Robust sparse estimation: An overview

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IBM Research

Workshop on New Frontiers in Robust Statistics, 2024

Overview

▶ **[Background](#page-1-0)**

- ▷ **[Algorithmic framework](#page-13-0)**
- ▶ **[Polynomial-time algorithms](#page-32-0)**
	- ▷ **[Some improvements](#page-51-0)**
- ▶ **[Quadratic-time algorithms](#page-81-0)**
- ▶ **[Subquadratic-time algorithms](#page-96-0)**

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► Sample complexity: $\Theta(d)$

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Can we reduce the sample complexity if μ is **structured**?

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Can we reduce the sample complexity if μ is **structured**? in this talk: sparsity

Motivating sparsity

 \blacktriangleright Many data distributions are sparse

- ▷ Images in wavelet basis
- ▷ Bioinformatics

Motivating sparsity

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- ▷ Images in wavelet basis
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▶ A classical concept in statistics

- \triangleright Extra information about the true parameter
- ▷ Allows us to get smaller error (alternatively, **lower sample complexity**)

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This talk: Utilizing the structure of sparsity **robustly**.

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Problem statement. (Robust sparse mean estimation) Let ${\mathcal P}$ be an unknown nice distribution over \mathbb{R}^d with a k -**sparse** mean μ Input: corrupted samples from P Output: $\hat{\mu}$ such that $\|\hat{\mu} - \mu\|_2$ is small w.h.p.

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Relaxed goal: Achieving poly(k, log d) sample complexity, **efficiently**

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Prelude: a path towards robust dense estimation

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 \blacktriangleright Suppose the inliers are sampled from $\mathcal{N}(\mu, I)$

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- **► (Reducing to one-dimension)** $\|\widehat{\mu} \mu\|_2 = \sup_v \langle v, \widehat{\mu} \mu \rangle$
	- \triangleright Equivalent to ensuring accurate estimates in all directions v

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- ▶ Key insight **[\[DKKLMS16;](#page-139-0) [LRV16\]](#page-139-1)**: For any direction v,
	- ▷ The sample mean is accurate **if** the sample variance is bounded
	- ▷ **Else if** the sample variance is large, we can filter the outliers

Algorithmic template: robust (dense) estimation

1. While there exists a direction v with large variance:

1.1 Filter each point x using $v^\top x$

2. $\hat{\mu} \leftarrow$ sample mean

[^{\[}DKKLMS16\]](#page-139-0) I. Diakonikolas, G. Kamath, D. Kane, J. Li, A. Moitra, A. Stewart. Robust estimators in high... *FOCS*. 2016 [\[LRV16\]](#page-139-1) K. A. Lai, A. B. Rao, S. Vempala. Agnostic Estimation of Mean and Covariance. *FOCS*. 2016

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sample mean and covariance should be accurate for **clean data** and **all large subsets** (termed **stability**)

[\[LRV16\]](#page-139-1) K. A. Lai, A. B. Rao, S. Vempala. Agnostic Estimation of Mean and Covariance. *FOCS*. 2016

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- **▶ (Projections)** $\|\text{HardThreshold}(\widehat{\mu}) \mu\|_2 \lesssim \sup_{v : k\text{-sparse}} \langle v, \widehat{\mu} \mu \rangle$
	- \triangleright Only the sparse directions matter

Next, a path towards robust sparse estimation

- Suppose the inliers are sampled from $\mathcal{N}(\mu, I)$, where μ is k-sparse
- (Projections) $\|\text{HardThresh}(\widehat{\mu}) \mu\|_2 \lesssim \sup_{v : k\text{-sparse}} \langle v, \widehat{\mu} \mu \rangle$

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Algorithmic template: robust **sparse** estimation

1. While there exists a **sparse** direction v with large variance:

1.1 Filter points after projecting onto v

2. Return HardThresh(sample mean)

Next, a path towards robust sparse estimation

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How to design an efficient subroutine?

 \blacktriangleright $\,$ Sparse operator norm $\|\mathbf{A}\|_{\mathrm{op},k}:=\max_{v:k\text{-sparse}} v^\top \mathbf{A} v$

Towards efficient estimation via relaxed certificates

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Instead, we design an efficient certificate $f(\cdot)$ such that:

1. $||{\bf A}||_{\text{on }k} \leq f({\bf A})$ and ...

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||A||_{op,k} \leq f(A)
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 and ...
2. $f(\hat{\Sigma} - I)$ is small for clean data

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Instead, we design an efficient certificate $f(\cdot)$ such that:

1. $||\mathbf{A}||_{\text{op.}k} \leq f(\mathbf{A})$ and ... **2.** $f($\hat{\Sigma}$ − **I**) is small for clean data and its all large subsets (*f*-stability)$

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 and ...
2. $f(\widehat{\boldsymbol{\Sigma}} - \mathbf{I})$ is small for clean data and its all large subsets (*f*-stability)

Algorithmic template: Robust sparse estimation, **efficiently**

1. While $f(\hat{\Sigma} - I)$ large:

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1.1 Filter points and update $\widehat{\mathbf{\Sigma}}$

2. Return HardThresh(sample mean)

- ▶ Sparse operator norm $\|\mathbf{A}\|_{\mathrm{op},k} := \max_{v:k\text{-sparse}} v^\top \mathbf{A} v$
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Algorithmic template: Robust sparse estimation, efficiently

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1.1 Filter points and update $\widehat{\mathbf{\Sigma}}$

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Better certificates =⇒ **better algorithms**

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An approach via semidefinite programs

▶ Efficient algorithms first developed in **[\[BDLS17\]](#page-139-2)**.

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- ▶ Efficient algorithms first developed in [\[BDLS17\]](#page-139-2).
- ▶ Recall $\|\mathbf{A}\|_{\text{op},k} := \max_{v:k\text{-sparse}} |\langle vv^\top, \mathbf{A} \rangle|$

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Theorem: (BDLS17)

Given ϵ -contaminated samples from an isotropic subgaussian distribution with k-sparse mean μ , a **polynomial-time** algorithm to compute $\hat{\mu}$:

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- \blacktriangleright (sample complexity) $n = \widetilde{O}\left(k^2/\epsilon^2\right)$ samples
- \blacktriangleright (error) $\|\widehat{\mu} \mu\|_2 = \widetilde{O}(\epsilon)$
- ▶ Near-optimal asymptotic error
- ▶ Near-optimal *computational* sample complexity

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\|\widehat{\mu} - \mu\|_2 = \widetilde{O}(\epsilon)
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- ▶ Near-optimal asymptotic error
- ▶ Near-optimal *computational* sample complexity
- ▶ Runtime: polynomial but existing SDP solvers are **impractical**
	- $\triangleright \;$ Current bounds: $\Omega(d^4)$ time
	- **Open problem:** design faster solvers for this SDP

[^{\[}BDLS17\]](#page-139-0) S. Balakrishnan, S. S. Du, J. Li, A. Singh. Computationally Efficient Robust Sparse Estimation.. *COLT*. 2017

 $\mathcal{X}_k := \{ \mathbf{M} \succ 0 : \text{tr}(\mathbf{M}) = 1, ||\mathbf{M}||_1 \leq k \}$

 $||\mathbf{A}||_{\mathcal{X}_k} := \sup_{\mathbf{M} \in \mathcal{X}_k}$

- Algorithm: Filtering (with SDP relaxation)
- \blacktriangleright **SDP-Stability**: For all large subsets S' of S :
	- \triangleright (Mean) $\sup_{v:\text{sparse}}\langle v,\mu_{S'}-\mu\rangle$ is small
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Proof sketch (of a weaker bound)

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\max_{S' \subset S: \text{large}} \|\mathbf{\Sigma}_{S'}\|_{\mathcal{X}_k}
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Proof sketch (of a weaker bound)

$$
\frac{\max\limits_{S' \subset S: \text{large}} \|\mathbf{\Sigma}_{S'}\|_{\mathcal{X}_k}}{\text{MPSD and } 0 \leq \mathbf{\Sigma}_{S'} \leq 2\mathbf{\Sigma}_S}
$$

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Proof sketch (of a weaker bound)

$$
\max_{S' \subset S: \text{large}} \|\mathbf{\Sigma}_{S'}\|_{\mathcal{X}_k} \ \lesssim \ \|\mathbf{\Sigma}_S\|_{\mathcal{X}_k} \ \leq \ 1 + \|\mathbf{\Sigma}_S - \mathbf{I}\|_{\mathcal{X}_k}
$$
\n
\ntriangle inequality

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13/30

Proof sketch (of a weaker bound)

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\max_{S' \subset S: \text{large}} \|\mathbf{\Sigma}_{S'}\|_{\mathcal{X}_k} \ \lesssim \ \|\mathbf{\Sigma}_S\|_{\mathcal{X}_k} \ \leq \ 1 + \|\mathbf{\Sigma}_S - \mathbf{I}\|_{\mathcal{X}_k} \\ \leq k \|\mathbf{\Sigma}_S - \mathbf{I}\|_{\infty} \\ \overbrace{\text{Hölder's inequality}}
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Overview

- ▶ **[Background](#page-1-0)**
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- ▶ **[Polynomial-time algorithms](#page-32-0)**
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To apply [\[BDLS17\]](#page-139-0) to heavy-tailed distributions, we need to ask:

Do heavy-tailed inliers satisfy SDP stability with **good** sample complexity?

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Can we close this gap?

Theorem: [DKL**P**22]

 $\mathcal{P}: k$ -sparse mean μ , bounded covariance, and degree-four* moments. An efficient algorithm to output $\widehat{\mu}$ from ϵ -contaminated data: w.p. $1-\delta$,

[^{\[}DKLP22\]](#page-139-2) I. Diakonikolas, D. Kane, J. Lee, A. Pensia. Outlier-Robust Sparse Estimation for Heavy-Tailed. *NeurIPS*. 2022

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▶ Near-optimal asymptotic error*, *computational* sample complexity*

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- **Open questions**
	- \triangleright removing bounded fourth-moment* condition
	- \triangleright faster runtime

[^{\[}DKLP22\]](#page-139-2) I. Diakonikolas, D. Kane, J. Lee, A. Pensia. Outlier-Robust Sparse Estimation for Heavy-Tailed. *NeurIPS*. 2022

Proof sketch of improved sample complexity

17/30

- ▶ Algorithm works even if inliers contains a **large stable subset**
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Let S be a set of n i.i.d. samples from P (heavy-tailed, bdd. coordinates)

$\mathcal{X}_k := \{ \mathbf{M} \succeq 0 : \text{tr}(\mathbf{M}) = 1, ||\mathbf{M}||_1 \leq k \}$

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holds at the population $(n\to\infty)$ by Markov

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Rounding analytically sparse PSD matrices to sparse matrices

Let S be a set of n i.i.d. samples from P (heavy-tailed, bdd. coordinates) Does the following hold with $n\approx k^2$?

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[^{\[}Li18\]](#page-139-3) J. Li. Principled Approaches to Robust Machine Learning and Beyond. PhD thesis. 2018
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Theorem: Sparse rounding (worst-case) [DKL**P**22]

Given $\mathbf{M} \in \mathcal{X}_k$, there is a random matrix \mathbf{Q}

$$
\blacktriangleright \ \ \text{w.h.p.,} \ \mathbf{Q} \in \mathcal{A}_{k,P}
$$

 $\blacktriangleright \; x^{\top} {\rm M} x \gg 1$ for clipped x implies $\mathbb{P}_{{\bf Q}}(x^{\top} {\bf Q} x \gg 1) \geq 0.4$

[^{\[}Li18\]](#page-139-0) J. Li. Principled Approaches to Robust Machine Learning and Beyond. PhD thesis. 2018

II. Adapting to unknown covariance

Suppose the distribution has bounded t-th moments; $t \gg 1$

- ▶ Optimal asymptotic error: $O(\epsilon^{1-\frac{1}{t}})$
- $▶$ However, for unknown covariance, [\[BDLS17\]](#page-139-2) gets stuck at $\Omega(\sqrt{\epsilon})$

[^{\[}BDLS17\]](#page-139-2) S. Balakrishnan, S. S. Du, J. Li, A. Singh. Computationally Efficient Robust Sparse Estimation.. *COLT*. 2017

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Theorem: [DKK**P**P22]

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21/30

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21/30

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 \triangleright $f(\Sigma - I)$ is bounded for clean data and all large subsets (stability)

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[^{\[}DKKPS19\]](#page-139-4) I. Diakonikolas, D. Kane, S. Karmalkar, E. Price, A. Stewart. Outlier-Robust Sparse Estimation... *NeurIPS*. 2019

21/30

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\|\mathbf{A}\|_{\mathrm{op},k}:=\sup\nolimits_{v:\mathsf{sparse}}|v^\top\mathbf{A}v|
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More practical certificates for the sparse operator norm?

We want a practical function $f(\cdot)$:

 \triangleright $||\mathbf{A}||_{\text{on }k} < f(\mathbf{A})$

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\blacktriangleright \text{ Suppose } f(\mathbf{A}) = \sup_{\mathbf{B}\in \mathcal{B}} \langle \mathbf{B}, \mathbf{A} \rangle.
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Desirable properties of B :

- \rhd sparsity-aware
- ▷ practical to search for B[∗]
- \triangleright (For stability) For all $\mathbf B$ in $\mathcal B$, $x^\top \mathbf B x$ has <mark>bdd. variance</mark>

▶ **[\[DKKPS19\]](#page-139-4):** $B := \{ B : ||B||_{\text{Fr}} = 1, ||B||_0 \le k^2 \}$

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Given $n \epsilon$ -contaminated samples from $\mathcal{N}(\mu, I)$ with k-sparse mean μ , a **practical** algorithm to compute $\widehat{\mu}$ such that w.h.p.,

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• (runtime) $d^2 \cdot \text{poly}(k, 1/\epsilon)$

▶ Near-optimal asymptotic error, computational sample complexity

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Overview

- ▶ **[Background](#page-1-0)**
	- ▷ **[Algorithmic framework](#page-13-0)**
- ▶ **[Polynomial-time algorithms](#page-32-0)**
	- ▷ **[Some improvements](#page-51-0)**
- ▶ **[Quadratic-time algorithms](#page-81-0)**
- ▶ **[Subquadratic-time algorithms](#page-96-0)**

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[^{\[}CDG19\]](#page-139-5) Y. Cheng, I. Diakonikolas, R. Ge. High-Dimensional Robust Mean Estimation in Nearly-Linear Time. *SODA*. 2019 [\[DL22\]](#page-139-6) J. Depersin, G. Lecué. Robust Subgaussian Estimation of a Mean Vector in Nearly Linear Time. *Ann. Stats.* 2022 [\[DHL19\]](#page-139-7) Y. Dong, S. Hopkins, J. Li. Quantum entropy scoring for fast robust mean estimation.. *NeurIPS*. 2019 [\[CMY20\]](#page-139-8) Y. Cherapanamjeri, S. Mohanty, M. Yau. List decodable mean estimation in nearly linear time. *FOCS*. 2020 [\[DKKLT22\]](#page-139-9) I. Diakonikolas, D. M. Kane, D. Kongsgaard, J. Li, K. Tian. Clustering Mixture Models in ..Linear.. *STOC*. 2022 [\[DKPP22\]](#page-139-10) I. Diakonikolas, D. Kane, A. Pensia, T. Pittas. Streaming Algorithms for .. Robust Statistics.. *ICML*. 2022

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- Analog of power iteration for sparse eigenvectors?
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[^{\[}Pen24\]](#page-139-11) A. Pensia. A Sub-Quadratic Time Algorithm for Robust Sparse Mean Estimation. *ICML*. 2024

Theorem: [**P**24]

Given ϵ -contaminated samples from $\mathcal{N}(\mu,I)$ on \mathbb{R}^d with k -sparse μ and a natural number **q**,

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	- $\triangleright\ \ k^2$ sample complexity
	- ▷ linear time
	- ▷ a wider family of distributions (same as [\[DKKPS19\]](#page-139-1))

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 $\|\mathbf{A}\|_{\mathrm{Fr},k^2}:=\ell_2$ norm of largest k^2 entries of \mathbf{A}

Algorithmic template from **[\[DKKPS19\]](#page-139-1)**.

- **1.** While $\|\mathbf{\Sigma} \mathbf{I}\|_{\text{Fr},k^2}$ large:
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\blacktriangleright H := \{ (i, j) : i \neq j , \ |\mathbf{\Sigma}_{i,j}| \gg 1/k \} .
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Strongly correlated coordinates

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▶ $H := \{(i, j) : i \neq j, |\sum_{i,j}| \gg 1/k\}$

 \blacktriangleright First observation: Coordinates in H^\complement are nice

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\triangleright \|\left(\mathbf{\Sigma} - \mathbf{I}\right)_{H}\mathbf{C}\|_{\text{Fr},k^2} \leq \sqrt{k^2} \cdot \frac{1}{k} = O(1)
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How to find H in subquadratic time?

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```
H := \{(i, j) : i \neq j, |\mathbf{\Sigma}_{i,j}| \gg \rho\}
```
Connections to correlation detection

Definition: Two vectors $x,y\in\mathbb{R}^n$ are ρ -correlated if $\big|\big\langle \frac{x}{\|x\|}$ $\frac{x}{\|x\|_2}, \frac{y}{\|y\|}$ $\frac{y}{\|y\|_2}\rangle$ $\geq \rho$

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 \blacktriangleright **Naïve algorithm:** try all possible pairs, runs in d^2 time \triangleright Likely to be optimal

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Problem statement. Correlation detection **with margin** Input: \blacktriangleright vectors $y_1,\ldots,y_d\in\mathbb{R}^n;\;\;n\ll d$ \triangleright a threshold $\rho \in (0,1)$, a threshold $\tau \ll \rho$ \blacktriangleright $\,$ **very few,** say $o(d)$ out of d^2 pairs, are τ -correlated Output: all ρ -correlated pairs $(i, j) \in [d] \times [d]$

 \blacktriangleright **Naïve algorithm:** try all possible pairs, runs in d^2 time

 \blacktriangleright [\[Val15\]](#page-139-2) gives an $o(d^2)$ algorithm if $\tau \ll \rho$

[^{\[}Val15\]](#page-139-2) G. Valiant. Finding Correlations in Subquadratic Time,... *J. ACM* (2015)

$H := \{(i, j) : i \neq j, |\mathbf{\Sigma}_{i,j}| \gg \rho\}$

Connections to correlation detection

Definition: Two vectors $x,y\in\mathbb{R}^n$ are ρ -correlated if $\big|\big\langle \frac{x}{\|x\|}$ $\frac{x}{\|x\|_2}, \frac{y}{\|y\|}$ $\frac{y}{\|y\|_2}\rangle$ $\geq \rho$

Problem statement. Correlation detection **with margin** Input: \blacktriangleright vectors $y_1,\ldots,y_d\in\mathbb{R}^n;\;\;n\ll d$ \triangleright a threshold $\rho \in (0,1)$, a threshold $\tau \ll \rho$ \blacktriangleright $\,$ **very few,** say $o(d)$ out of d^2 pairs, are τ -correlated Output: all ρ -correlated pairs $(i, j) \in [d] \times [d]$

► [Val15] gives an
$$
o(d^2)
$$
 algorithm if $\tau \ll \rho$
▶ runtime $\approx d^{1.6 + \frac{1}{q}}$ if $\tau = \text{poly}(\rho^q)$

[^{\[}Val15\]](#page-139-2) G. Valiant. Finding Correlations in Subquadratic Time,... *J. ACM* (2015)

Filtering using fast correlation detection

 $\tau = \rho^{100}$

Filter outliers

Algorithm outline.

28/30

- **1.** $H \leftarrow \{(i, j) : |\Sigma_{i,j}| \ge \rho\}$ $\rho = 1/k$
- **2.** $J \leftarrow \{(i, j) : |\Sigma_{i,j}| \geq \tau\}$
- **3.** While $|H| \gg \text{poly}(k)$:

► If
$$
|J| = o(d)
$$
:
\n▶ Use [Val15] to find *H* and filter
\n▶ Else
\n▶ ????

Filtering using fast correlation detection

28/30

While $\|\mathbf{\Sigma} - \mathbf{I}\|_{\text{Fr.}k^2}$ large:

Filter outliers

Algorithm outline. 1. $H \leftarrow \{(i, j) : |\Sigma_{i,j}| \ge \rho\}$ $\rho = 1/k$ **2.** $J \leftarrow \{(i, j) : |\Sigma_{i,j}| \geq \tau\}$ $\tau = \rho^{100}$ **3.** While $|H| \gg \text{poly}(k)$: \triangleright **If** $|J| = o(d)$: \triangleright Use **[\[Val15\]](#page-139-2)** to find H and filter ▷ **Else** ▷ ???? How to calculate size of J

Filtering using fast correlation detection

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- **1.** $H \leftarrow \{(i, j) : |\Sigma_{i,j}| \ge \rho\}$ $\rho = 1/k$
- **2.** $J \leftarrow \{(i, j) : |\Sigma_{i,j}| \geq \tau\}$ $\tau = \rho^{100}$
- **3.** While $|H| \gg \text{poly}(k)$:

Size of J : randomly sample $d^{1.5}$ many $\{(i,j)\}$ & count τ -correlation

$$
\blacktriangleright \text{ whp, }\Omega(\sqrt{d}) \text{ hits iff } |J| = \Omega(d)
$$

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Filter outliers

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3. While
$$
|H| \gg \text{poly}(k)
$$
:
 $\triangleright R \leftarrow \text{a set of } d^{1.5} \text{ randomly sampled } (i, j)$

$$
\triangleright \quad \widehat{J} \leftarrow \{ (i,j) \in R : |\mathbf{\Sigma}_{i,j}| \ge \tau \}
$$

$$
\triangleright \quad \mathbf{If} \quad |\widehat{J}| = o(\sqrt{d}) :
$$

 \triangleright **If** $|J| = o($ \triangleright Use **[\[Val15\]](#page-139-2)** to find H and filter

▷ **Else**

 \triangleright ????

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$$
\n
$$
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$$

 \triangleright Use [Val₁₅] to find H and filter

▷ **Else**

$$
\triangleright \quad \textbf{????} \qquad \qquad \text{How to make progress when } |J| \text{ large?}
$$

28/30

Filtering using fast correlation detection

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\n
$$
\triangleright \text{ If } |\widehat{J}| = o(\sqrt{d}).
$$

 \triangleright **If** $|J| = o($ $d)$: \triangleright Use **[\[Val15\]](#page-139-2)** to find H and filter

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 \triangleright ????

Filter: If many entries bigger than τ , then $||\mathbf{\Sigma} - I||_{\text{Frnolv}(1/\tau)} \gg 1$

Can filter if stability holds with $k' = \text{poly}(1/\tau)$

Filtering using fast correlation detection

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\n
$$
\triangleright \text{ If } |\hat{J}| = o(\sqrt{d}) :
$$

 \triangleright **If** $|J| = o($ \triangleright Use **[\[Val15\]](#page-139-2)** to find H and filter

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 \triangleright - Filter using $\operatorname{poly}(1/\tau)$ coordinates in R

Filter: If many entries bigger than τ , then $||\mathbf{\Sigma} - I||_{\text{Fr.poly}(1/\tau)} \gg 1$

Can filter if stability holds with $k' = \text{poly}(1/\tau)$

Filtering using fast correlation detection

While $\|\mathbf{\Sigma} - \mathbf{I}\|_{\text{Fr.}k^2}$ large:

Filter outliers

The complete algorithm.

28/30

1. $H \leftarrow \{(i, j) : |\Sigma_{i,j}| \ge \rho\}$ $\rho = 1/k$

$$
\mathbf{2.} \ \ J \leftarrow \{ (i,j) : |\mathbf{\Sigma}_{i,j}| \geq \tau \} \tag{7}
$$

How to calculate size of J

3. While
$$
|H| \gg \text{poly}(k)
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:
 $\triangleright R \leftarrow \text{a set of } d^{1.5} \text{ randomly sampled } (i, j)$

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\triangleright \widehat{I} \leftarrow \{ (i,j) \in R : |\Sigma_{i,j}| \ge \tau \}
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 \triangleright Use [Val₁₅] to find H and filter

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Conclusion

- \blacktriangleright Today: robust sparse estimation through the lens of mean estimation
- \triangleright What we didn't discuss?
	- ▷ Sparsity in other contexts: PCA, linear regression, covariance,. . .
	- ▷ Privacy
	- ▷ Information-computation tradeoffs

Conclusion

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- Open questions:
	- ▷ Similar progress on sparse PCA, linear regression,
	- Custom SDP solvers for ${M \succeq 0; \text{tr}(M) = 1; ||M||_1 \leq k}$
	- ▷ Relaxing assumptions on data distributions
	- ▷ Linear-time/Practical algorithms

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Happy to chat more

Thank You

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