

# Learning without correspondence

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# Introduction

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## Example #1: unlinked data sources

- Two separate data sources about same entities:

Sex	Age	Height
M	20	180
F	24	162.5
F	22	160
F	23	167.5

Disease
1
0
0
1

- First source contains covariates (sex, age, height, ...).
- Second source contains response variable (disease status).

## Example #1: unlinked data sources

- Two separate data sources about same entities:

Sex	Age	Height		Disease
M	20	180	???	1
F	24	162.5		0
F	22	160		0
F	23	167.5		1

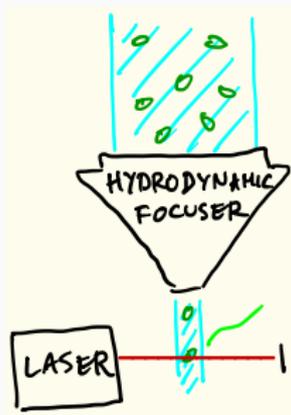
- First source contains covariates (sex, age, height, ...).
- Second source contains response variable (disease status).

**To learn:** relationship between response and covariates.

**Record linkage unknown.**

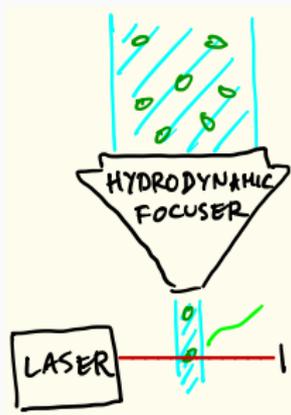
## Example #2: flow cytometry

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2. Cells pass through laser, one at a time; measure emitted light.



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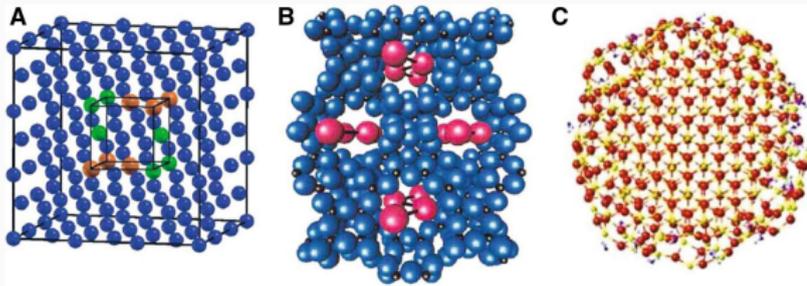


**To learn:** relationship between measurements and cell properties.

**Order in which cells pass through laser is unknown.**

## Example #3: unassigned distance geometry

1. Unknown arrangement of  $n$  points in Euclidean space.

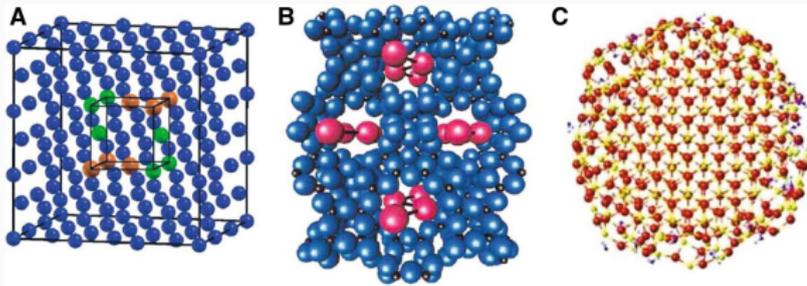


(Image credit: Billinge, Duxbury, Gonçalves, Lavor, & Mucherino, 2016)

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2. Measure distribution of *pairwise distances* among the  $n$  points  
(using high-energy X-rays).

**To learn:** original arrangement of the  $n$  points.

**Assignment of distances to pairs of points is unknown.**

# Learning without correspondence

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Correspondence information is missing in many natural settings.

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We give a theoretical treatment in context of two simple problems:

1. **Linear regression without correspondence**

(Joint work with Kevin Shi and Xiaorui Sun; NIPS 2017.)

2. **Correspondence retrieval** (generalization of *phase retrieval*)

(Joint work with Alexandr Andoni, Kevin Shi, and Xiaorui Sun; COLT 2017.)

## 1. **Linear regression without correspondence**

- Strong NP-hardness of least squares problem.
- Polynomial-time approximation scheme in constant dimensions.
- Information-theoretic signal-to-noise lower bounds.
- Polynomial-time algorithm in noise-free average case setting.

## 2. **Correspondence retrieval**

- Measurement-optimal recovery algorithm in noise-free setting.
- Robust recovery algorithm in noisy setting.

# Linear regression without correspondence

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## Linear regression without correspondence

$y_1$	$\mathbf{x}_1^\top$
$y_2$	$\mathbf{x}_2^\top$
$\vdots$	$\vdots$
$y_n$	$\mathbf{x}_n^\top$

**Feature vectors:**  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n \in \mathbb{R}^d$

**Labels:**  $y_1, y_2, \dots, y_n \in \mathbb{R}$

## Linear regression without correspondence

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**Classical linear regression:**

$$y_i = \mathbf{x}_i^\top \boldsymbol{\beta}^* + \varepsilon_i, \quad i = 1, \dots, n.$$

# Linear regression without correspondence

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**Linear regression without correspondence:**

$$y_i = \mathbf{x}_{\pi^*(i)}^\top \beta^* + \varepsilon_i, \quad i = 1, \dots, n.$$

# Model for linear regression without correspondence

Unnikrishnan, Haghigatshoar, & Vetterli, 2015; Pananjady, Wainwright, & Courtade 2016; Elhami, Scholefield, Haro, & Vetterli, 2017; Abid, Poon, & Zou, 2017; ...

- **Feature vectors:**  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n \in \mathbb{R}^d$
- **Labels:**  $y_1, y_2, \dots, y_n \in \mathbb{R}$
- **Model:**

$$y_i = \mathbf{x}_{\pi^*(i)}^\top \boldsymbol{\beta}^* + \varepsilon_i, \quad i = 1, \dots, n.$$

- Linear function:  $\boldsymbol{\beta}^* \in \mathbb{R}^d$
- Permutation:  $\pi^* \in S_n$
- Errors:  $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_n \in \mathbb{R}$ .

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- **Goal:** “learn”  $\boldsymbol{\beta}^*$ .

Correspondence between  $(\mathbf{x}_i)_{i=1}^n$  and  $(y_i)_{i=1}^n$  is **unknown**.

# Questions

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(Least squares approximation.)
2. When is it possible to recover the “correct”  $\beta^*$ ?  
(When is the “best” linear fit actually meaningful?)

# Least squares approximation

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## Least squares problem

Given  $(\mathbf{x}_i)_{i=1}^n$  from  $\mathbb{R}^d$  and  $(y_i)_{i=1}^n$  from  $\mathbb{R}$ , minimize

$$F(\boldsymbol{\beta}, \pi) := \sum_{i=1}^n \left( \mathbf{x}_i^\top \boldsymbol{\beta} - y_{\pi(i)} \right)^2 .$$

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Reduction from 3-PARTITION ([H., Shi, & Sun, 2017](#)).

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**Naïve brute-force search:**  $\Omega(|S_n|) = \Omega(n!)$ .

**Least squares with known correspondence:**  $O(nd^2)$  time.

## Least squares problem ( $d = 1$ )

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$$\begin{array}{c} (x_1 \beta - y_1)^2 \\ (x_2 \beta - y_2)^2 \\ \vdots \\ (x_n \beta - y_n)^2 \end{array}$$

Cost with  $\pi(i) = i$  for all  $i = 1, \dots, n$ .

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If  $\beta > 0$ , then can improve cost with  $\pi(1) = 2$  and  $\pi(2) = 1$ .

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$$25\beta^2 - 20\beta + 5 + \dots > 25\beta^2 - 22\beta + 5 + \dots$$

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**What about  $d > 1$ ?**

## Alternating minimization

Pick initial  $\hat{\beta} \in \mathbb{R}^d$  (e.g., randomly).

Loop until convergence:

$$\hat{\pi} \leftarrow \arg \min_{\pi \in S_n} \sum_{i=1}^n \left( \mathbf{x}_i^\top \hat{\beta} - y_{\pi(i)} \right)^2 .$$

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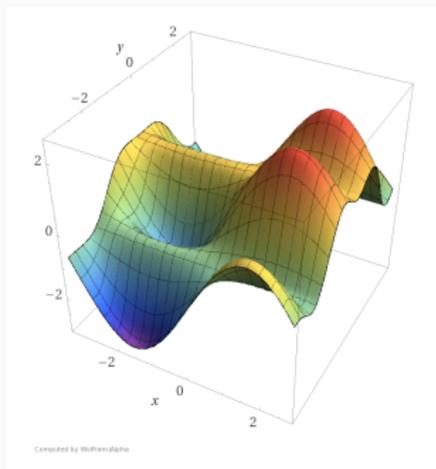
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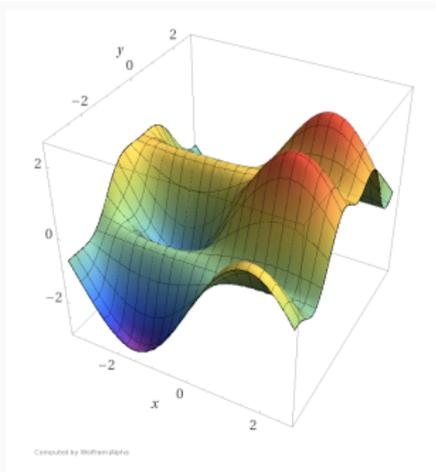
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(Image credit: Wolfram|Alpha)

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- Each loop-iteration efficiently computable.
- But can get stuck in local minima. So try many initial  $\hat{\beta} \in \mathbb{R}^d$ .  
(**Open:** How many restarts? How many iterations?)

### Theorem (H., Shi, & Sun, 2017)

*There is an algorithm that given any inputs  $(\mathbf{x}_i)_{i=1}^n$ ,  $(y_i)_{i=1}^n$ , and  $\epsilon \in (0, 1)$ , returns a  $(1 + \epsilon)$ -approximate solution to the least squares problem in time*

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$$\left(\frac{n}{\epsilon}\right)^{O(d)} + \text{poly}(n, d).$$

**Recall:** Brute-force solution needs  $\Omega(n!)$  time.

(No other previous algorithm with approximation guarantee.)

# Statistical recovery of $\beta^*$ : algorithms and lower-bounds

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**Approach:** Study question in context of statistical model for data.

1. Understand information-theoretic limits on recovering truth.
2. Natural “average-case” setting for algorithms.

# Statistical model

$$\begin{array}{|c|} \hline y_1 \\ \hline y_2 \\ \hline \vdots \\ \hline y_n \\ \hline \end{array} = \begin{array}{|c|} \hline \mathbf{x}_{\pi^*}^\top(1) \\ \hline \mathbf{x}_{\pi^*}^\top(2) \\ \hline \vdots \\ \hline \mathbf{x}_{\pi^*}^\top(n) \\ \hline \end{array} \begin{array}{|c|} \hline \beta^* \\ \hline \end{array} + \begin{array}{|c|} \hline \varepsilon_1 \\ \hline \varepsilon_2 \\ \hline \vdots \\ \hline \varepsilon_n \\ \hline \end{array}$$

Assume  $(\mathbf{x}_i)_{i=1}^n$  iid from  $\mathbb{P}$  and  $(\varepsilon_i)_{i=1}^n$  iid from  $N(0, \sigma^2)$ .

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Recoverability of  $\beta^*$  depends on **signal-to-noise ratio**:

$$\text{SNR} := \frac{\|\beta^*\|_2^2}{\sigma^2}.$$

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Recoverability of  $\beta^*$  depends on **signal-to-noise ratio**:

$$\text{SNR} := \frac{\|\beta^*\|_2^2}{\sigma^2}.$$

**Classical setting (where  $\pi^*$  is known):**

Just need  $\text{SNR} \gtrsim d/n$  to approximately recover  $\beta^*$ .

## High-level intuition

$$\begin{array}{|c|} \hline y_1 \\ \hline y_2 \\ \hline \vdots \\ \hline y_n \\ \hline \end{array} = \begin{array}{|c|} \hline \mathbf{x}_{\pi^*}^\top(1) \\ \hline \mathbf{x}_{\pi^*}^\top(2) \\ \hline \vdots \\ \hline \mathbf{x}_{\pi^*}^\top(n) \\ \hline \end{array} \begin{array}{|c|} \hline \\ \hline \beta^* \\ \hline \\ \hline \end{array} + \begin{array}{|c|} \hline \varepsilon_1 \\ \hline \varepsilon_2 \\ \hline \vdots \\ \hline \varepsilon_n \\ \hline \end{array}$$

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Suppose  $\beta^*$  is either  $e_1 = (1, 0, 0, \dots, 0)$  or  $e_2 = (0, 1, 0, \dots, 0)$ .

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$\pi^*$  **known**: distinguishability of  $e_1$  and  $e_2$  can improve with  $n$ .

## High-level intuition

Suppose  $\beta^*$  is either  $e_1 = (1, 0, 0, \dots, 0)$  or  $e_2 = (0, 1, 0, \dots, 0)$ .

$$\begin{array}{|c|} \hline y_1 \\ \hline y_2 \\ \hline \vdots \\ \hline y_n \\ \hline \end{array} = \begin{array}{|c|c|} \hline & \mathbf{x}_{\pi^*}^\top(1) \\ \hline & \mathbf{x}_{\pi^*}^\top(2) \\ \hline & \vdots \\ \hline & \mathbf{x}_{\pi^*}^\top(n) \\ \hline \end{array} \beta^* + \begin{array}{|c|} \hline \varepsilon_1 \\ \hline \varepsilon_2 \\ \hline \vdots \\ \hline \varepsilon_n \\ \hline \end{array}$$

$\pi^*$  **known**: distinguishability of  $e_1$  and  $e_2$  can improve with  $n$ .

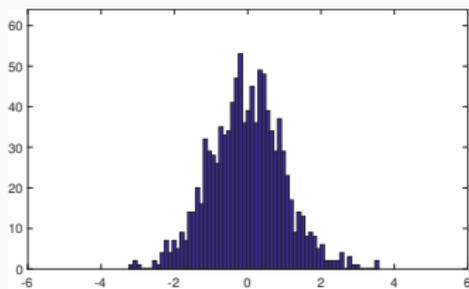
$\pi^*$  **unknown**: distinguishability is less clear.

$$\{y_i\}_{i=1}^n = \begin{cases} \{\mathbf{x}_{i,1}\}_{i=1}^n + N(0, \sigma^2) & \text{if } \beta^* = e_1, \\ \{\mathbf{x}_{i,2}\}_{i=1}^n + N(0, \sigma^2) & \text{if } \beta^* = e_2. \end{cases}$$

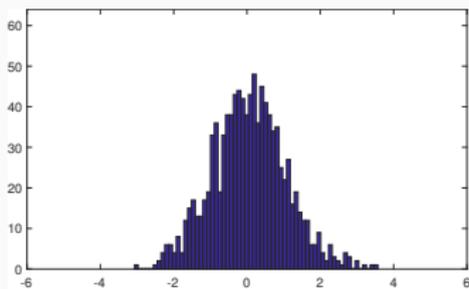
( $\{\cdot\}$  denotes *unordered multi-set*.)

# Effect of noise

Without noise ( $\mathbb{P} = \mathcal{N}(0, \mathbf{I}_d)$ )



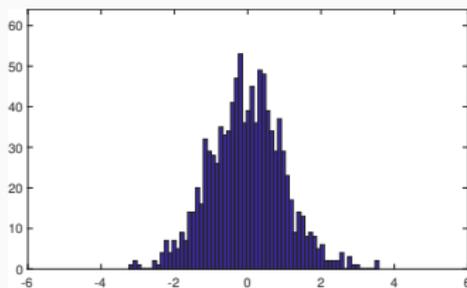
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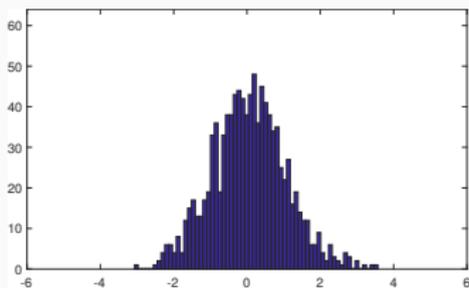
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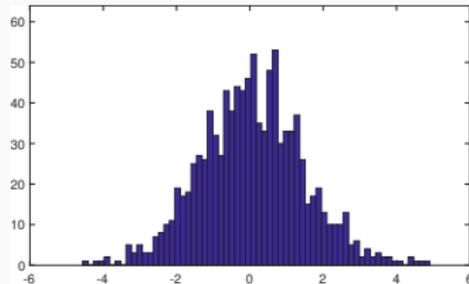


$\{x_{i,1}\}_{i=1}^n$



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With noise



??? +  $\mathcal{N}(0, \sigma^2)$

### Theorem (H., Shi, & Sun, 2017)

For  $\mathbb{P} = \mathcal{N}(0, \mathbf{I}_d)$ , no estimator  $\hat{\beta}$  can guarantee

$$\mathbb{E} \left[ \|\hat{\beta} - \beta^*\|_2 \right] \leq \frac{\|\beta^*\|_2}{3}$$

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Another theorem: for  $\mathbb{P} = \text{Uniform}([-1, 1]^d)$ , must have

$\text{SNR} \geq 1/9$ , even as  $n \rightarrow \infty$ .

## High SNR regime

**Previous works** (Unnikrishnan, Haghghatshoar, & Vetterli, 2015; Pananjady, Wainwright, & Courtade, 2016):

If  $\text{SNR} \gg \text{poly}(n)$ , then can recover  $\pi^*$  (and  $\beta^*$ , approximately) using Maximum Likelihood Estimation, i.e., least squares.

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Estimate sign of correlation between  $x_i$  and  $y_i$ .

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**Does high SNR also permit efficient algorithms?**

(Recall: our approximate MLE algorithm has running time  $n^{O(d)}$ .)

## **Average-case recovery with very high SNR**

---

## Noise-free setting ( $\text{SNR} = \infty$ )

$$\begin{array}{|c|} \hline y_0 \\ \hline y_1 \\ \hline \vdots \\ \hline y_n \\ \hline \end{array} = \begin{array}{|c|} \hline \mathbf{x}_{\pi^*}^\top(0) \\ \hline \mathbf{x}_{\pi^*}^\top(1) \\ \hline \vdots \\ \hline \mathbf{x}_{\pi^*}^\top(n) \\ \hline \end{array} \begin{array}{|c|} \hline \beta^* \\ \hline \end{array}$$

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**Claim:**  $n \geq d$  suffices to recover  $\pi^*$  with high probability.

**Theorem (H., Shi, & Sun, 2017)**

*In the noise-free setting, there is a  $\text{poly}(n, d)$ -time\* algorithm that returns  $\pi^*$  and  $\beta^*$  with high probability.*

\*Assuming problem is appropriately discretized.

## Main idea: hidden subset

Measurements:

$$y_0 = \mathbf{x}_0^\top \boldsymbol{\beta}^*; \quad y_i = \mathbf{x}_{\pi^*(i)}^\top \boldsymbol{\beta}^*, \quad i = 1, \dots, n.$$

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## Reduction to Subset Sum

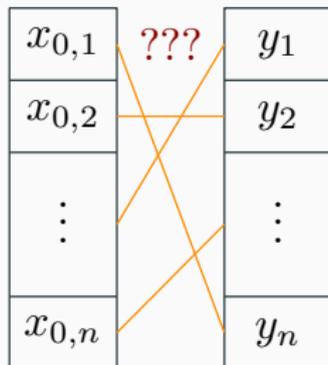
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$x_{0,2}$
$\vdots$
$x_{0,n}$

$y_1$
$y_2$
$\vdots$
$y_n$

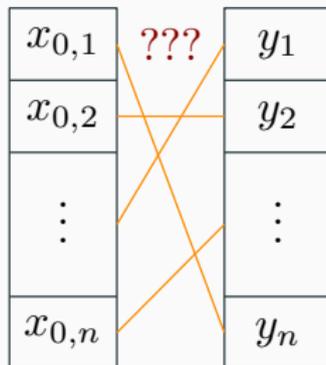
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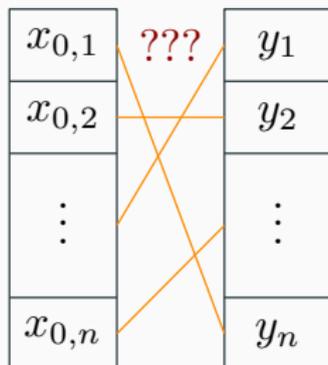
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- $d^2$  “source” numbers  $c_{i,j} := x_{0,j} y_i$ , “target” sum  $y_0$ .  
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**Subset Sum problem.**

## REDUCIBILITY AMONG COMBINATORIAL PROBLEMS<sup>†</sup>

Richard M. Karp

University of California at Berkeley

### 18. KNAPSACK

INPUT:  $(a_1, a_2, \dots, a_r, b) \in \mathbb{Z}^{n+1}$

PROPERTY:  $\sum_j a_j x_j = b$  has a 0-1 solution.

(Karp, 1972)

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- Our algorithm is based on similar reduction but requires a somewhat different analysis.

## Reducing subset sum to shortest vector problem

**Lagarias & Odlyzko (1983)**: random instances of Subset Sum *efficiently solvable* when  $N$  **source numbers**  $c_1, \dots, c_N$  chosen independently and u.a.r. from sufficiently wide interval of  $\mathbb{Z}$ .

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*Reduction*: construct lattice basis in  $\mathbb{R}^{N+1}$  such that

- **correct subset** of basis vectors gives short lattice vector  $\mathbf{v}_*$ ;
- **any other lattice vector**  $\not\propto \mathbf{v}_*$  is more than  $2^{N/2}$ -times longer.

$$\left[ \mathbf{b}_0 \mid \mathbf{b}_1 \mid \cdots \mid \mathbf{b}_N \right] := \left[ \begin{array}{c|ccc} 0 & & & \mathbf{I}_N \\ \hline MT & -Mc_1 & \cdots & -Mc_N \end{array} \right]$$

for sufficiently large  $M > 0$ .

## Our random subset sum instance

**Catch:** Our source numbers  $c_{i,j} = y_i \mathbf{x}_j^\top \mathbf{x}_0$  are **not independent**, and **not uniformly distributed** on some wide interval of  $\mathbb{Z}$ .

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- To show that Lagarias & Odlyzko reduction still works, use Gaussian anti-concentration for quadratic and quartic forms.

**Key lemma:** (w.h.p.) for every  $\mathbf{Z} \in \mathbb{Z}^{d \times d}$  that is not an integer multiple of **permutation matrix corresponding to  $\pi^*$** ,

$$\left| y_0 - \sum_{i,j} Z_{i,j} \cdot c_{i,j} \right| \geq \frac{1}{2^{\text{poly}(d)}} \cdot \|\beta^*\|_2.$$

## Some remarks

- In general,  $\mathbf{x}_1, \dots, \mathbf{x}_n$  are not  $\mathbf{e}_1, \dots, \mathbf{e}_d$ , but similar reduction works via Moore-Penrose pseudoinverse.

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- Algorithm strongly exploits assumption of noise-free measurements. **Unlikely to tolerate much noise.**

### Open problem:

*robust* efficient algorithm in high SNR setting.

# Correspondence retrieval

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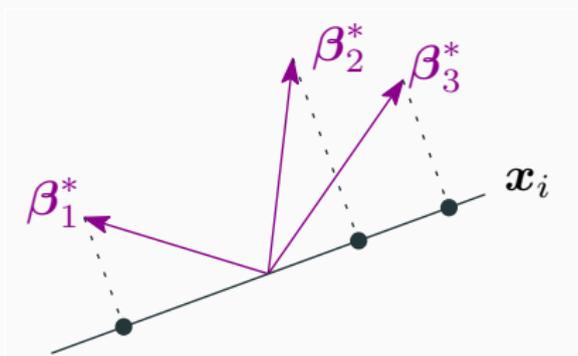
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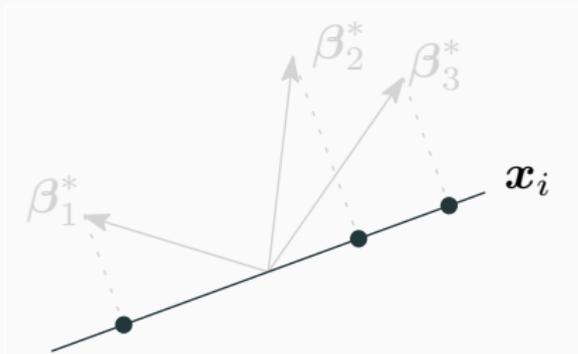
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## Special cases

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- $k = 2$  and  $\beta_1^* = -\beta_2^*$ : (real variant of) *phase retrieval*.

Note that  $\{\mathbf{x}_i^\top \beta^*, -\mathbf{x}_i^\top \beta^*\}$  has same information as  $|\mathbf{x}_i^\top \beta^*|$ .

Existing methods require  $n > 2d$ .

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Algorithm based on reduction to Subset Sum that requires  $n \geq d + 1$ , which is optimal.

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**Questions:** SNR limits? Sub-optimality of “method-of-moments”?

## **Closing remarks and open problems**

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  - Close gap between SNR lower and upper bounds?
  - Lower bounds for correspondence retrieval?
  - Faster/more robust algorithms?
  - (Smoothed) analysis of alternating minimization?

# Acknowledgements

**Collaborators:** Alexandr Andoni (Columbia), Kevin Shi (Columbia), Xiaorui Sun (Microsoft Research).

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**Hospitality:** Simons Institute for the Theory of Computing (UCB).

Thank you



## Beating brute-force search: “realizable” case

“Realizable” case: Suppose there exist  $\beta_\star \in \mathbb{R}^d$  and  $\pi_\star \in S_n$  s.t.

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- Find subset of  $d$  linearly independent points  $\mathbf{x}_{i_1}, \mathbf{x}_{i_2}, \dots, \mathbf{x}_{i_d}$ .
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## Beating brute-force search: “realizable” case

“Realizable” case: Suppose there exist  $\beta_\star \in \mathbb{R}^d$  and  $\pi_\star \in S_n$  s.t.

$$y_{\pi_\star(i)} = \mathbf{x}_i^\top \beta_\star, \quad i \in [n].$$

Solution is determined by action of  $\pi_\star$  on  $d$  points

(assume  $\dim(\text{span}(\mathbf{x}_i)_{i=1}^d) = d$ ).

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“Guess” means “enumerate over  $\binom{n}{d}$  choices”; rest is  $\text{poly}(n, d)$ .

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**Better way to get  $1+\epsilon$ :** exploit first-order optimality conditions (i.e., “normal equations”) and  $\epsilon$ -nets.

**Overall time:**  $(n/\epsilon)^{O(k)} + \text{poly}(n, d)$  for  $k = \dim(\text{span}(\mathbf{x}_i)_{i=1}^n)$ .

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**Task:** show  $P_{e_1}$  and  $P_{-e_1}$  are “close”, then appeal to Le Cam’s standard “two-point argument”:

$$\max_{\beta^* \in \{e_1, -e_1\}} \mathbb{E}_{P_{\beta^*}} \|\hat{\beta} - \beta^*\|_2 \geq 1 - \|P_{e_1} - P_{-e_1}\|_{\text{tv}}.$$

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**Key idea:** conditional means of  $\{y_i\}_{i=1}^n$  given  $(\mathbf{x}_i)_{i=1}^n$ , under  $P_{e_1}$  and  $P_{-e_1}$ , are close *as unordered multi-sets*.

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Conditional distribution of  $\mathbf{y} = (y_1, y_2, \dots, y_n)$  given  $(\mathbf{x}_i)_{i=1}^n$ :

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**Data processing:** Lose information by going from  $\mathbf{y}$  to  $(y_i)_{i=1}^n$ .

## Proof sketch (continued)

By data processing inequality,

$$\begin{aligned} & \text{KL} \left( P_{e_1}(\cdot \mid (\mathbf{x}_i)_{i=1}^n), P_{-e_1}(\cdot \mid (\mathbf{x}_i)_{i=1}^n) \right) \\ & \leq \text{KL} \left( \text{N}(\mathbf{u}^\uparrow, \sigma^2 \mathbf{I}_n), \text{N}(-\mathbf{u}^\downarrow, \sigma^2 \mathbf{I}_n) \right) \end{aligned}$$

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By conditioning + Pinsker's inequality,

$$\|P_{e_1} - P_{-e_1}\|_{\text{tv}} \leq \frac{1}{2} + \frac{1}{2} \text{med} \sqrt{\frac{\text{SNR}}{4} \cdot \|\mathbf{u}^\uparrow + \mathbf{u}^\downarrow\|_2^2} \leq \frac{1}{2} + \frac{1}{2} \sqrt{\text{SNR}}.$$

□

### Theorem (H., Shi, & Sun, 2017)

Fix any  $\beta^* \in \mathbb{R}^d$  and  $\pi^* \in S_n$ , and assume  $n \geq d$ . Suppose  $(\mathbf{x}_i)_{i=0}^n$  are drawn iid from  $N(0, \mathbf{I}_d)$ , and  $(y_i)_{i=0}^n$  satisfy

$$y_0 = \mathbf{x}_0^\top \beta^*; \quad y_i = \mathbf{x}_{\pi^*(i)}^\top \beta^*, \quad i = 1, \dots, n.$$

There is a  $\text{poly}(n, d)$ -time<sup>‡</sup> algorithm that, given inputs  $(\mathbf{x}_i)_{i=0}^n$  and  $(y_i)_{i=0}^n$ , returns  $\pi^*$  and  $\beta^*$  with high probability.

<sup>‡</sup>Assuming problem is appropriately discretized.

## Reducing subset sum to shortest vector problem

**Lagarias & Odlyzko (1983)**: random instances of Subset Sum *efficiently solvable* when  $N$  **source numbers** chosen independently and u.a.r. from sufficiently wide interval of  $\mathbb{Z}$ .

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*Main idea*: (w.h.p.) every incorrect subset will “miss” the target sum  $T$  by noticeable amount.

*Reduction*: construct lattice basis in  $\mathbb{R}^{N+1}$  such that

- **correct subset** of basis vectors gives short lattice vector  $\mathbf{v}_*$ ;
- **any other lattice vector**  $\not\propto \mathbf{v}_*$  is more than  $2^{N/2}$ -times longer.

$$\left[ \mathbf{b}_0 \mid \mathbf{b}_1 \mid \cdots \mid \mathbf{b}_N \right] := \left[ \begin{array}{c|ccc} 0 & & & \mathbf{I}_N \\ \hline MT & -Mc_1 & \cdots & -Mc_N \end{array} \right]$$

for sufficiently large  $M > 0$ .

## Our random subset sum instance

**Catch:** Our source numbers  $c_{i,j} = y_i \mathbf{x}_j^\top \mathbf{x}_0$  are **not independent**, and **not uniformly distributed** on some wide interval of  $\mathbb{Z}$ .

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- To show that Lagarias & Odlyzko reduction still works, need Gaussian anti-concentration for quadratic and quartic forms.

**Key lemma:** (w.h.p.) for every  $\mathbf{Z} \in \mathbb{Z}^{d \times d}$  that is not an integer multiple of **permutation matrix corresponding to  $\pi^*$** ,

$$\left| y_0 - \sum_{i,j} Z_{i,j} \cdot c_{i,j} \right| \geq \frac{1}{2^{\text{poly}(d)}} \cdot \|\beta^*\|_2.$$