Algorithms and Algorithmic Intractability in High Dimensional Linear Regression

Ilias Zadik

Massachusetts Institute of Technology (MIT)

Stanford Theory Seminar
1/18/19

Introduction- Big Data Challenges

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Required heavy **statistical and computational tools** on dealing with issues such as high dimensionality, large noise, missing entries.

Still **many open problems**
even for *simple high dimensional statistical models!*

Overview

This talk

Algorithms and **algorithmic barriers**
for *high dimensional linear regression*.

- Improve **information-theory upper bounds**
  through *tight analysis of MLE. ("All or Nothing Property")*
- Explain **computational-statistical gap**,
  through *statistical-physics* based methods. *("Overlap Gap Property")*
- Offer new **polynomial time algorithm** for noiseless case
  using *lattice basis reduction ("One Sample Suffices")*

Papers:
(Gamarnik, Z. *Annals of Stats* (major revision) '17+, *COLT* '17)
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(Gamarnik, Z. *NeurIPS* '18)

Outline of the Talk

(1) Introduction
(2) Background in High Dimensional Linear Regression
(3) Information Theory Limits: MLE performance
(4) Computational-Statistical Gap: a statistical-physics perspective
(5) The Noiseless Case: A lattice basis reduction approach
(6) Conclusion

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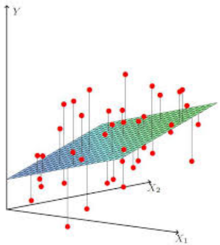
Linear Regression

Let (unknown) $\beta^* \in \mathbb{R}^p$. p number of features.
For **data matrix** $X \in \mathbb{R}^{n \times p}$, and **noise** $W \in \mathbb{R}^n$,
observe n noisy linear samples of β^*, $Y = X\beta^* + W$.

Goal: Given (Y, X), **recover** β^*.



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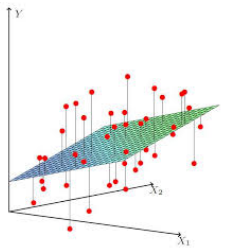

Simplifying assumption between dependent Y and independent X.

Main Question

Setting: $Y = X\beta^* + W$, $X \in \mathbb{R}^{n \times p}, W \in \mathbb{R}^n$.

Main Question: Sample Complexity

What is the **minimum** n so that β^* is (efficiently) recoverable?

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Main Question: Sample Complexity

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An immediate answer under full generality: *at least* p.

Reason: Even if $W = 0$, we have $Y = X\beta^*$,
a **linear system** with p unknowns and n equations!
To solve it, we need at least p equations, i.e. $n \geq p$.

Problem: A High Dimensional Reality

In many **real-life applications** of Linear Regression
(e.g. computer vision, digital economy, computational biology)
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To be well-posed, **need additional assumptions.**

Structural Assumptions on β^*

Assumptions:

(1) β^* is k-**sparse**: k non-zero coordinates, $k = o(p)$.
(A lot of research: e.g. *Compressed Sensing.*)

(2) β^* is **binary valued**: $\beta^* \in \{0,1\}^p$. (†)

(†) (non-trivial) *simplification* of **well-studied** $\beta^*_{\min} := \min_{\beta^*_i \neq 0} |\beta^*_i| = \Theta(1)$ and *support recovery task.*

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Assume: X iid $\mathcal{N}(0,1)$ entries, W iid $\mathcal{N}(0,\sigma^2)$ entries.

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The Model

Setup

Let $\beta^* \in \{0,1\}^p$ be a **binary** k-**sparse** vector, $k = o(p)$. For

- $X \in \mathbb{R}^{n \times p}$ consisting of i.i.d $\mathcal{N}(0,1)$ entries
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Goal

Minimum n so that given (Y, X), β^* is **(efficiently) recoverable** with probability tending to 1 as $n, p, k \to +\infty$ **(w.h.p.)**.

A Computational-Statistical Gap

Algorithmic Results ([Wainwright '09],[Fletcher et al '11])

Set $n_{\text{alg}} = 2k \log p$. Assume $\text{SNR} = \frac{k}{\sigma^2} \to +\infty$.
If

$$n > (1+\epsilon) n_{\text{alg}}$$

LASSO *(convex relaxation)* and OMP *(greedy algorithm)* succeed w.h.p.

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Information-Theoretic Bounds

Let $n^* := 2k \log \frac{p}{k} / \log\left(\frac{k}{\sigma^2}+1\right)$. Assume $\mathrm{SNR} = \frac{k}{\sigma^2} \to +\infty$.

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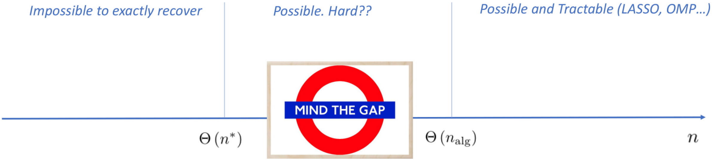

Figure: Computational-Statistical Gap

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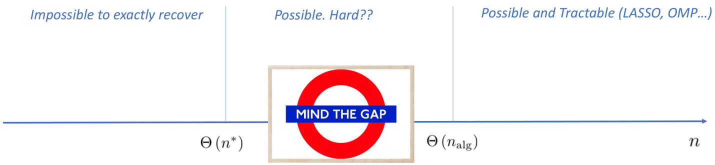

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Questions

(1) Can we find the **exact information theoretic bound** of the problem?

(2) Is there some **fundamental** explanation for the apparent *computational-statistical gap*?

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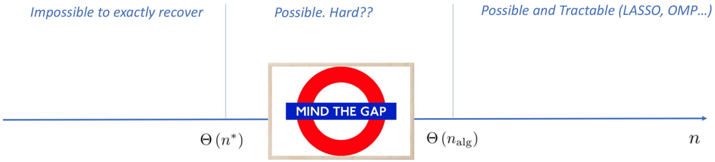

Figure: Computational-Statistical Gap

Questions/Contributions

(1) Can we find the **exact information theoretic bound** of the problem?
Contribution: n*, in an (asymptotic) strong sense.

(2) Is there some **fundamental** explanation for the apparent *computational-statistical gap*?
Contributions: Stat physics-based evidence for (landscape) hardness.
If $\sigma = 0$, β^* **truly** binary: gap closes using lattice basis reduction.

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Maximum Likelihood Estimator (MLE)

$Y = X\beta^* + W$ with W iid $N(0, \sigma^2)$ entries.

The MLE

$\hat{\beta}_{\text{MLE}}$ is the optimal solution of least-squares

$$(\text{LS}) : \min_{\beta \in \{0,1\}^p, \|\beta\|_0 = k} \|Y - X\beta\|_2$$

[Rad '11]: *success* with Cn^* samples.

“All or Nothing” Theorem [Gamarnik, Z. ’17]

Definition

For $\beta \in \{0,1\}^p$, k-sparse we define

$$\mathrm{overlap}(\beta) := |\mathrm{Support}(\beta^*) \cap \mathrm{Support}(\beta)|.$$

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Theorem ("All or Nothing" (Gamarnik, Z. COLT '17))

Let $\epsilon > 0$ be arbitrary.

- *If* $\mathsf{n} > (1+\epsilon)\,\mathsf{n}^*$, *then* $\frac{1}{\mathsf{k}}\text{overlap}(\hat{\beta}_{\text{MLE}}) \to 1$ *whp.*
- *If* $\mathsf{n} < (1-\epsilon)\,\mathsf{n}^*$, *(†) then* $\frac{1}{\mathsf{k}}\text{overlap}(\hat{\beta}_{\text{MLE}}) \to 0$ *whp.*

(†) $\mathsf{k} \leq \exp(\sqrt{\log \mathsf{p}})$

"All or Nothing Theorem" - Comments

An "All or Nothing" phase transition!

- With $n = (1+\epsilon)n^*$, MLE recovers **all but** $o(1)$-fraction of the support.

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- Delicate argument: **novel conditional second moment method** for the existence of “low overlap” β with “small” $\|Y - X\beta\|_2$.

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For $Z = |\{$ "low-overlap" β : "small" $\|Y - X\beta\|_2\}|$,

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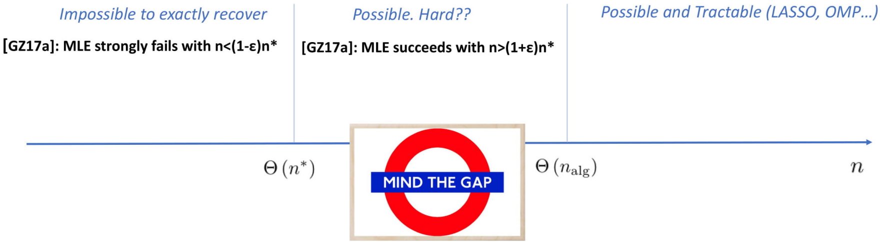
We use

$$\mathbb{P}\left[Z \geq 1\right] = \mathbb{E}_Y[\mathbb{P}[Z \geq 1|Y]] \geq \mathbb{E}_Y[\frac{\mathbb{E}[Z|Y]^2}{\mathbb{E}[Z^2|Y]}] \quad \textit{(conditional 2nd MM)}$$

Summary for n* contribution



Sharp Information-Theoretic Limit n*

$(1+\epsilon)$n* samples MLE (asymptotically) succeeds.
$(1-\epsilon)$n* samples MLE strongly fails.

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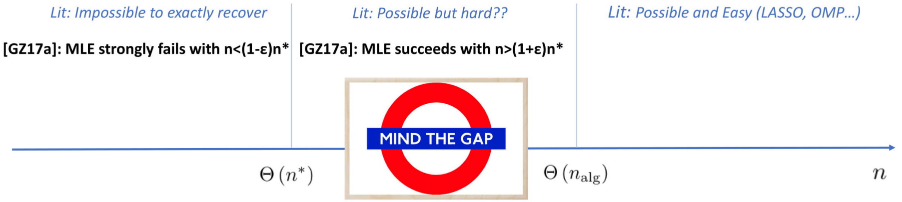
Computational-Statistical Gap



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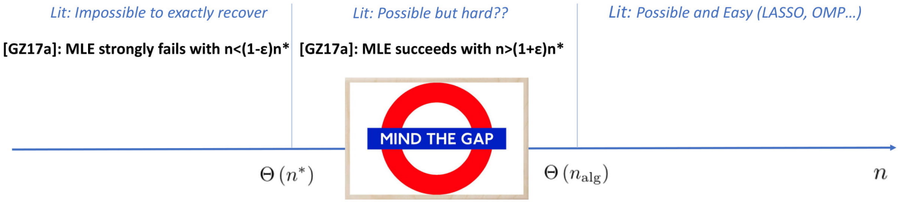

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Contribution through Landscape Analysis

n_{alg} is a **phase transition point** for certain Overlap Gap Property (OGP) on the space of binary k-sparse vectors (origin in *spin glass theory*).
Conjecture computational hardness!

Computational Hardness: A Spin Glass Perspective

Computational gaps appear frequently in random environments

(1) *randoms CSPs*,
such as random-k-SAT (e.g. [MMZ '05], [ACORT '11])

(2) *average-case combinatorial opt problems*
such as max-independent set in ER graphs (e.g. [GS '17], [RV '17])

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Between easy and hard regime there is an **"abrupt change in the geometry of the space of (near-optimal) solutions"** [ACO '08].

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(Vague) Strategy of Studying the Geometry

Study **realizable overlap sizes** between "near-optimal" solutions.
Algorithms appear to work as long as there are **no gaps** in the overlaps.

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Overlap Gap Property, Shattering, Clustering, Free Energy Wells etc

The Overlap Gap Property (OGP) for Linear Regression

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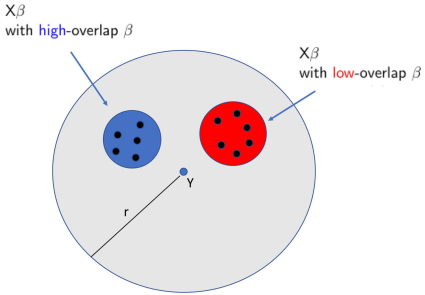
"Near-optimal solutions" $\{\beta \in \{0,1\}^p : \|\beta\|_0 = k, \text{ "small" } \|Y - X\beta\|_2\}$.
Idea: Study overlaps between β and β^*.
$\text{overlap}(\beta) = |\text{Support}(\beta) \cap \text{Support}(\beta^*)|$.

The OGP (informally)

The set of β's with "small" $\|Y - X\beta\|_2$ partitions in
one group where β have **low** overlap with the ground truth β^* and
the other group where β have **high** overlap with the ground truth β^*.



The Overlap Gap Property for Linear Regression-definition

For $r > 0$, set $S_r := \{\beta \in \{0,1\}^p : \|\beta\|_0 = k, n^{-\frac{1}{2}}\|Y - X\beta\|_2 < r\}$.

Definition (The Overlap Gap Property)

The linear regression problem satisfies OGP if there exists $r > 0$ and $0 < \zeta_1 < \zeta_2 < 1$ such that

(a) For every $\beta \in S_r$,

$$\frac{1}{k}\text{overlap}(\beta) < \zeta_1 \text{ or } \frac{1}{k}\text{overlap}(\beta) > \zeta_2.$$

(b) Both the sets

$$S_r \cap \{\beta : \frac{1}{k}\text{overlap}(\beta) < \zeta_1\} \text{ and } S_r \cap \{\beta : \frac{1}{k}\text{overlap}(\beta) > \zeta_2\}$$

are non-empty.

OGP Phase Transition at $\Theta(n_{alg})$

Theorem (Gamarnik, Z COLT '17a), (Gamarnik, Z '17b)

Suppose $k \leq \exp(\sqrt{\log p})$. *There exists* $C > 1 > c > 0$ *such that,*

- *If* $n < cn_{alg}$ *then w.h.p. OGP holds.*
- *If* $n > Cn_{alg}$ *then w.h.p. OGP does* **not** *hold.*

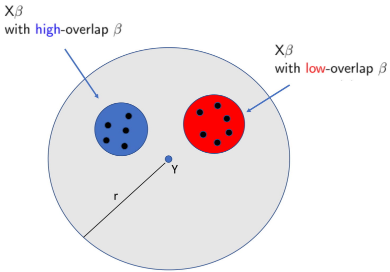
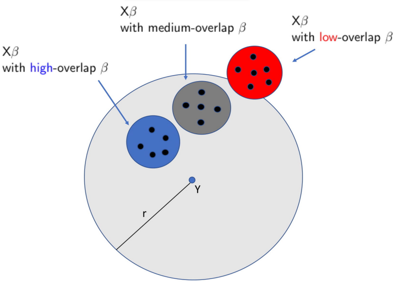


Figure: $n < cn_{alg}$



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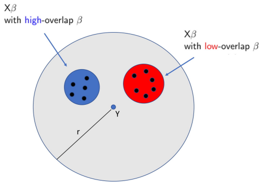
OGP coincides with the failure of
convex relaxation and **compressed sensing** methods!



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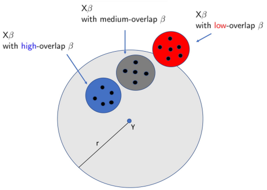

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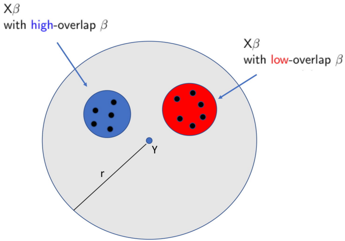
OGP and Local Search

Local Step: $\beta \to \beta'$ if $\mathrm{d_H}(\beta, \beta') = 2$. E.g. $\begin{bmatrix} * \\ 0 \\ 1 \\ * \end{bmatrix} \to \begin{bmatrix} * \\ 1 \\ 0 \\ * \end{bmatrix}$



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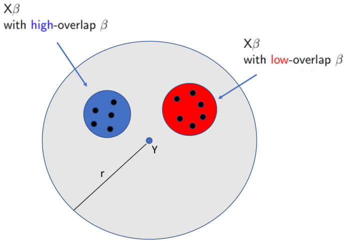


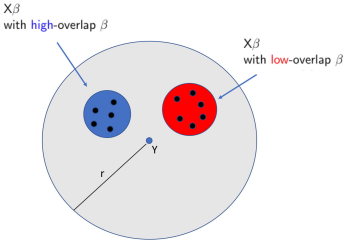
OGP and Local Search

Local Step: $\beta \to \beta'$ if $d_H(\beta, \beta') = 2$. E.g. $\begin{bmatrix} * \\ 0 \\ 1 \\ * \end{bmatrix} \to \begin{bmatrix} * \\ 1 \\ 0 \\ * \end{bmatrix}$

(LS): $\min_{\beta \in \{0,1\}^p, \|\beta\|_0 = k} \|Y - X\beta\|_2$.

Local Search Barrier

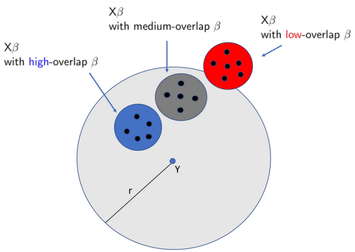
Under OGP, there are **low-overlap local minima** in (LS).
If $n < cn_{alg}$, greedy local-search algorithm **fails** (worst-case) w.h.p.



OGP and Local Search

Theorem (Gamarnik, Z '17b)

If $n > Cn_{alg}$, *the* **only local minimum** *in (LS) is* β^* *whp and greedy local search algorithm* **succeeds** *in* $O(k/\sigma^2)$ *iterations whp.*



Summary of Contribution

Lit: Impossible to exactly recover

[RXZ18]:Weak recovery fails with n<(1-ε)n*

Lit: Possible but hard??

[GZ17a]: MLE succeeds with n>(1+ε)n*

[GZ17a]: OGP appears

[GZ17b]: LS has low overlap local min

Lit: Possible and Easy (LASSO, OMP...)

[GZ17b]: OGP disappears and greedy local search works

[GZ17b]: LS has only the trivial local min

$\Theta(n^*)$ $\Theta(n_{\text{alg}})$ n

Sharp Information-Theoretic Limit n^*

$(1+\epsilon)n^*$ samples MLE (asymptotically) succeeds.
$(1-\epsilon)n^*$ samples MLE strongly fails.

OGP Phase Transition at n_{alg}

$n < cn_{\text{alg}}$ OGP holds and $n > Cn_{\text{alg}}$ OGP does not hold.
Computational Hardness conjectured!

Outline of the Talk

(1) Introduction
(2) Background in High Dimensional Linear Regression
(3) Information Theory Limits: MLE performance
(4) Computational-Statistical Gap: a statistical-physics perspective
(5) **The Noiseless Case: A lattice basis reduction approach**
(6) Conclusion

Noiseless Case: One Sample Suffices

Fact

Under $X \in \mathbb{R}^{n \times p}$ iid $\mathcal{N}(0,1)$, one samples suffices for $\sigma = 0$. $(n^* = 1)$

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For any $\beta \neq \beta^*$ $\mathbb{P}\left[y_1 = \langle X_1, \beta \rangle\right] = 0$ *(no sparsity needed.)*

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Can we make brute-force search efficient?

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$n_{\text{alg}} = 2k \log p$ and OGP for $n < n_{\text{alg}}$.

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Contribution: Beyond the sparsity constraint

Offer an **efficient algorithm**
which recovers any **rational-valued** β^* (no-sparsity)
from $n = 1$ **noiseless sample** $y_1 = \langle X_1, \beta^* \rangle$ and $p \to +\infty$.

Generalizes to higher n *and tolerates small noise.*

Regression using Lattice Based Methods

Suppose β^* has Q-rational entries: $\beta_i^* \in \frac{1}{Q}\mathbb{Z}$.

Theorem ("One Sample Suffices", (Gamarnik, Z. NeurIPS '18))

Assume **any** $n = o(p)$ *samples and* $\sigma \le e^{-p \max\{p, \log Q\}/n}$.
Then there exists a **polynomial-in-**$n, p, \log Q$ *time algorithm with input* (Y, X) *ouputs* β^* *w.h.p. as* $p \to +\infty$.

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The Algorithm: Lattice-Based Method

Reduces to **Shortest Vector Problem** on a lattice
and uses **lattice basis reduction** technique.

Based on pioneering work [Lagarias, Odlyzko '83], [Frieze '86]
on *randomly generated subset-sum problems.*

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- *Lattice* produced by matrix $A \in \mathbb{Z}^{d \times d}$: $\mathcal{L} = \{Aw : w \in \mathbb{Z}^d\}$.

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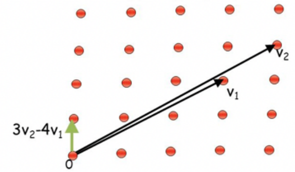

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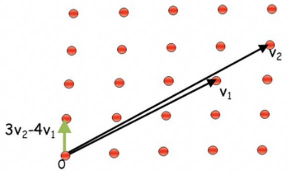
- *Shortest Vector Problem:* $\min \|z\|_2 : z \in \mathcal{L} \setminus \{0\}$, say optimum z_{SV}.
- *NP-hard*,
  but **Lenstra-Lenstra-Lovász** efficiently approximates it,
  outputs $\hat{z} \in \mathcal{L} \setminus \{0\}$ with $\|\hat{z}\|_2 \leq 2^{d/2}\|z_{SV}\|_2$.



Shortest Vector Problem (SVP): given a lattice, find a shortest (nonzero) vector

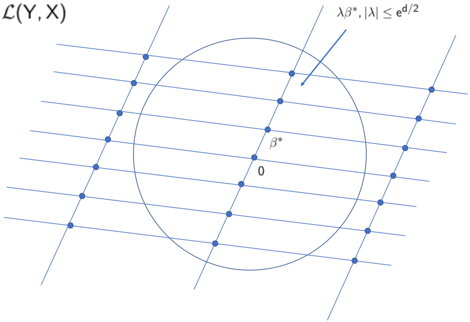
Algorithm Ideas

Main Idea (High Level)

Construct lattice $\mathcal{L}(Y, X)$ where

- **shortest vector** is β^*
- **all "approximately" short** vectors are multiples of β^*.

Use **Lenstra-Lenstra-Lovász** to recover β^*.



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Conclusion - Overview

This talk

Algorithms and **algorithmic barriers**
for *high dimensional linear regression*.

- Improve **information-theory upper bounds**
  through tight analysis of MLE. *("All or Nothing Property")*
- Explain **computational-statistical gap**,
  through *statistical-physics* based methods. *("Overlap Gap Property")*
- Offer new **polynomial time algorithm** for noiseless case
  using *lattice basis reduction ("One Sample Suffices")*

Papers:
(Gamarnik, Z. *Annals of Stats* (major revision) '17+, *COLT* '17)
(Gamarnik, Z. *Annals of Stats* (major revision) '17+)
(Gamarnik, Z. *NeurIPS* '18)

Conclusion - Future Directions

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Thank you!!

The Algorithm (special case, [F '84])

Assume

- $n = 1$, $\sigma = 0$, β^* binary: $y = \langle X_1, \beta^* \rangle$.
- $X_1 \in \mathbb{Z}^p$ with iid **uniform in** $[2^N]$ **entries** for large N (say $N = p^2$).

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Intuition:

$$z = A_M \begin{bmatrix} \beta \\ \lambda \end{bmatrix} = \begin{bmatrix} M\langle X_1, \beta \rangle - M\lambda y_1 \\ \beta \end{bmatrix} = \begin{bmatrix} M\langle X_1, \beta - \lambda\beta^* \rangle \\ \beta \end{bmatrix},$$

$\mathbb{P}\,(\text{Lemma is false}) \leq \mathbb{P}\,(\exists \beta \neq \lambda\beta^* : \|\beta\|_2 < M, \langle X_1, \beta - \lambda\beta^* \rangle = 0) \to 0.$

“All or Nothing” Theorem [Gamarnik, Z. ’17]

Definition

For $\beta \in \{0,1\}^p$, k-sparse we define

$$\text{overlap}(\beta) := |\text{Support}(\beta^*) \cap \text{Support}(\beta)|.$$

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Theorem ("All or Nothing" (Gamarnik, Z. COLT '17))

Let $\epsilon > 0$ be arbitrary.

- *If* $n > (1+\epsilon)\, n^*$, *then* $\frac{1}{k}\text{overlap}(\hat{\beta}_{MLE}) \to 1$ *whp.*
- *If* $n < (1-\epsilon)\, n^*$, *(†) then* $\frac{1}{k}\text{overlap}(\hat{\beta}_{MLE}) \to 0$ *whp.*

(†) $k \leq \exp(\sqrt{\log p})$

Proof Ideas-1

- Set $\mathrm{OPT} = \min_{\beta \in \{0,1\}^p, \|\beta\|_0 = k} \left(\|Y - X\beta\|_2 \right)$.

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Proof Ideas-2

- We show that w.h.p. for all $\ell = 0, 1, \ldots, k$,

$$\mathrm{OPT}_\ell \sim \sqrt{2k(1-\frac{\ell}{k}) + \sigma^2} \exp\left(-\frac{k(1-\frac{\ell}{k})\log p}{n}\right).$$

(requires **novel conditional second moment method**)

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- So, w.h.p. for all $\ell = 0, 1, \ldots, k$,

$$\mathrm{OPT}_\ell \sim f\left(1 - \frac{\ell}{k}\right),$$

for $f(\alpha) := \sqrt{2\alpha k + \sigma^2} \exp\left(-\alpha \frac{k \log p}{n}\right), \alpha \in [0, 1]$

Proof Ideas-3

- So w.h.p. for $\alpha = 1 - \frac{\ell}{k}$ (false detection rate - FDR) ,

$$\mathsf{OPT} = \min_{\ell=0,1,\ldots,k} \mathsf{OPT}_\ell \sim \min_{\ell=0,1,\ldots,k} f\left(1 - \frac{\ell}{k}\right) \sim \min_{\alpha\in[0,1]} f(\alpha)\,.$$

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- *"All or Nothing Phase Transition":*
  $n < n^*$ **full FDR or zero overlap**
  but $n > n^*$ **zero FDR or full overlap.**

OGP curve

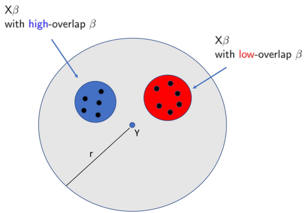
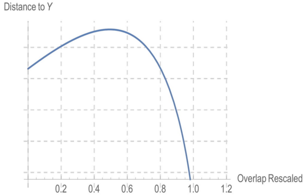


Figure: OGP



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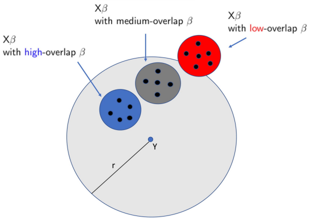

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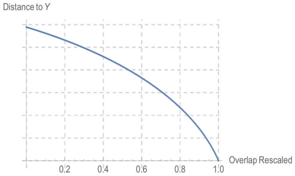

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