNPs; (2) linking range ~ 100 SNPs

Modeling locality via graphs

• Constraint graph ${\mathcal G}$



Modeling locality via graphs

• Constraint graph ${\mathcal G}$



• Random sampling: pick m randomly chosen edges of $\mathcal G$

Modeling locality via constraint graph

Global / long-range measurements







randomly picked edges

Modeling locality via constraint graph

Global / long-range measurements



randomly picked edges



constraint graph

Local measurements



1. How many samples are needed to recover $\{x_i\}$ reliably (up to global offset)?

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Encouraging news: one can obtain efficient recovery within linear time

Start by running spectral method on core complete subgraphs



• Compute low-rank approximation of L (sample matrix restricted to the subgraph)

Split all nodes into overlapping subsets and run spectral methods separately



Split all nodes into overlapping subsets and run spectral methods separately



• Approximate solution within each subgraph

Split all nodes into overlapping subsets and run spectral methods separately



- Approximate solution within each subgraph
- Inconsistent global phases across subgraphs

Calibrate phases across subgraphs by checking their correlations



Calibrate phases across subgraphs by checking their correlations



Calibrate phases across subgraphs by checking their correlations



Purpose of Stages 1-2: obtain approximate solution of all nodes

Clean up all remaining errors by iterative refinement (e.g. projected power method)

• local refinement using *all* samples



Main results: rings



Main results: rings





Main results: rings













Info and comput. limits are identical for many spatially invariant graphs

Empirical success rate vs. sample size



n = 100,000, input error rate = 0.2

10 Monte Carlo runs to get each point Each run takes \sim 6.4 sec on a Mac Pro

Projected power method

Extension: beyond spatially invariant graphs


Extension: beyond spatially invariant graphs



Infomation and comput. limits achievable by same algorithm

Extension: beyond pairwise measurements

New technologies (e.g. 10x) provide multi-linked reads from same chromosome, not just two



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New technologies (e.g. 10x) provide multi-linked reads from same chromosome, not just two



Algorithm and theory can be easily extended to see performance gain



Real data (haplotype phasing)

NA12878_WGS dataset from 10x genomics (# SNPs $n: 34240 \sim 191829$)



Short switch error rate vs. coverage depth (Spectral-Stitching vs. 10X algorithm) (green circle: improvement; red circle: loss of performance)

Fig. credit: Prof. David Tse, Stanford $_{49/50}$

Projected power method

Real data (haplotype phasing)

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Fig. credit: Prof. David Tse, Stanford

Concluding remarks

- Nonconvex procedures are efficient for many discrete optimization problems
- Information limits can be achieved in linear time for a broad family of models

Papers:

1. "The projected power method: an efficient algorithm for joint alignment from pairwise differences", $\,$ Y. Chen and E. Candès, 2016

2. "Community recovery in graphs with locality", Y. Chen, G. Kamath, C. Suh, and D. Tse, International Conference on Machine Learning, 2016

3. "Resolving phase ambiguity in dual-echo Dixon imaging using a projected power method", T. Zhang et al, Magnetic Resonance in Medicine, 2016