STAT 37797: Mathematics of Data Science

Introduction

../Figures/UC_logo.png

Cong Ma

University of Chicago, Autumn 2021

An article in Harvard Data Science Review

stat_comp_HDSR.jpg

Key messages

- Statistical efficiency is still relevant in big data era

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- "A ... procedure is far from optimal in practice if it relies on optimization of a highly nonconvex and nonsmooth objective function"

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- Statistical efficiency is still relevant in big data era
  — *big data vs big parameters (high-dimensional statistics)*
- Computational efficiency cannot be ignored
  — *due to limited computation/memory*
- "A ... procedure is far from optimal in practice if it relies on optimization of a highly nonconvex and nonsmooth objective function"
  — *hmm...nonconvexity maybe our friend*

Main theme of this course

By blending statistical and computational theory, we can extract useful information from big data more efficiently

../Figures/opt_Stat.pdf

Outline

- A motivating example: low-rank matrix completion
- Topics covered in this course
- Course logistics

A motivating example:
low-rank matrix completion

Noisy low-rank matrix completion

../Figures/rankr_matrix.pdf

unknown rank-r matrix $\boldsymbol{\Theta}^{\star} \in \mathbb{R}^{d\times d}$

$$\begin{bmatrix} \checkmark & ? & ? & ? & \checkmark & ? \\ ? & ? & \checkmark & \checkmark & ? & ? \\ \checkmark & ? & ? & \checkmark & ? & ? \\ ? & ? & \checkmark & ? & ? & \checkmark \\ \checkmark & ? & ? & ? & ? & ? \\ ? & \checkmark & ? & ? & \checkmark & ? \\ ? & ? & \checkmark & \checkmark & ? & ? \end{bmatrix}$$

sampling set Ω

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sampling set Ω

observations: $Y_{i,j} = \Theta^\star_{i,j} + \text{noise}, \quad (i,j) \in \Omega$

goal: estimate $\boldsymbol{\Theta}^\star$

Motivation 1: recommendation systems

- Netflix challenge: Netflix provides highly incomplete ratings from nearly 0.5 million users & 20k movies
- How to predict unseen user ratings for movies?

In general, we cannot infer missing ratings

$$\begin{bmatrix} \checkmark & ? & ? & ? & \checkmark & ? \\ ? & ? & \checkmark & \checkmark & ? & ? \\ \checkmark & ? & ? & \checkmark & ? & ? \\ ? & ? & \checkmark & ? & ? & \checkmark \\ \checkmark & ? & ? & ? & ? & ? \\ ? & \checkmark & ? & ? & \checkmark & ? \\ ? & ? & \checkmark & \checkmark & ? & ? \end{bmatrix}$$

Underdetermined system (more unknowns than equations)

... unless rating matrix has some structure

../Figures/matrix_factorization.jpg

Motivation 2: sensor localization

../Figures/localization_sensor.png

- Observe partial pairwise distances
- Goal: infer distance between every pair of nodes

Motivation 2: sensor localization

Introduce location matrix

$$\boldsymbol{X} = \begin{bmatrix} - & \boldsymbol{x}_1^\top & - \\ - & \boldsymbol{x}_2^\top & - \\ - & \vdots & - \\ - & \boldsymbol{x}_d^\top & - \end{bmatrix} \in \mathbb{R}^{d\times 3}$$

then distance matrix $\boldsymbol{D} = [D_{i,j}]_{1\le i,j\le d}$ can be written as

$$\boldsymbol{D} = \underbrace{\underbrace{\begin{bmatrix} \|\boldsymbol{x}_1\|_2^2 \\ \vdots \\ \|\boldsymbol{x}_d\|_2^2 \end{bmatrix} \boldsymbol{1}^\top}_{\text{rank 1}} + \underbrace{\boldsymbol{1} \cdot \left[\|\boldsymbol{x}_1\|_2^2, \cdots, \|\boldsymbol{x}_d\|_2^2\right]}_{\text{rank 1}} - \underbrace{2\boldsymbol{X}\boldsymbol{X}^\top}_{\text{rank 3}}}_{\text{low rank}}$$

$\text{rank}(\boldsymbol{D}) \ll d \quad \longrightarrow \quad$ low-rank matrix completion

Least-squares estimator

$$
\begin{aligned}
\underset{\boldsymbol{\Theta} \in \mathbb{R}^{d \times d}}{\text{minimize}} \qquad & f(\boldsymbol{\Theta}) = \sum_{(i,j) \in \Omega} (\Theta_{i,j} - Y_{i,j})^2 \\
\text{subject to} \qquad & \text{rank}(\boldsymbol{\Theta}) = r
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— *This is also MLE when noise follows Gaussian*

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Challenge: nonconvexity $\Longrightarrow$ computational hardness

Popular workaround: convex relaxation

../Figures/cvx_relaxation.pdf

Convex relaxation for matrix completion

Replace rank constraint by nuclear norm constraint

$$\underset{\boldsymbol{\Theta}\in\mathbb{R}^{d\times d}}{\text{minimize}} \quad f(\boldsymbol{\Theta}) = \sum_{(i,j)\in\Omega} (\Theta_{i,j} - Y_{i,j})^2$$

$$\text{subject to} \quad \cancel{\mathrm{rank}(\boldsymbol{\Theta}) = r} \quad \|\boldsymbol{\Theta}\|_* \le t$$

— $\|\boldsymbol{\Theta}\|_* = \sum_{i=1}^{d} \sigma_i(\boldsymbol{\Theta})$

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convex relaxation (regularized version):

$$\underset{\boldsymbol{\Theta} \in \mathbb{R}^{d \times d}}{\text{minimize}} \quad \sum_{(i,j) \in \Omega} (\Theta_{i,j} - Y_{i,j})^2 + \lambda \|\boldsymbol{\Theta}\|_*$$

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Pro: often achieve statistical optimality

Issue: expensive in computation/memory

Can we solve matrix completion with lower computational cost?

Spectral methods

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— simple, but sometimes statistically inefficient

Nonconvex optimization

Represent low-rank matrix by $\boldsymbol{L}\boldsymbol{R}^\top$ with $\underbrace{\boldsymbol{L}, \boldsymbol{R} \in \mathbb{R}^{d\times r}}_{\text{low-rank factors}}$

../Figures/XY_factor-plain.pdf

$$\underset{\boldsymbol{L},\boldsymbol{R}\in\mathbb{R}^{d\times r}}{\text{minimize}} \quad f(\boldsymbol{L},\boldsymbol{R}) = \sum_{(i,j)\in\Omega} \Big[\big(\boldsymbol{L}\boldsymbol{R}^\top\big)_{i,j} - Y_{i,j} \Big]^2$$

Two-stage algorithm

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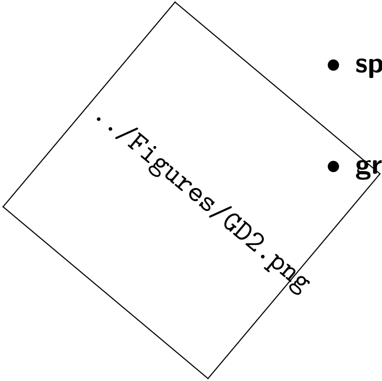

- **spectral initialization:** $(\boldsymbol{L}^0, \boldsymbol{R}^0)$
  — top singular vectors of $\hat{\boldsymbol{Y}}$
- **gradient descent:** for $t = 0, 1, \ldots$

$$\boldsymbol{L}^{t+1} = \boldsymbol{L}^t - \eta_t \nabla_{\boldsymbol{L}} f(\boldsymbol{L}^t, \boldsymbol{R}^t)$$
$$\boldsymbol{R}^{t+1} = \boldsymbol{R}^t - \eta_t \nabla_{\boldsymbol{R}} f(\boldsymbol{L}^t, \boldsymbol{R}^t)$$

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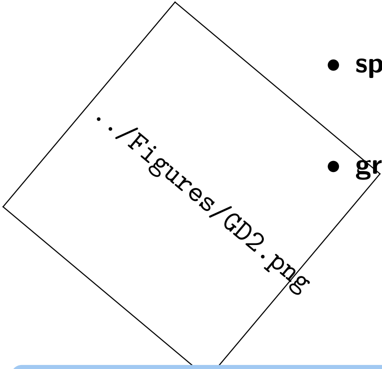

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nonconvex estimator achieves optimal estimation error

— *Ma, Wang, Chi, Chen '17*

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Tentative topics

- Spectral methods
  - Classic ℓ_2 matrix perturbation theory
  - Matrix concentration inequalities
  - Applications of spectral methods (ℓ_2 theory)
  - ℓ_∞ matrix perturbation theory
  - Applications of spectral methods (ℓ_∞ theory)
- Nonconvex optimization
  - Basic optimization theory
  - Generic local analysis for regularized gradient descent (GD)
  - Refined local analysis for vanilla GD
  - Global landscape analysis
  - Gradient descent with random initialization
- Convex relaxation
  - Compressed sensing and sparse recovery
  - Phase transition and convex geometry
  - Low-rank matrix recovery
  - Robust principal component analysis
- Minimax lower bounds (maybe)

Logistics

Why you **should not** take this course

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  - promote deeper understanding of scientific results
- Nonrigorous/heuristic arguments from time to time
  - "nonrigorous" but grounded in rigorous theory
  - help develop intuition

Prerequisites

- linear algebra
- probability theory
- a programming language (e.g., Matlab, Python, Julia, . . .)
- *knowledge in convex optimization*

Textbooks

We recommend these books, but will not follow them closely

high-dim-stats-Wainwright.jpg high-dim-prob-Vershynin.jpg jianqing-book.jpeg

Useful references

- *Spectral Methods for Data Science: A Statistical Perspective*, Yuxin Chen, Yuejie Chi, Jianqing Fan, and Cong Ma
- *Nonconvex optimization meets low-rank matrix factorization: An overview*, Yuejie Chi, Yue M. Lu, and Yuxin Chen
- *Convex optimization*, Stephen Boyd, and Lieven Vandenberghe

Grading

- Homework: 3 problem sets involving proofs and simulations
  - Due on Thursdays

- Course project
  - Either individually or in groups of two

- Your grade: $\max\{0.4 \times \text{HW} + 0.6 \times \text{project}, \text{project}\}$

Course project

Two forms

- literature review
- original research
  - *You are strongly encouraged to combine it with your own research*

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Three milestones

- proposal (due Oct. 28st): up to 1 page
- in-class presentation: last week of class
- report (due Dec. 13th): up to 4 pages with unlimited appendix