University of Colorado **Boulder**

Randomization methods for big-data
(other than SGD)

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Applied Math and Statistics colloquium, Colorado School of Mines

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Joint work with several authors, mostly former PhD students:

(and colleagues at CU & the Colorado School of Mines)

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(Asst. Prof at UC Denver)

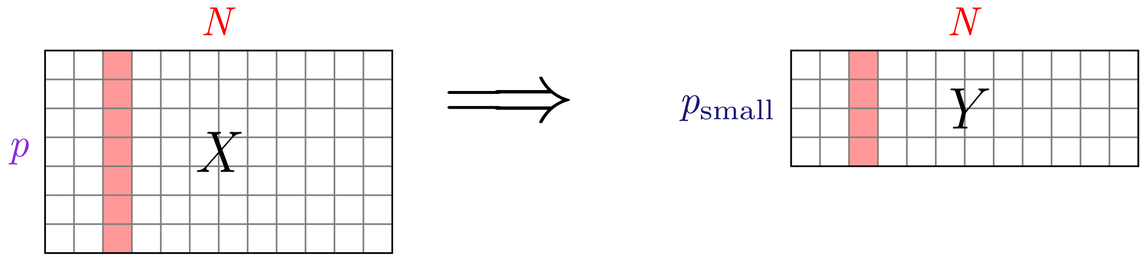
David Kozak
(private sector)

Osman Asif Malik
(was Alvarez postdoc at Berkeley Labs, now private sector)

OUTLINE

1. Randomized "sketches"
   a. Warmup: PCA
   b. Classical sketches
   c. Structured sketches
2. Applications
   a. Warmup: linear algebra
   b. K-means clustering
   c. Tensor factorizations
   d. Gradient-free optimization

Reducing the dimensionality of data



$x_i \in \mathbb{R}^p, \quad i = 1, \ldots, N$ is converted to $y_i \in \mathbb{R}^{p_{\text{small}}}, \quad i = 1, \ldots, N$

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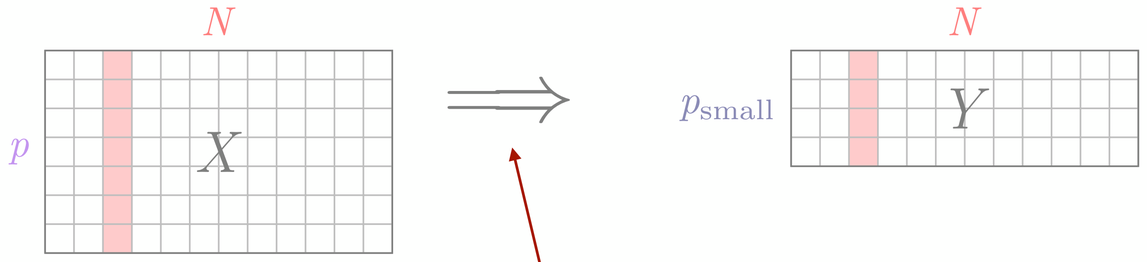

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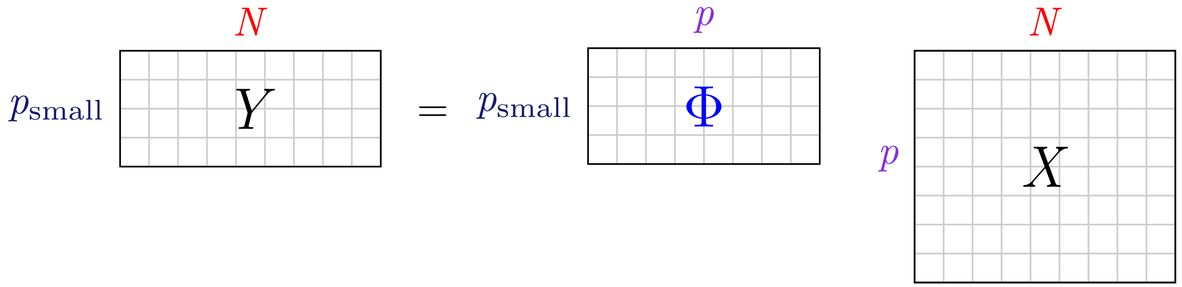
this reduction is often linear, in which case can write as



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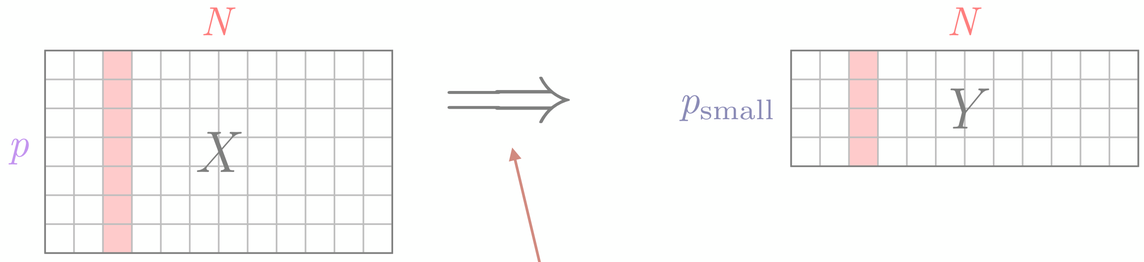

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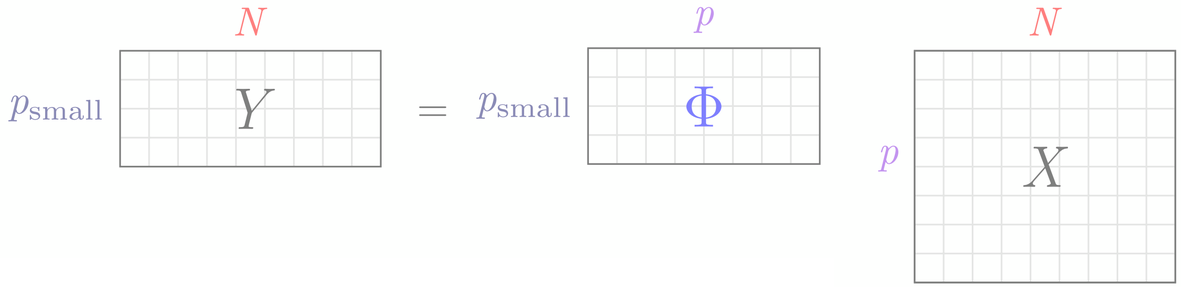


Why?

- Faster computation
  - Especially if the complexity of subsequent processing is $\mathcal{O}(p^2 N)$
  - If $p_{\text{small}} = 0.05p$ then speedup is $400\times$
- Denoising (remove irrelevant components)
- Fewer degrees-of-freedom reduces chance of overfitting models
- Visual interpretation (e.g., $p_{\text{small}} = \{2, 3\}$) ⟵ This is "multidimensional scaling". Specialized techniques (tSNE, UMAP) are best

... or for storage reasons

(especially to create **one-pass methods**)

Method 1: PCA (non-linear)

Principal Component Analysis (aka Hotelling or Karhunen-Loeve transform)

Take SVD

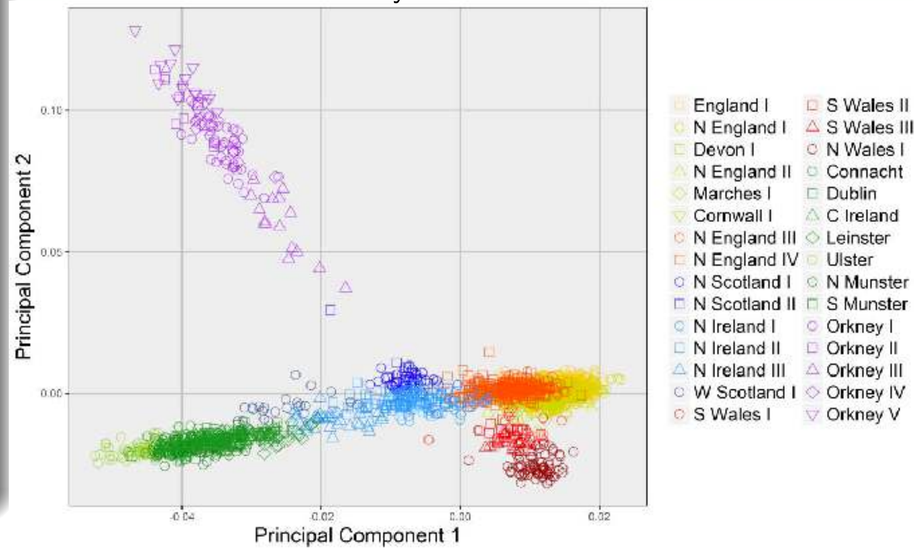
$$X = \begin{bmatrix} U_1 \, U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix}$$

where $\|\Sigma_2\| \approx$ small. Then PCA takes the form of

$$Y \leftarrow \Phi_{\text{PCA}} \cdot X$$

where $\Phi_{\text{PCA}} = {U_1}^T$.

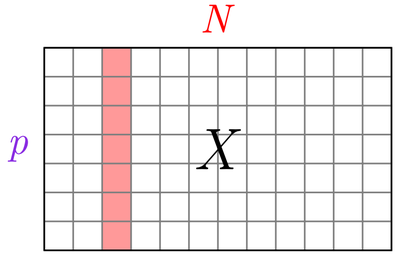
Principal component analysis of the fineStructure co-ancestry matrix



https://commons.wikimedia.org/wiki/File:PCA_of_British_people.png
Gilbert, E., O'Reilly, S., Merrigan, M. et al. The Irish DNA Atlas: Revealing Fine-Scale Population Structure and History within Ireland. Sci Rep 7, 17199 (2017)

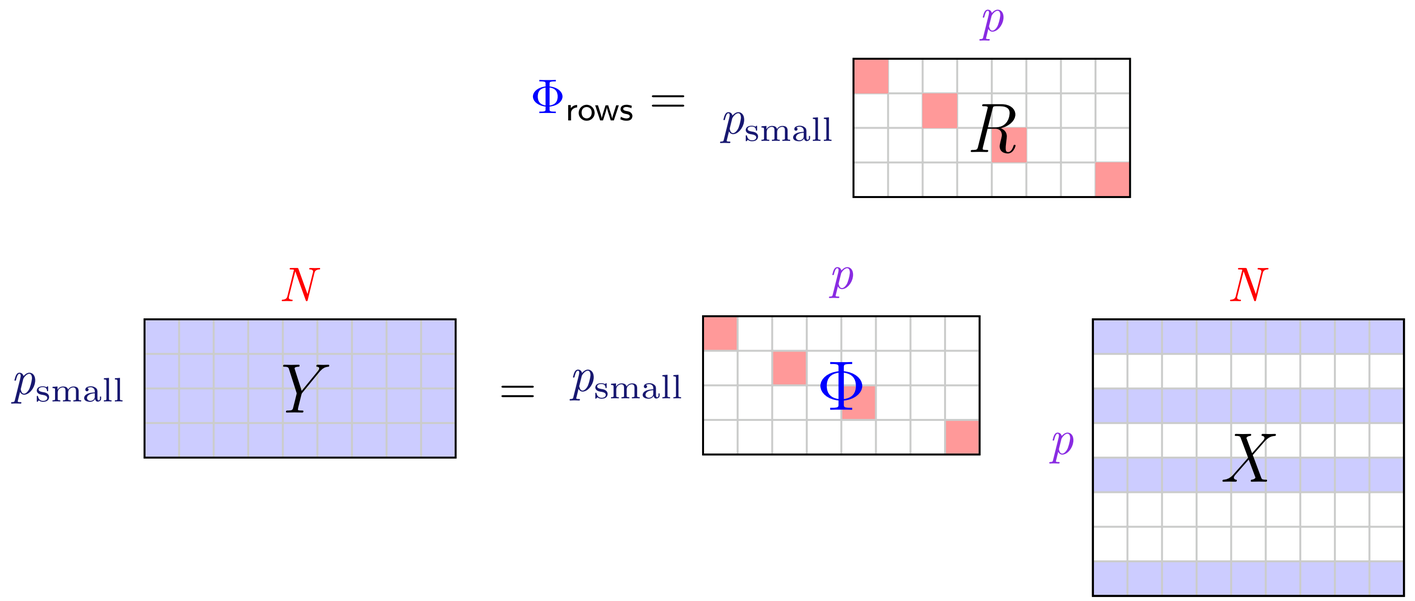
Note:

- Costly but linear in N: ($\mathcal{O}(p^2 N)$ direct, or about $\mathcal{O}(p_{\text{small}} p N)$ Krylov)
- Non-linear, since Φ_{PCA} is determined by X
- Need to process all of X before we can apply $y_i \leftarrow \Phi_{\text{PCA}} \cdot x_i$



Method 2: sub-sample dimensions (i.e., rows)

R *randomly* samples rows



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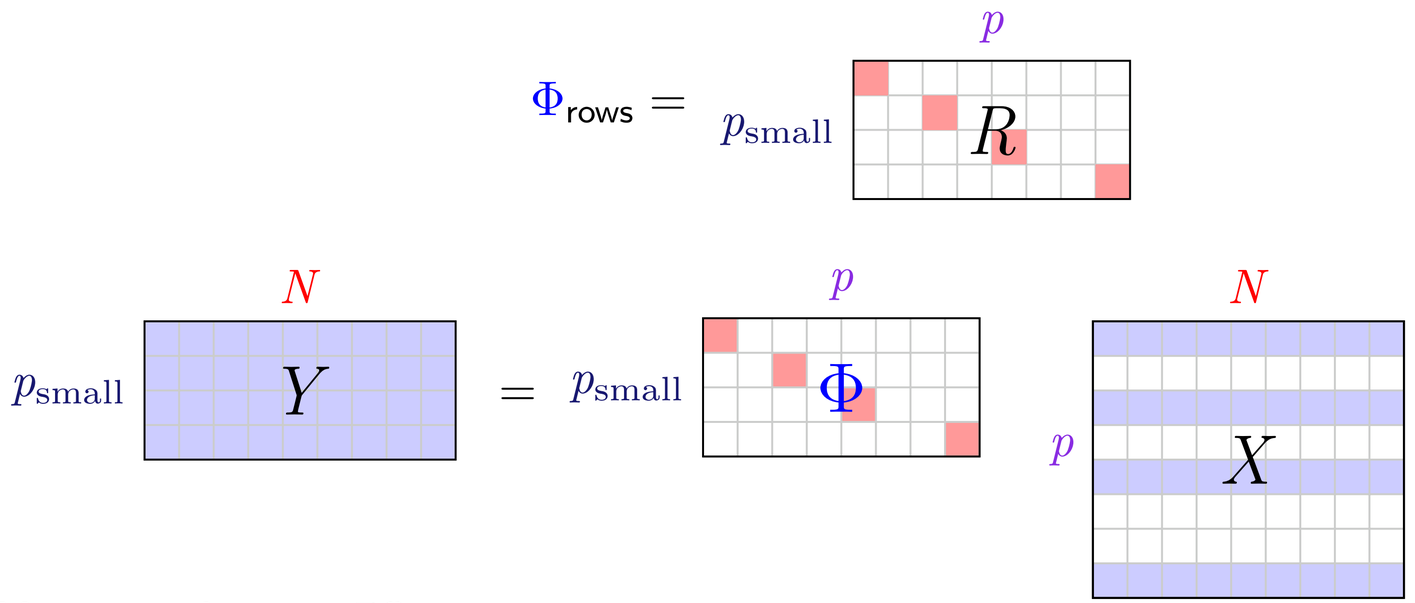

How to choose R?

- Uniformly at random (... poor performance) ← "oblivious"
- According to row-norm (... better, not great, and slower)
- According to *leverage scores* based on partial SVD (... better, slow) ← "non-oblivious" (like PCA)

One benefit: for many applications, this avoids computing all entries of the RHS in the first place!

That's sometimes the bottleneck...

Method 2: sub-sample dimensions (i.e., rows)

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p_{sma}

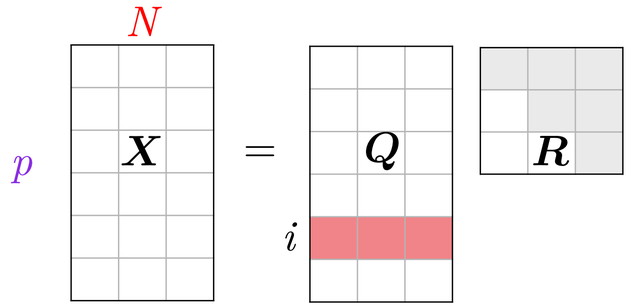
How

- U
- Ac
- According to *leverage scores* based on partial SVD (. . . better, slow)

"oblivious"

"non-oblivious"

Leverage scores



i^{th} leverage score is Euclidean norm squared of the i^{th} row of $\boldsymbol{Q}$

[For keen observers: this isn't useful if $N > p$. What to do then?
Can essentially prove separately for all pairs of points (so $N = 2$)
and then take union bound (not an issue, since failure decays fast).
Technically, usually prove via subspace embeddings]

Method 3: dense random matrix

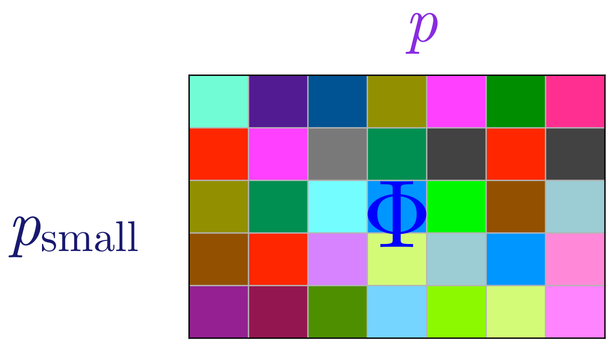
Theorem (Johnson-Lindenstrauss, 1984 (and Indyk-Motwani, 1998))

Choose $\Phi = \Phi_{randn}$ *with* $p_{small} \propto \varepsilon^{-2} \log N$ *iid rows each* $\mathcal{N}(0, p/p_{small})$*, then for all* $x_i, x_j \in \{x_1, \ldots, x_N\} \subset \mathbb{R}^p$*,*

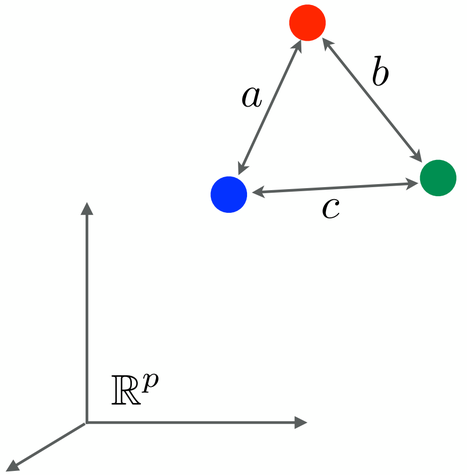
$$1 - \varepsilon \leq \frac{\|\Phi x_i - \Phi x_j\|_2}{\|x_i - x_j\|_2} \leq 1 + \varepsilon$$

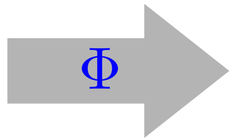
with constant probability.

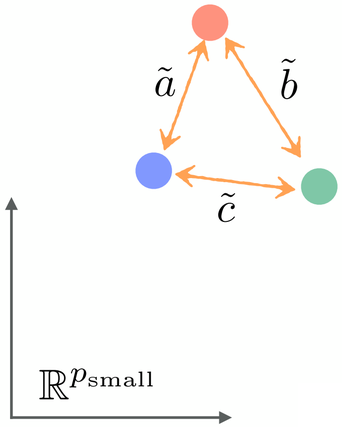
"gold standard" for accuracy among randomized data-oblivious sketches (for any Euclidean norm results)

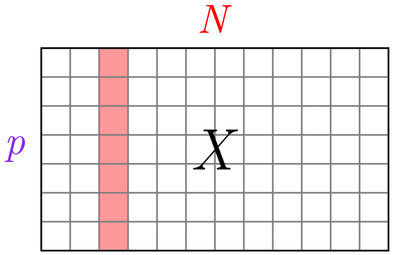


$\Phi_{ij} \sim \mathcal{N}(0, p/p_{\text{small}})$









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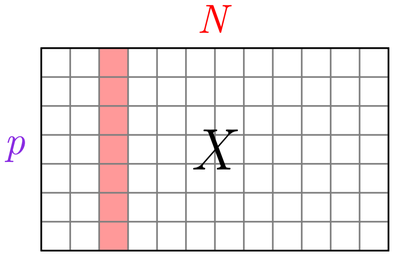
with constant probability.

- Φ is linear and data-independent (unlike PCA)
- but Φ is not orthogonal (unlike PCA) (though variants can be made to be orthogonal)
- Independent of original dimension p
- Independent of conditioning of X (unlike PCA)
- Probabilistic (unlike PCA)

Usually not practical since too costly since computing ΦX is $\mathcal{O}(pp_{\text{small}}N)$

Depends on what its purpose is...



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Bipartite Expander graphs

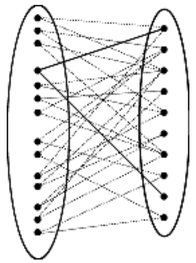

image: De Castro, IEEE TIT 2010

example

CountSketch

example

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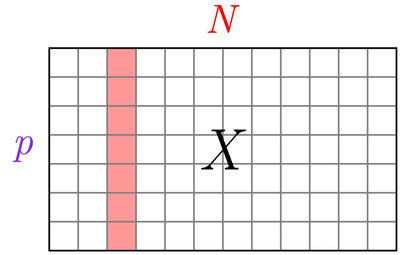
Usually not practical since too costly since computing ΦX is $\mathcal{O}(pp_{\text{small}}N)$

Extensions of **applicability**, for example:

- entire subspaces and manifolds (using covering-number arguments)

Many **extensions**, for example:

- sub-Gaussian entries, and/or dependent rows (e.g., columns uniform on sphere)
- dependent columns, e.g., Haar measure on orthogonal matrices
- sparse matrix (worse performance though)



Method 4: Fast Johnson-Lindenstrauss Transforms

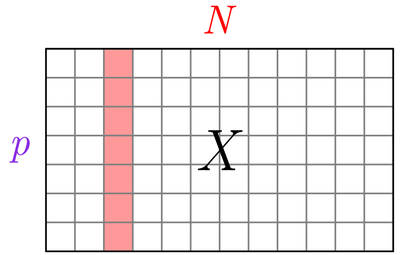
R samples rows; $\mathcal{F}$ Fourier-like; D diag. w/ random ± 1 entries ("Rademacher")

(uniformly)

$$\Phi_{\text{FFT}} = p_{\text{small}} \underbrace{\begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix}}_{R} \; p \underbrace{\begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix}}_{\mathcal{F}} \; p \underbrace{\begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix}}_{D}$$

Orthogonal/unitary, ideally with small max entry

(so *identity matrix* is bad)



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$$\Phi_{\text{FFT}} = p_{\text{small}} \underbrace{\boxed{R}}_{p} \; p \underbrace{\boxed{\mathcal{F}}}_{p} \; p \underbrace{\boxed{D}}_{p}$$

Cost:

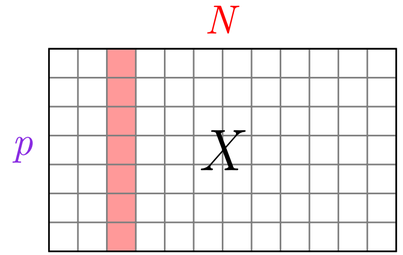
- $\mathcal{F}(x)$ costs $p \log p$ (vs p^2 naively)
- hence $\mathcal{O}(pN \log p)$ to compute ΦX

Guarantees: almost as good as classical Johnson-Lindenstrauss
First guarantees in the Fast Johnson-Lindenstrauss paper

Ailon and Chazelle, "Approximate nearest neighbors and the fast Johnson-Lindenstrauss transform", STOC 2006

Think of $\mathcal{F}$ as FFT or DCT or Hadamard transform

also known under many names, e.g., Random Orthogonal System (**ROS**), FJLT



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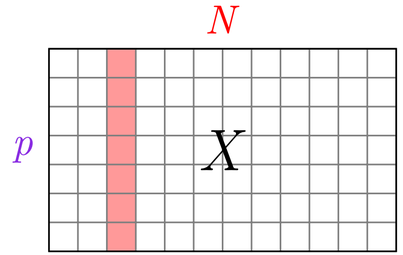
How to get guarantees?

Basic idea is that after applying the first two steps, resulting matrix has (almost) uniform leverage scores...

... so uniform subsampling is (almost) leverage score sampling.



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More intuition

Suppose we want to estimate $\|\boldsymbol{x}\|_2^2$ for $\boldsymbol{x} \in \mathbb{R}^p$ by sampling just p_{small} entries (and multiplying by p/p_{small}). Wlog, let $\|\boldsymbol{x}\|_2 = 1$.

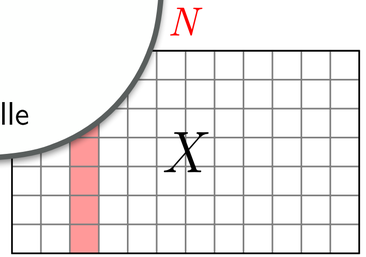
- High variance if $\boldsymbol{x}$ has a few large components
- Intuition: the matrix $\mathcal{F}D$ flattens out input vectors
  - Components of $\boldsymbol{x}$ can be as large as 1
  - Average component of $\boldsymbol{x}$ is $p^{-1/2}$
- Define $\boldsymbol{y} = \mathcal{F}D\boldsymbol{x}$, so $\|\boldsymbol{y}\|_2 = \|\boldsymbol{x}\|_2$. Then $y_1 = \sum_{j=1}^p \mathcal{F}_{1,j}\varepsilon_j x_j$
  - $\mathbb{E}\, y_1 = 0$ since $\mathbb{E}\, \varepsilon_j = 0$
  - $\text{Var}(y_1) = p^{-1}$ since $\mathcal{F}_{1,j}^2 \le \eta = p^{-1}$ and $\|\boldsymbol{x}\|_2 = 1$ and ε_j independent
- Hoeffding inequality:

$$\mathbb{P}\left(|y_1| \ge t\right) \le 2e^{-pt^2/2}$$

- So chance that one of y_j for $j = 1, \ldots, p$ is $\ge t$ is less than $p2e^{-pt^2/2}$
- So with constant probability, can choose $t \approx \sqrt{p^{-1}\log(p)}$
- Conclusion: the max component of $\boldsymbol{y}$ is about the same as its average component. Subsampling $\boldsymbol{y}$ will have much less variance than subsampling $\boldsymbol{x}$.

from "Improved analysis of the subsampled randomized Hadamard transform" (Tropp, 2010); see also Ailon and Chazelle

also kn

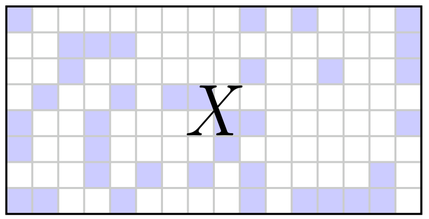


Method 5: subsample entries of a matrix

Keep $x_i' \in \mathbb{R}^p$ but with only p_{small} nonzeros

Idea goes back to landmark Achlioptas/McSherry paper (2001)

$$X' = \quad p \overbrace{\quad\quad\quad\quad}^{N} \begin{bmatrix} \\ \\ \\ \\ \\ \\ \\ \end{bmatrix} X$$



This is the odd-one-out so far, because it's not the same linear operator applied to every column

Method 6: "**precondition**," *then* subsample entries of a matrix

Our new twist: first precondition with Random Orthogonal System (ROS)

(i.e., first 2 matrices from the Fast JLT)

$$Y = \underset{p}{\underset{\uparrow}{\mathcal{F}}} \; \underset{p}{\underset{\uparrow}{D}} \; \underset{N}{\underset{\uparrow}{X}}$$

$$Y' = \underset{N}{\underset{\uparrow}{Y}}$$

Why precondition?

Easy to see that better than uniform sampling of X is **non-uniform** sampling, with probability proportional to magnitude of entry

cf. Achlioptas, Z. Karnin, and E. Liberty 2013

Disadvantage of weighted sampling is the extra pass through data

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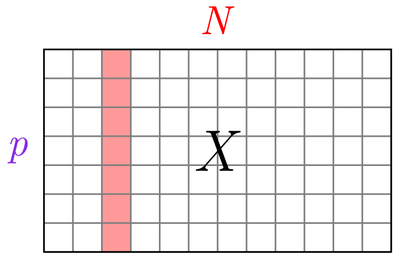
Disadvantage of weighted sampling is the extra pass through data

In our analysis, we have terms like (want this small)

$$\|X\|_{\text{max-entry}} = \max_{\substack{i=1,\ldots,N \\ j=1,\ldots,p}} |X_{ij}|$$

Assuming $\|x_i\|_2 = 1$,

- it is possible for $\|X\|_{\text{max-entry}} = 1$ (BAD)
- best case is $\|X\|_{\text{max-entry}} = 1/\sqrt{p}$



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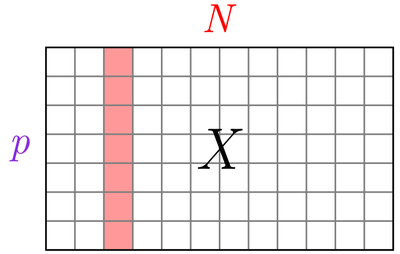
Benefit of preconditioning
After applying ROS, exponentially small chance that

$$\|Y\|_{\text{max-entry}} > \sqrt{\log(Np)}/\sqrt{p}$$

N.B. Since $\mathcal{F}D$ is unitary, bounds in spectral/Frobenius norm are unchanged



Theory: estimating the mean

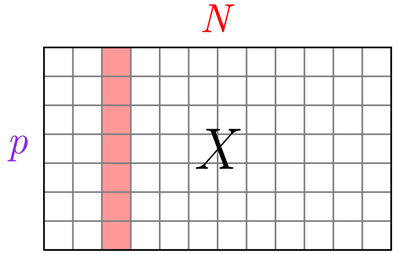
Given a true mean $\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$, and our estimate of it $\hat{\bar{x}}$ from sampled data,

Theorem (Pourkamali-Anaraki & B., *IEEE Trans. Info Theory* 2017)

$\mathbb{E}\,\hat{\bar{x}} = \bar{x}$ *and* $\|\hat{\bar{x}} - \bar{x}\|_\infty \leq t$ *with probability greater than*

$$1 - 2p\,exp\left(\frac{-N\gamma t^2/2}{\|X\|^2_{\text{max-row}} + t/3\|X\|_{\text{max-entry}}}\right)$$

where $\gamma = p_{small}/p$ *(simplifying to* $p_{small} \ll p \ll N$*)*



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where $\gamma = p_{small}/p$ *(simplifying to $p_{small} \ll p \ll N$)*

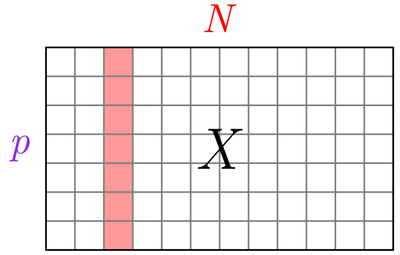
If X has normalized columns, then $\|X\|_{\text{max-entry}} = 1$ and $\|X\|_{\text{max-row}} = \sqrt{N}$ are possible, which is bad.

Lemma

If X is preconditioned, then *(for $Np = 10^{10}$, $\sqrt{\log(2Np) + 1000} = 32$)*

$$\mathbb{P}\left\{\|X\|_{\text{max-entry}} \ge \frac{\sqrt{2}}{\sqrt{p}} \cdot \sqrt{\log(2Np) + 1000}\right\} \le .001$$

$$\mathbb{P}\left\{\|X\|_{\text{max-row}} \ge \frac{\sqrt{2N}}{\sqrt{p}} \cdot \sqrt{\log(2Np) + 1000}\right\} \le .001$$



Theory: estimating the mean

Given a tru

Theor

$\mathbb{E}\,\hat{\bar{x}} =$

where

If X ha
possibl

Lemm

If X is

Probability theory aside

(symmetric Bernoulli, aka Rademacher)

Let $y_i = \pm 1$ be iid Bernoulli, $\hat{\bar{x}} = \frac{1}{N}\sum_{i=1}^{N} y_i$ (transform of Binomial)

- $\mathbb{E}(\hat{\bar{x}}) = 0$
- $\mathrm{Var}(\hat{\bar{x}}) = 1/N$

Chebyshev, Markov inequalities

$$\mathbb{P}(|\hat{\bar{x}}| \geq t) \leq \frac{1}{Nt^2}$$

Example: $N = 10^4$ and $t = 0.1$, $\mathbb{P}(|\hat{\bar{x}}| \geq t) \leq 0.01$

Markov
$X \geq 0,\ \mathbb{P}(X \geq t) \leq \frac{\mu}{t}$

Chebyshev
$\mathbb{P}\left(|X - \mu| \geq t\sigma^2\right) \leq \frac{1}{t^2}$

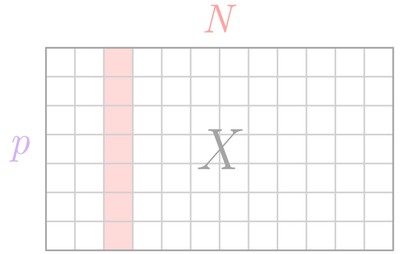
Concentration ineq.

Bernstein, Hoeffding, Chernoff

$$\mathbb{P}(|\hat{\bar{x}}| \geq t) \leq 2\exp\left(\frac{-Nt^2/2}{1 + t/3}\right)$$

Example: $N = 10^4$ and $t = 0.1$, $\mathbb{P}(|\hat{\bar{x}}| \geq t) \leq 2 \cdot 10^{-21}$

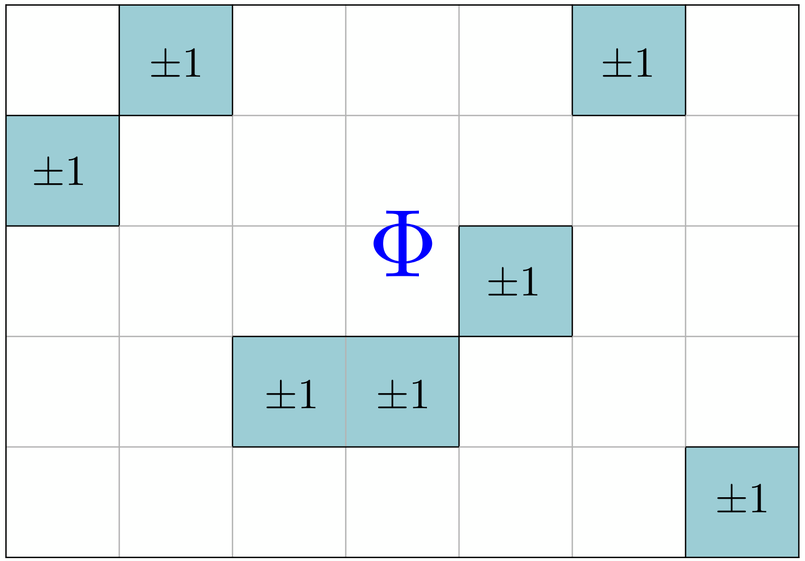
intuition: central limit theorem says random sums of iid rv should look Gaussian, and for a Gaussian, we have exponential concentration

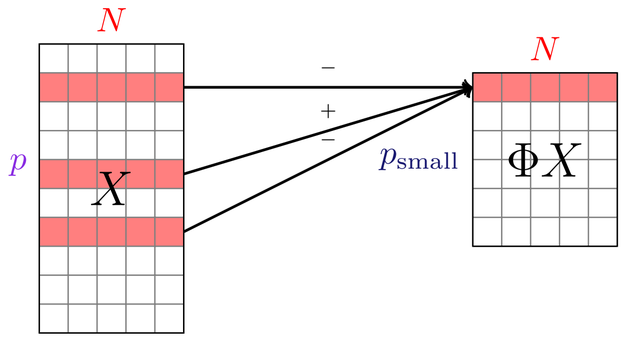


Method 7: CountSketch

p

p_{small}





Introduced in Charikar et al. (2004), more analysis in, e.g., Clarkson and Woodruff (2017)

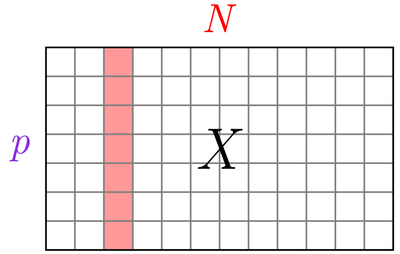
Based on **hash functions**
(as a side-effect, doesn't need full iid random variables for analysis to work)

See "appendix" of these slides for more details

Every column has exactly 1 nonzero entry, location chosen uniformly at random (and value is a Rademacher r.v.)

Has some guarantees, though not as good as a Gaussian (and not a JLT)
... but it's very fast to apply
cost: nnz(X), so no more than pN (vs $p_{\text{small}}pN$ with a Gaussian)

new linear algebra application in: Malik & B. "Fast randomized matrix and tensor interpolative decomposition using CountSketch", *Adv. Comp. Math* (2020)



Method 8: TensorSketch

Introduced in Pham, & Pagh (2013), more analysis in, e.g., Diao, Zong, Sun, Woodruff (2018)

TensorSketch is just CountSketch when the input can be written as a tensor product (for a special choice of the hash and sign functions)

$$\Phi_{\mathcal{T}} : \mathbb{R}^{p} \to \mathbb{R}^{p_{\text{small}}}$$

$$\boldsymbol{v} = \boldsymbol{v}^{(1)} \otimes \boldsymbol{v}^{(2)} \qquad \text{where size is} \quad p = p^{(1)} \cdot p^{(2)}$$

Not (yet!) related to tensors

Two tricks:

- **Computationally**, combine small sketches in a convenient way
- For **analysis**, we lose independence, but CountSketch analysis didn't require full independence!

Method 8: TensorSketch

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Kronecker/tensor product of vectors

$$\boldsymbol{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}, \ \boldsymbol{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \qquad \boldsymbol{a} \otimes \boldsymbol{b} = \begin{bmatrix} a_1 \boldsymbol{b} \\ a_2 \boldsymbol{b} \\ a_3 \boldsymbol{b} \end{bmatrix} = \begin{bmatrix} a_1 b_1 \\ a_1 b_2 \\ a_1 b_3 \\ a_2 b_1 \\ a_2 b_2 \\ a_2 b_3 \\ a_3 b_1 \\ a_3 b_2 \\ a_3 b_3 \end{bmatrix}$$

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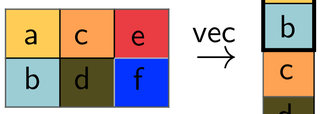
another equivalent definition:

$$\boldsymbol{a} \otimes \boldsymbol{b} = \text{vec}_{\text{col}}\left(\boldsymbol{b}\boldsymbol{a}^T\right)$$

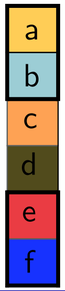
$$\boldsymbol{b}\boldsymbol{a}^T = \begin{bmatrix} b_1 a_1 & b_1 a_2 & b_1 a_3 \\ b_2 a_1 & b_2 a_2 & b_2 a_3 \\ b_3 a_1 & b_3 a_2 & b_3 a_3 \end{bmatrix} = \begin{bmatrix} a_1 b_1 & a_2 b_1 & a_3 b_1 \\ a_1 b_2 & a_2 b_2 & a_3 b_2 \\ a_1 b_3 & a_2 b_3 & a_3 b_3 \end{bmatrix}$$

vec: $\mathbb{R}^{p^{(1)} \times p^{(2)}} \to \mathbb{R}^{p^{(1)} p^{(2)}}$

mat = vec^{-1}



vec $\to$



more generally,

$$(\boldsymbol{A} \otimes \boldsymbol{B})\, \text{vec}_{\text{col}}(\boldsymbol{X}) = \text{vec}_{\text{col}}\left(\boldsymbol{B}\boldsymbol{X}\boldsymbol{A}^T\right)$$

TensorSketch: applying to matrices

From vector case $\boldsymbol{v} = \boldsymbol{v}^{(1)} \otimes \boldsymbol{v}^{(2)}$ to matrix case $\mathbf{A} = \mathbf{A}^{(1)} \otimes \mathbf{A}^{(2)} \otimes \cdots \otimes \mathbf{A}^{(N)}$

Recall the Kronecker product:

$$\underset{I \times J}{\mathbf{A}} \otimes \underset{K \times L}{\mathbf{B}} = \begin{bmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \cdots & a_{1J}\mathbf{B} \\ a_{21}\mathbf{B} & a_{22}\mathbf{B} & \cdots & a_{2J}\mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ a_{I1}\mathbf{B} & a_{I2}\mathbf{B} & \cdots & a_{IJ}\mathbf{B} \end{bmatrix} \in \mathbb{R}^{IK \times JL}$$

$$= \begin{bmatrix} \mathbf{a}_1 \otimes \mathbf{b}_1 & \mathbf{a}_1 \otimes \mathbf{b}_2 & \mathbf{a}_1 \otimes \mathbf{b}_3 & \cdots & \mathbf{a}_J \otimes \mathbf{b}_{L-1} & \mathbf{a}_J \otimes \mathbf{b}_L \end{bmatrix}$$

Khatri-Rao product $\mathbf{A} \odot \mathbf{B} = \begin{bmatrix} \mathbf{a}_1 \otimes \mathbf{b}_1 & \mathbf{a}_2 \otimes \mathbf{b}_2 \cdots \mathbf{a}_L \otimes \mathbf{b}_L \end{bmatrix} \in \mathbb{R}^{IK \times L} \quad (J = L)$

pointwise multiplication (aka Hadamard product)

Observe $\mathbf{a} \circ \mathbf{b} = \left(\mathbf{a}^\top \odot \mathbf{b}^\top\right)^\top$

and with some work, $\Phi_{\mathcal{T}}(\mathbf{A}) = \mathrm{FFT}^{-1}\left(\left(\bigodot_{n=1}^{N}\left(\mathrm{FFT}\left(\mathbf{S}^{(n)}\mathbf{A}^{(n)}\right)\right)^\top\right)^\top\right)$

if $\mathbf{A} = \mathbf{A}^{(1)} \otimes \mathbf{A}^{(2)} \otimes \cdots \otimes \mathbf{A}^{(N)}$

small countSketch

FFTs are doing circular convolution, i.e., multiplying polynomials modulo a fixed modulus. See appendix

TensorSketch: complexity analysis

$$\Phi_{\mathcal{T}} : \mathbb{R}^{p} \to \mathbb{R}^{p_{\text{small}}}$$

$$p = p^{(1)} \cdot p^{(2)}$$

Complexity (per mat-vec):

CountSketch applied as TensorSketch: $\mathcal{O}\big(p^{(1)} + p^{(2)} + p_{\text{small}} \log p_{\text{small}}\big)$ vs CountSketch applied naively: $\mathcal{O}\big(p^{(1)} \cdot p^{(2)}\big)$ vs generic dense matrix multiply: $\mathcal{O}\big(p^{(1)} \cdot p^{(2)} \cdot p_{\text{small}}\big)$

small CountSketches; polynomial multiplication via FFTs

Savings grow as we have more tensor products

If $p = p^{(1)} p^{(2)} \cdots p^{(q)}$

$$\mathcal{O}\big(p^{(1)} + p^{(2)} + \ldots p^{(q)} + p_{\text{small}} \log p_{\text{small}}\big) \quad \text{vs} \quad \mathcal{O}\big(p^{(1)} p^{(2)} \cdots p^{(q)}\big)$$

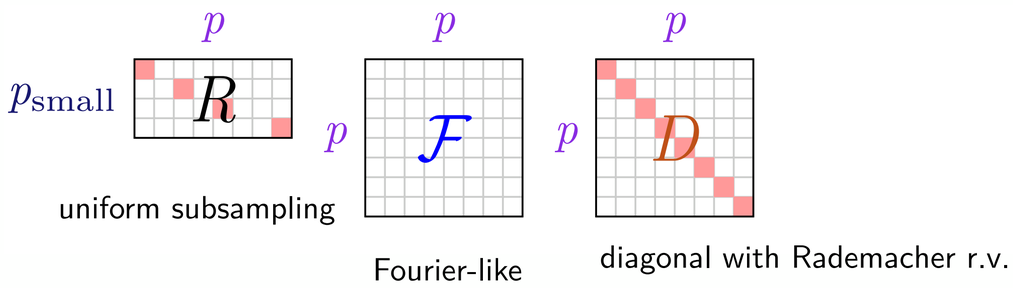
(Even larger savings if input factor matrices are **sparse**)

Method 9: Kronecker Fast Johnson-Lindenstrauss sketch

As for TensorSketch, suppose each column of data looks like $\boldsymbol{v} = \boldsymbol{v}^{(1)} \otimes \boldsymbol{v}^{(2)}$

sizes: $p = p^{(1)} \cdot p^{(2)}$

Recall the Fast Johnson-Lindenstrauss (FJLT): $\Phi = R\mathcal{F}D$



The **Kronecker** FJLT has a similar structure:

$$\Phi_{\text{KFJLT}} = R\left(\mathcal{F}^{(1)}D^{(1)} \otimes \mathcal{F}^{(2)}D^{(2)}\right)$$

($\mathcal{F}^{(1)}D^{(1)}$: size $p^{(1)} \times p^{(1)}$; $\mathcal{F}^{(2)}D^{(2)}$: size $p^{(2)} \times p^{(2)}$)

which is efficient to apply since

$$R\left(\mathcal{F}^{(1)}D^{(1)} \otimes \mathcal{F}^{(2)}D^{(2)}\right)\cdot\left(\boldsymbol{v}^{(1)} \otimes \boldsymbol{v}^{(2)}\right) = R\left(\left(\mathcal{F}^{(1)}D^{(1)}\boldsymbol{v}^{(1)}\right) \otimes \left(\mathcal{F}^{(2)}D^{(2)}\boldsymbol{v}^{(2)}\right)\right)$$

and uniform subsampling can be done implicitly without forming this

- Battaglino, Ballard, Kolda, "A practical randomized CP tensor decomposition", *SIAM J. Matrix Anal. Appl.* (2018)
- Jin, Kolda, Ward. "Faster Johnson–Lindenstrauss transforms via Kronecker products," *Information and Inference: A Journal of the IMA* (2021)
- Malik & B. "Guarantees for the Kronecker fast Johnson–Lindenstrauss transform using a coherence and sampling argument," *Lin. Alg. & its Applications* (2020)

Method 9: Kronecker Fast Johnson-Lindenstrauss sketch

$$\Phi_{\mathrm{KFJLT}} = R\left(\mathcal{F}^{(1)}D^{(1)} \otimes \mathcal{F}^{(2)}D^{(2)} \otimes \ldots \otimes \mathcal{F}^{(q)}D^{(q)}\right) \qquad p = p^{(1)}p^{(2)}\ldots p^{(q)}$$

Theorem (Thm 4.2 in Malik & B. 2020)

If all datapoints have a Kronecker structure, $p_{\mathrm{small}} > \frac{16}{2}\frac{4^q}{\varepsilon^2}\log\left(\frac{4N^2(q+1)}{\delta}\right)\log\left(\frac{4p^{(1)}N^2(q+1)}{\delta}\right)\cdots\log\left(\frac{4p^{(q)}N^2(q+1)}{\delta}\right)$

and $\Phi = \Phi_{\mathrm{KFJLT}}$

then with probability at least $1-\delta$

$$\forall x_i, x_j \in \{x_1, \ldots, x_N\} \subset \mathbb{R}^p \qquad 1-\varepsilon \leq \frac{\|\Phi x_i - \Phi x_j\|_2^2}{\|x_i - x_j\|_2^2} \leq 1+\varepsilon$$

proof idea: FJLT keeps leverage scores almost uniform. With Kronecker product structure, this is (almost) true also, due to properties of leverage scores of Kronecker products

in fact, can extend. See: Malik, Xu, Cheng, B., Doostan, Narayan. "Fast Algorithms for Monotone Lower Subsets of Kronecker Least Squares Problems", https://arxiv.org/abs/2209.05662

- Malik & B. "Guarantees for the Kronecker fast Johnson–Lindenstrauss transform using a coherence and sampling argument," *Lin. Alg. & its Applications* (2020)

Method 9: Kronecker Fast Johnson-Lindenstrauss sketch

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no dependence on p

for reference:

Theorem (Johnson-Lindenstrauss, 1984 (and Indyk-Motwani, 1998))

Choose $\Phi = \Phi_{randn}$ with $p_{small} \propto \varepsilon^{-2}\log N$ iid rows each $\mathcal{N}(0, p/p_{small})$, then for all $x_i, x_j \in \{x_1, \ldots, x_N\} \subset \mathbb{R}^p$,

$$1-\varepsilon \leq \frac{\|\Phi x_i - \Phi x_j\|_2}{\|x_i - x_j\|_2} \leq 1+\varepsilon$$

with constant probability.

OUTLINE

1. Randomized "sketches"
   a. Warmup: PCA
   b. Classical sketches
   c. Structured sketches
2. Applications
   a. Warmup: linear algebra
   b. K-means clustering
   c. Tensor factorizations
   d. Gradient-free optimization

One application of sketching: least-squares

Least-squares

Solve $x_{\mathrm{LS}} = \operatorname{argmin} \|Ax - b\|$, A is $p \times N$ with $p \gg N$

Approach 1: randomization to quickly find preconditioner BLENDENPIK, LSRN

"sketch-to-precondition"

- If $A = QR$ is a QR-decomposition, then AR^{-1} is well-conditioned
- Idea: do QR-decomp on reduced-dimension matrix ΦA
- On large, very ill-conditioned matrices (and tall), about $4\times$ faster than LAPACK

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Approach 2: directly solve sketched problem Sarlos, Woodruff, Mahoney, etc.

"sketch-to-solve"

- Directly sove $\min_x \|\Phi(Ax - b)\|$
- Theoretical bounds on objective error if Φ has $p_{\mathrm{small}} = N\mathrm{polylog}(N)$ rows
  - i.e., p_{small} is independent of p

For a sub-sampling sketch, this lets you avoid even computing some entries of b, which can be very useful when each entry of b is, e.g., the output of a simulation

One application of sketching: least-squares

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Solve $x_{\text{LS}} = \text{argmin} \|Ax - b\|$, A is $p \times N$ with $p \gg N$

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Other applications: SVDs, matrix multiplies, Nystrom/CUR/Interpolative Decompositions, QR without pivoting

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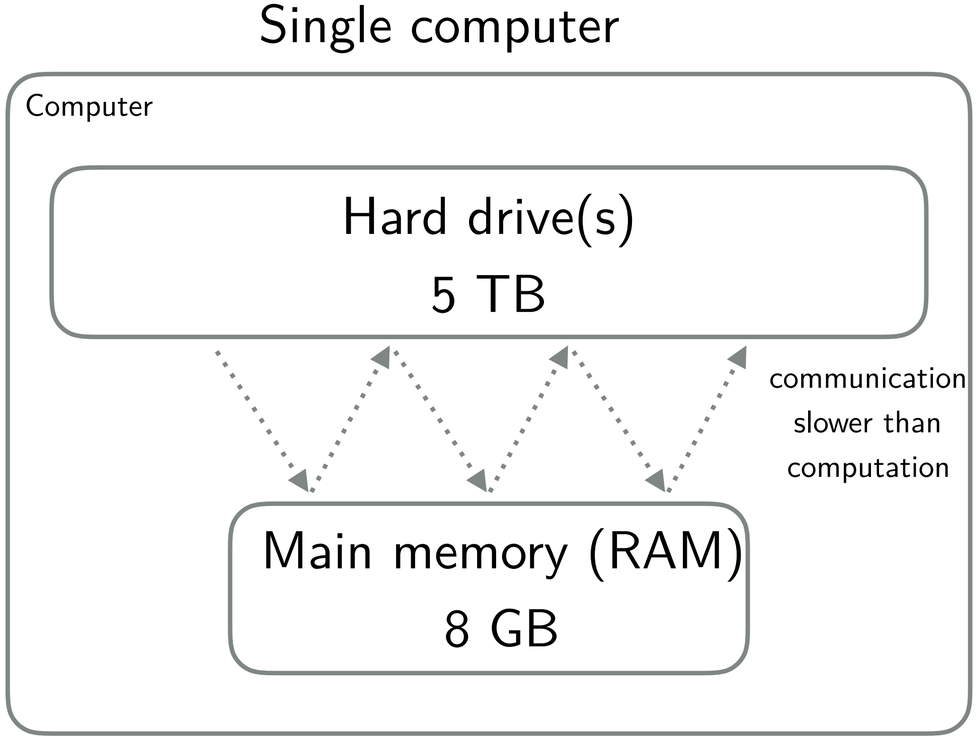
Interlude: one-pass methods



Often want to minimize number of **passes** through a dataset if it's large

- *communication cost* can be significant
- in the extreme case, new data is constantly **streaming** in and we could never store it all

Think of a **pass** as a "for" loop through the dataset

Streaming is a special case of a "**one-pass**" method

Example: google indexing the web is streaming

1. Google finds a website and downloads the site
2. Applies algorithm to index/categorize/rank it
3. Discards the website (keeps only meta-data, ranking, etc.)
4. Never has to store entire WWW *all at once*

Interlude: one-pass methods

Example: computing the sample variance $\hat{\sigma}^2$

2-pass method

pass #1 $\quad \hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i$

pseudocode

$$\begin{cases} \hat{\mu} = 0 \\ \texttt{for } i = 1, \dots, n \\ \qquad \hat{\mu} \leftarrow \hat{\mu} + x_i \\ \hat{\mu} \leftarrow \frac{1}{n}\hat{\mu} \end{cases}$$

pass #2 $\quad \hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n} (x_i - \hat{\mu})^2$

pseudocode

$$\begin{cases} \hat{\sigma}^2 = 0 \\ \texttt{for } i = 1, \dots, n \\ \qquad \hat{\sigma}^2 \leftarrow \hat{\sigma}^2 + (x_i - \hat{\mu})^2 \\ \hat{\sigma}^2 \leftarrow \frac{1}{n-1}\hat{\sigma}^2 \end{cases}$$

1-pass method

motivation: $\quad \mathrm{Var}[X] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$

pass #1

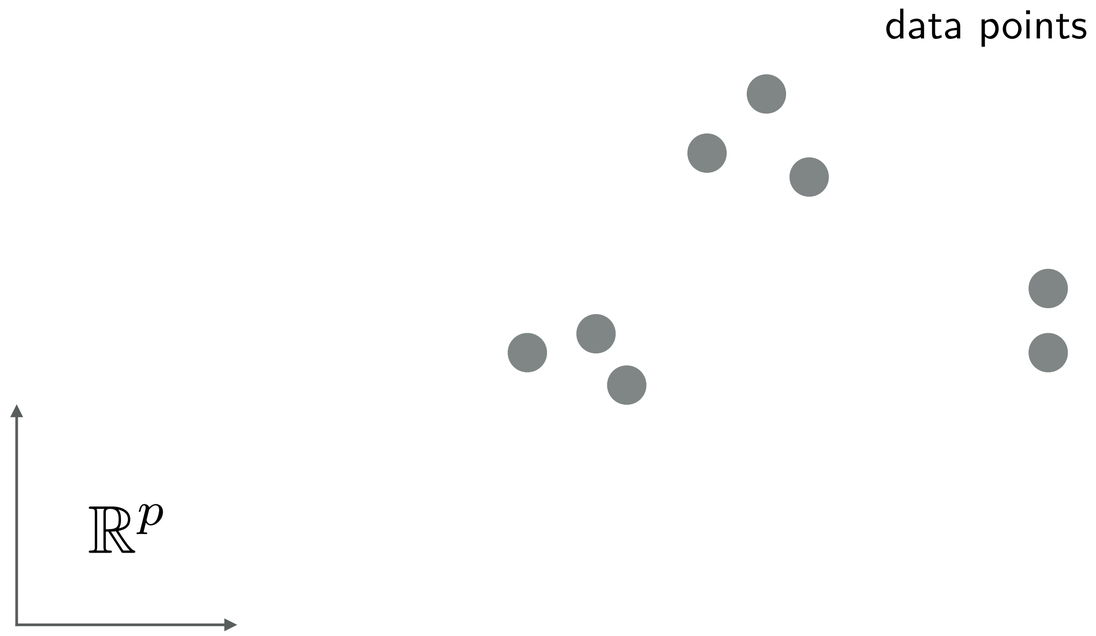
$$\begin{cases} \hat{\mu} = 0, \ s = 0 \\ \texttt{for } i = 1, \dots, n \\ \qquad \hat{\mu} \leftarrow \hat{\mu} + x_i \\ \qquad s \leftarrow s + x_i^2 \\ \hat{\sigma}^2 \leftarrow \frac{1}{n-1}(s - \hat{\mu}^2) \end{cases}$$

Interlude: one-pass methods

A major application of **sketching** is to create **one-pass** algorithms:

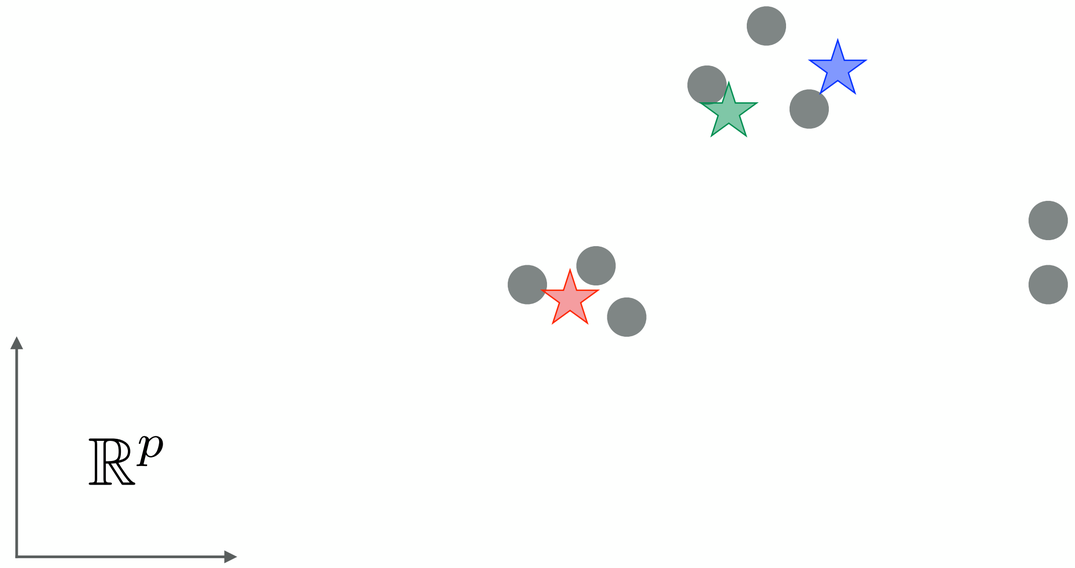
we spend one-pass to apply the sketch, and the sketched data is then small enough that we don't "count it" in our budget anymore

Machine Learning 101: K-means clustering



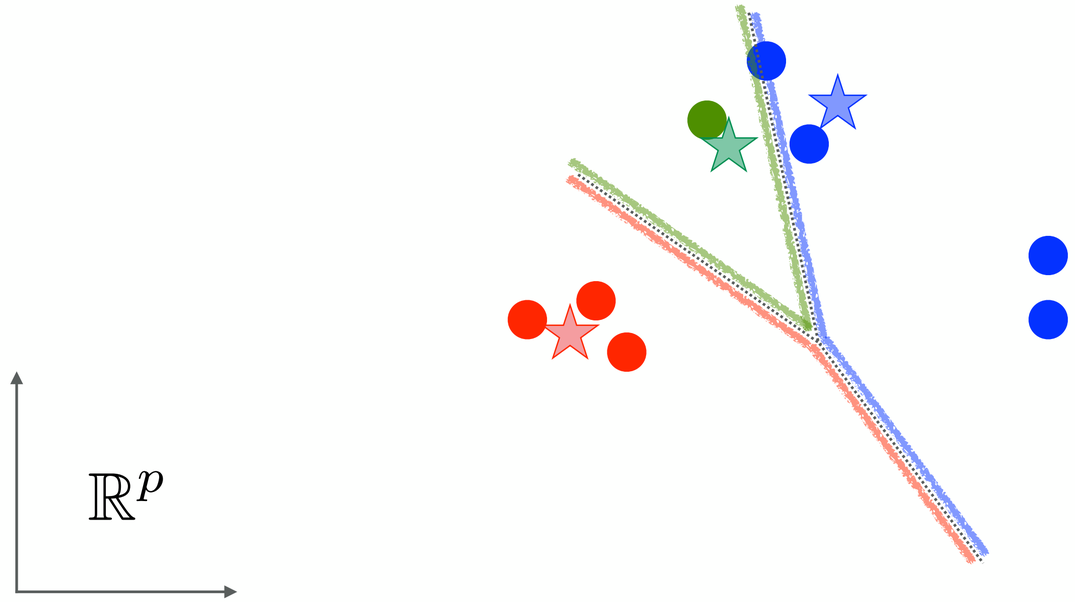
Machine Learning 101: K-means clustering

Step: initialize with guesses for cluster **centers**



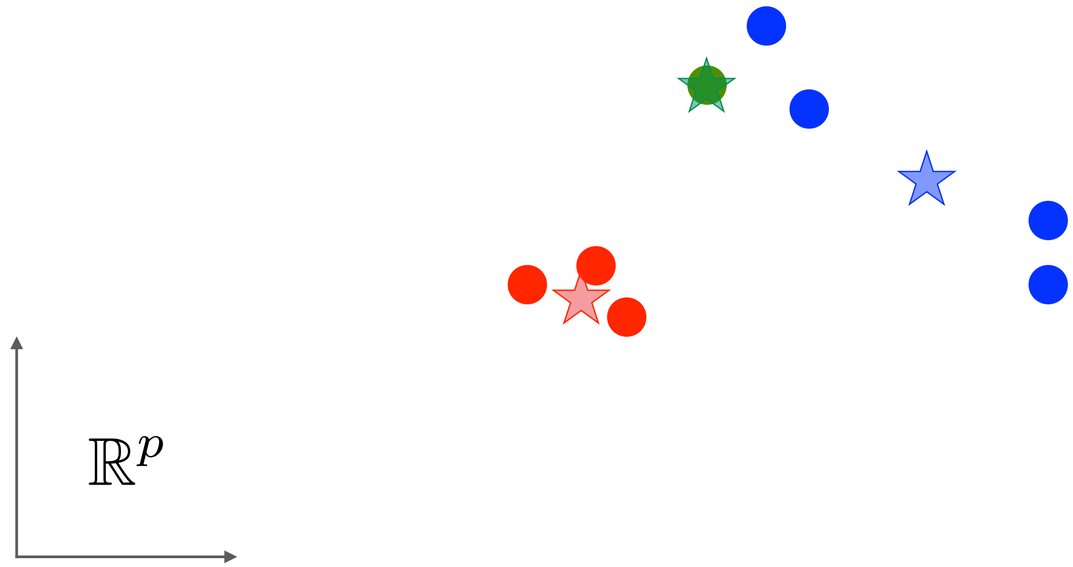
Machine Learning 101: K-means clustering

Step: update **assignments**



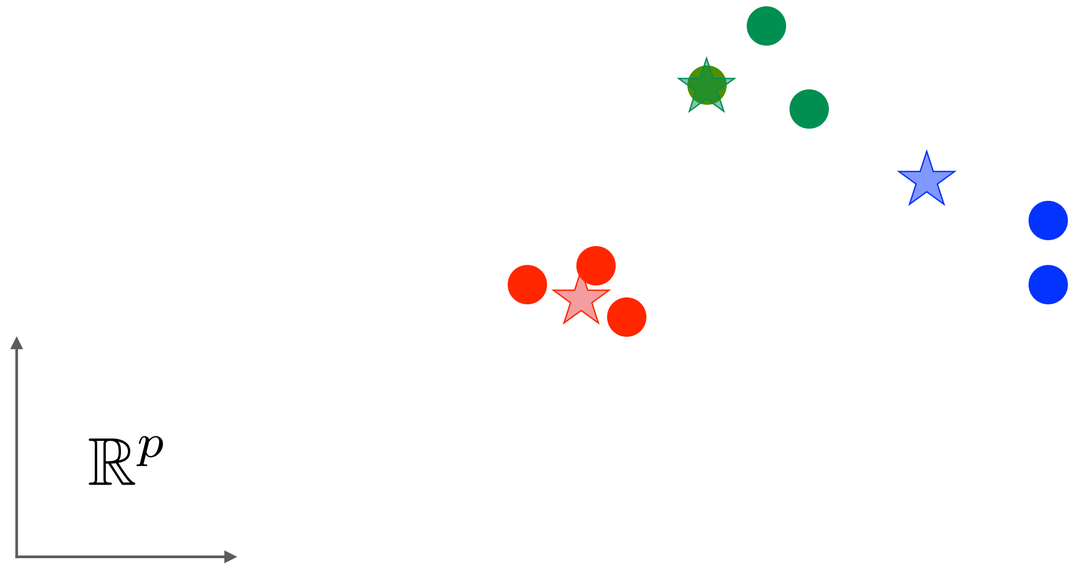
Machine Learning 101: K-means clustering

Step: recompute **cluster means**



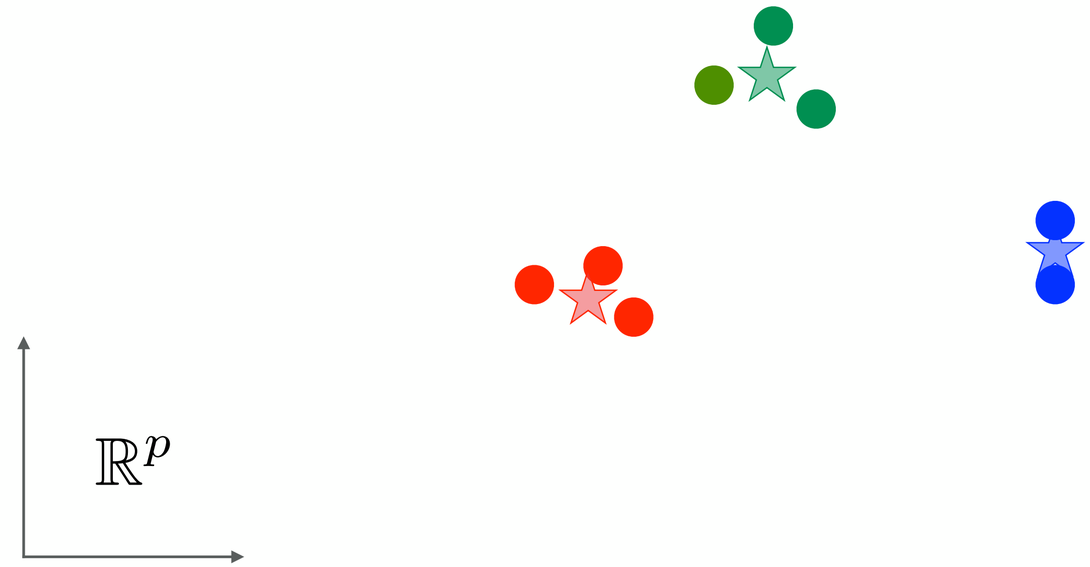
Machine Learning 101: K-means clustering

Step: update **assignments**



Machine Learning 101: K-means clustering

Step: recompute **cluster means**



Machine Learning 101: K-means clustering

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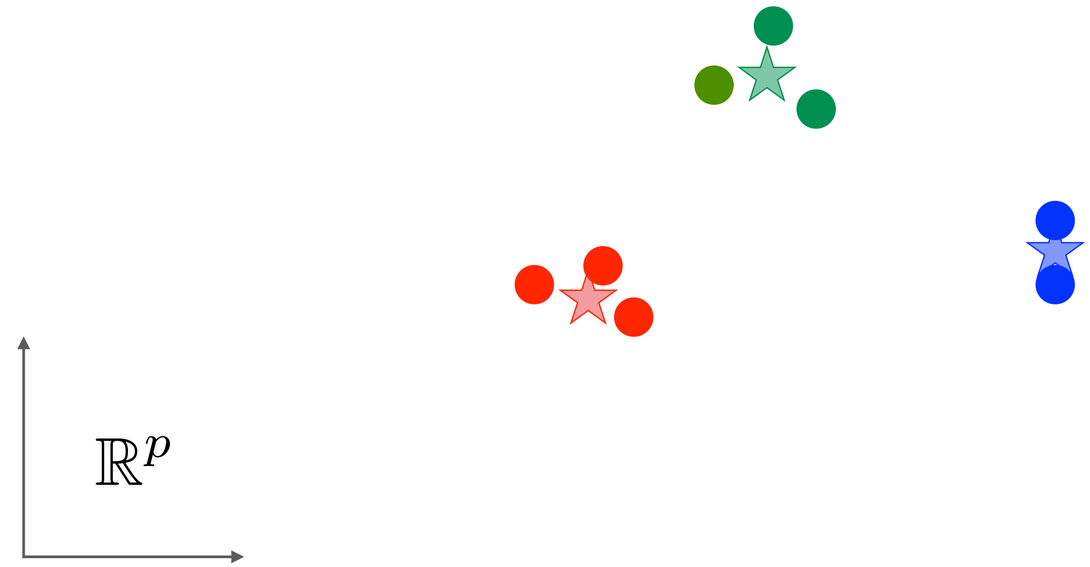


Theorem:

K-means procedure (Lloyd's algorithm) converges*

Proof:

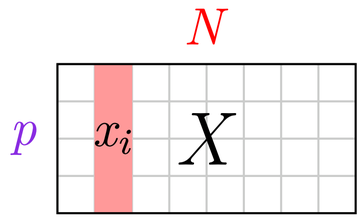
There are only a finite number of assignments, and we can never cycle since each iteration is an improvement

* *but it need not converge to the optimal solution!*

K-means clustering: complexity

Hard K-means / Lloyd's algorithm:
$\{x_i\}_{i=1,\dots,N} \subset \mathbb{R}^p$

1. Update cluster centers $\mu_k \in \mathbb{R}^p$ for $k = 1, \dots, K$
2. Update assignments $c_i \in \{1, \dots, K\}$ for $i = 1, \dots, N$



Let $X = (x_i)_{i=1,\dots,N}$
To update assignment of x_i:

- Compute $\|x_i - \mu_k\|$ (cost: p flops).
- For all k, and all i, this means $\mathcal{O}(KNp)$ cost.

K-means clustering: complexity

Hard K-means / Lloyd's algorithm:
$\{x_i\}_{i=1,\dots,N} \subset \mathbb{R}^p$

1. Update cluster centers $\mu_k \in \mathbb{R}^p$ for $k = 1, \dots, K$
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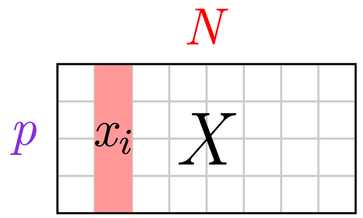

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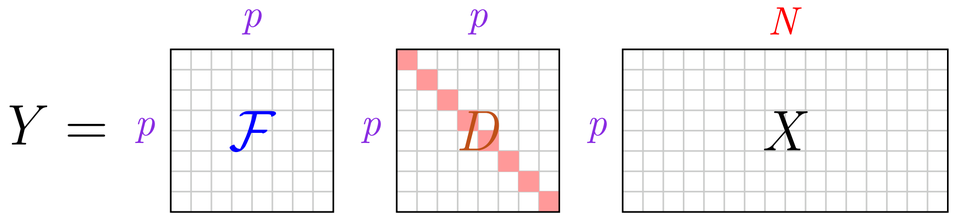
To update assignment of x_i:

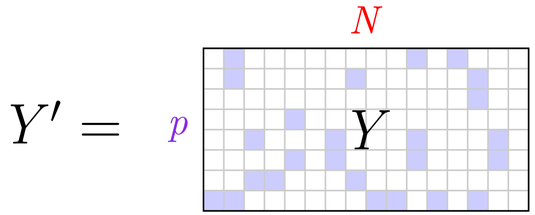
- Compute $\|x_i - \mu_k\|$ (cost: p flops).
- For all k, and all i, this means $\mathcal{O}(KNp)$ cost.

Because we're estimating the mean, we can use the theorems discussed earlier!

Our sampling is suitable for **streaming** data

Our idea: apply "preconditioned" entry-wise subsampling





Given a true mean $\bar{x} = \frac{1}{N}\sum_{i=1}^N x_i$, and our estimate of it $\hat{\bar{x}}$ from sampled data,

Theorem (Pourkamali-Anaraki & B., *IEEE Trans. Info Theory* 2017)
$\mathbb{E}\,\hat{\bar{x}} = \bar{x}$ *and* $\|\hat{\bar{x}} - \bar{x}\|_\infty \le t$ *with probability greater than*

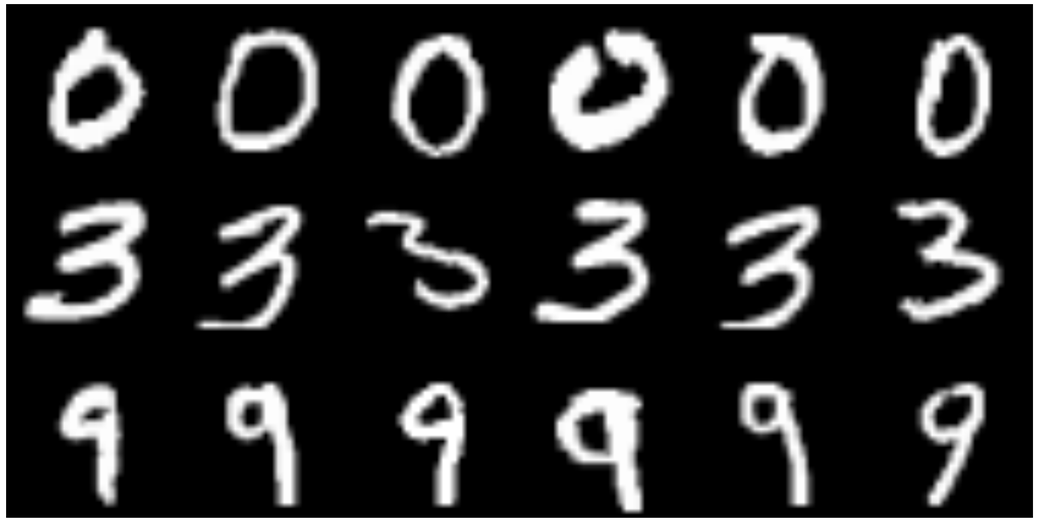
$$1 - 2p\exp\left(\frac{-N\gamma t^2/2}{\|X\|^2_{\text{max-row}} + t/3\|X\|_{\text{max-entry}}}\right)$$

where $\gamma = p_{small}/p$ *(simplifying to* $p_{small} \ll p \ll N$*)*

MNIST handwritten digits

Goal: recover cluster centers, using K-means clustering algorithm

Data: $N = 21{,}002$ examples of 28×28 pixel images ($p = 784$)



Experiments: MNIST handwritten digits

(a) true cluster centers

(b) K-means, many passes

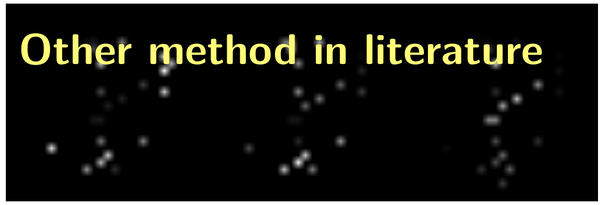
Experiments: MNIST handwritten digits

(a) true cluster centers

(b) K-means, many passes

(c) sparsified K-means, 1 pass, no preconditioning

(g) feature extraction, 1 pass



(h) feature selection, 3 passes

Experiments: MNIST handwritten digits

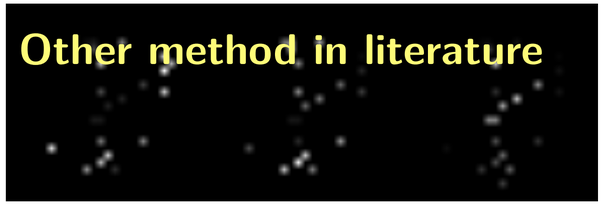
(a) true cluster centers

(b) K-means, many passes

(c) sparsified K-means, 1 pass, no preconditioning

(g) feature extraction, 1 pass

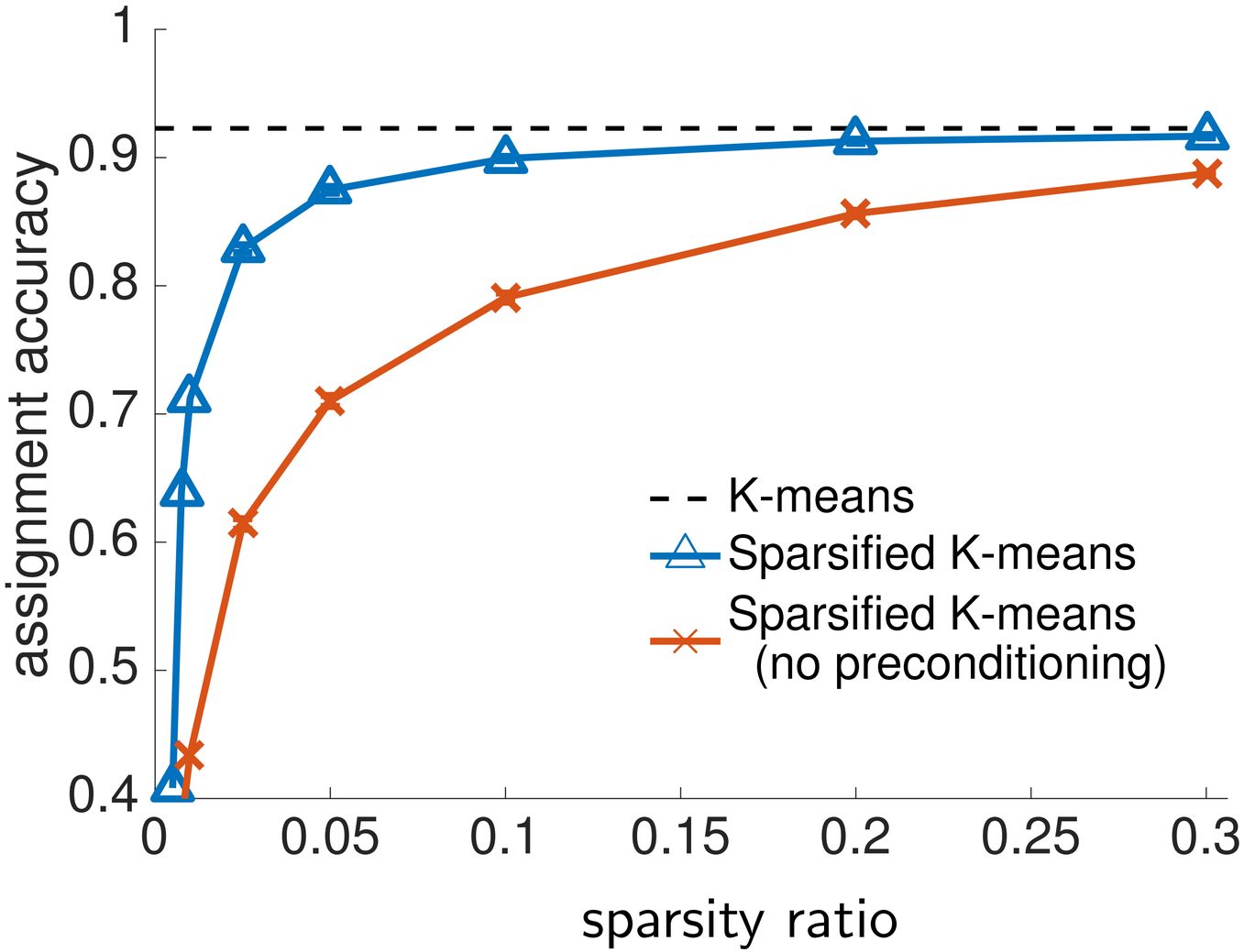
(d) sparsified K-means, 1 pass, preconditioned



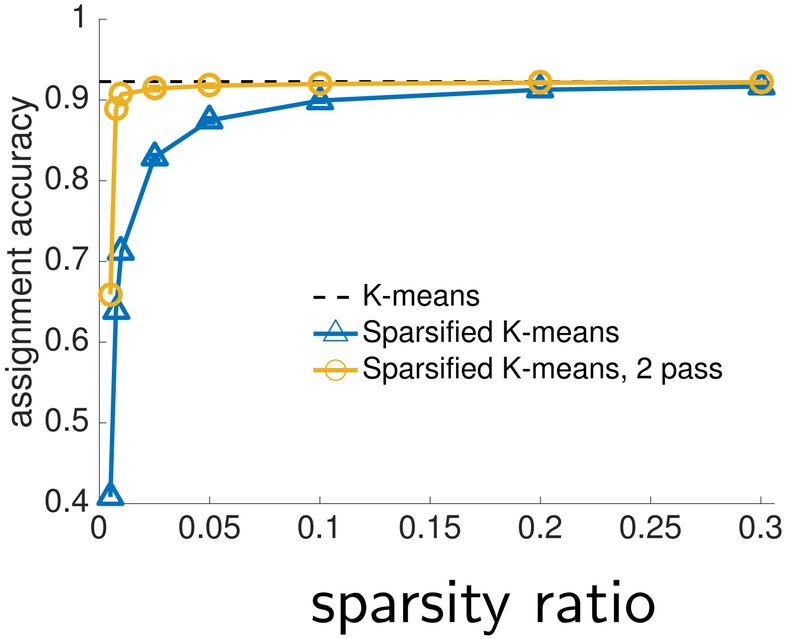
(h) feature selection, 3 passes

Accuracy on MNIST

Now look at **classification** accuracy (averaged over 50 trials)



"two-pass" version even more accurate



Speed on "Infinite MNIST"

"Infinite MNIST", $p = 784$, but now $N = 9{,}631{,}605$ instead of $21{,}002$

56 GB data, split into 58 chunks to keep RAM usage around 1 GB

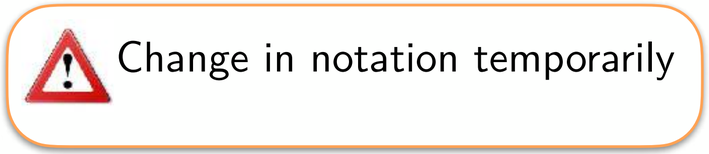
	Time to find assignments		Time to update all centers		Combined time	
Algorithm	Absolute	Speedup	Absolute	Speedup	Absolute	Speedup
K-means	130.0s	1×	150.8s	1×	280.8s	1×
Sparsified	1.3s	100×	5.7s	26.4×	7.0s	40.1×

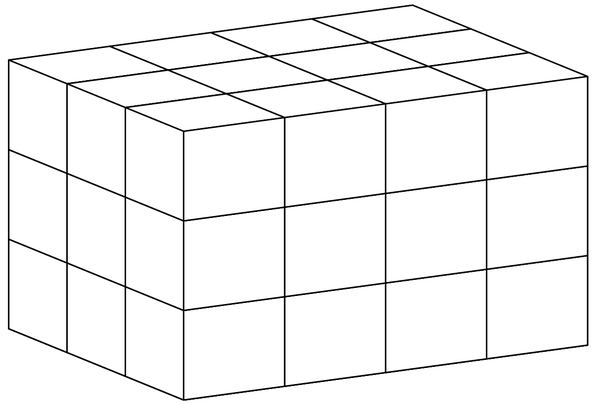
at 20x undersampling; accuracy is 89% (vs 92% for K-means)

OUTLINE

1. Randomized "sketches"
   a. Warmup: PCA
   b. Classical sketches
   c. Structured sketches
2. Applications
   a. Warmup: linear algebra
   b. K-means clustering
   c. Tensor factorizations
   d. Gradient-free optimization

Tensor Background: what is a tensor?





- A *tensor* $\mathcal{X} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ is an array of dimension N, also called an *N-way tensor* or *order N tensor*.
- A matrix $\mathbf{X} \in \mathbb{R}^{I_1 \times I_2}$ is a 2-way tensor.
- A vector $\mathbf{x} \in \mathbb{R}^{I_1}$ is a 1-way tensor.
- A scalar $x \in \mathbb{R}$ is a 0-way tensor.

Examples of tensors

For example, [Kolda & Sun, '08] consider these datasets:

- **The Enron dataset** has size $1K \times 1K \times 1.1K \times 200$ and consists of elements of the form (user,user,keyword,day). Element (i, j, k, l) is 1 if user i sent an email to user j with keyword k on day l, 0 otherwise.
- **The DBLP dataset** has size $5K \times 1K \times 1K$ and consists of elements of the form (author,conference,keyword). Element (i, j, k) is 1 if author i published a paper at conference j containing the keyword k in the title, 0 otherwise.

These are examples of **sparse** tensors

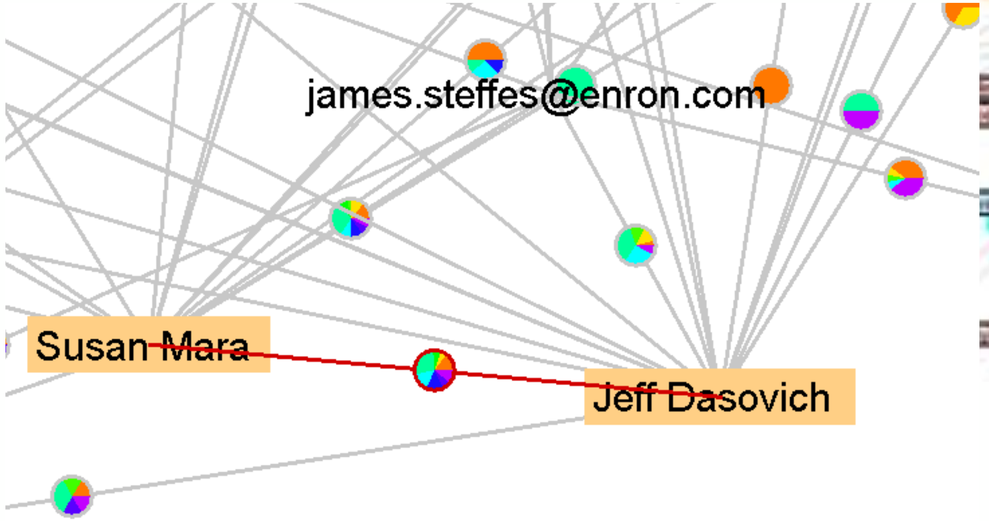


Image: https://homes.cs.washington.edu/~jheer/projects/enron/

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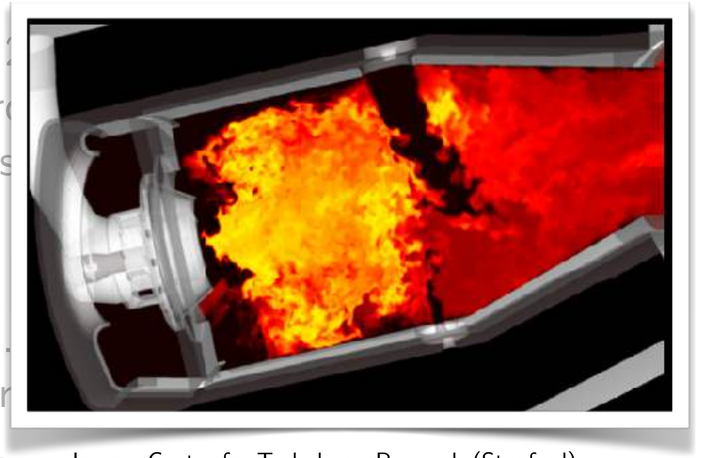
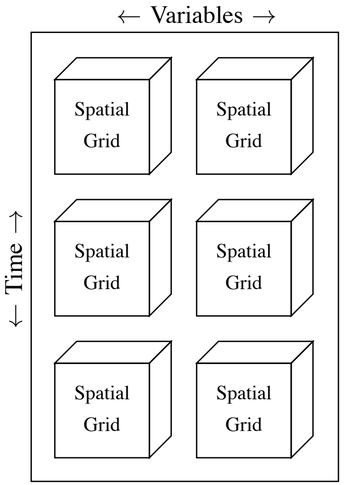


Image: Center for Turbulence Research (Stanford)

[Austin et al., '16] consider tensor data produced by high-fidelity combustion simulations with the following properties:

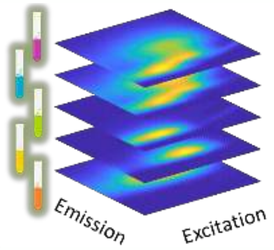
- 3-dimensional spatial grid with 512 points per dimension
- 64 variables are tracked per grid point
- 128 time steps 512 x 512 x 512 x 64 x 128 (8 TB)



This is a **dense** tensor

... we'll want methods that work with both sparse and dense tensors

Examples of tensors



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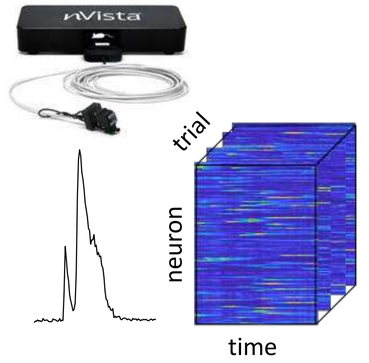

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Others:

- Chemometrics (emission x excitation x samples, for fluorescence spectroscopy)
- Neuroscience (neuron x time x trial/stimulus, for calcium imaging)
- Criminology (day x hour x location x crime, e.g., Chicago crime dataset)

Images: Tamara Kolda

Examples of tensors

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[Austin et al.,
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One-pass methods

All these tensors have a **time** or **sample** index

As time/samples increase, we don't want to store old ones

i.e., want a **streaming/one-pass method**

THIS IS A BIG MOTIVATION FOR SKETCHING

Tensor operations 1: matricization

Matricization (i.e., flattening) turns a tensor $\mathcal{X}$ into a matrix $\mathbf{X}_{(n)}$

Same idea as turning a matrix (e.g., an image) into a vector

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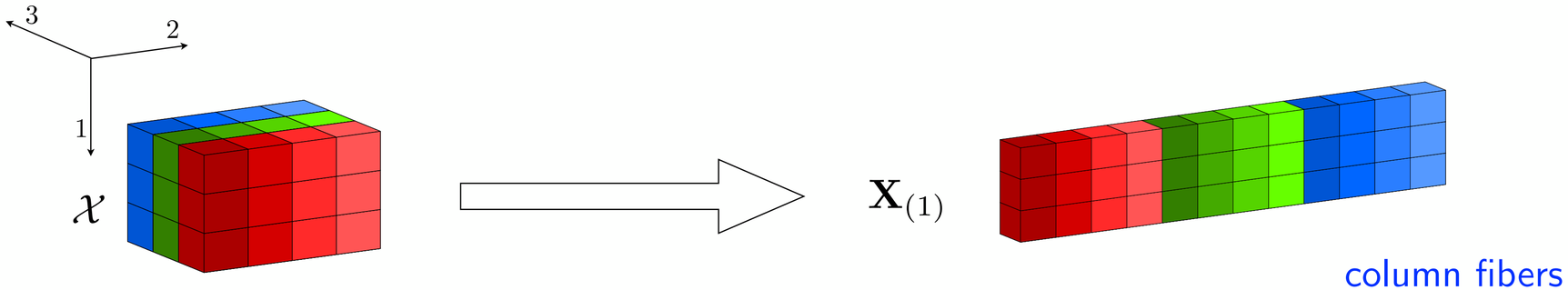

column fibers

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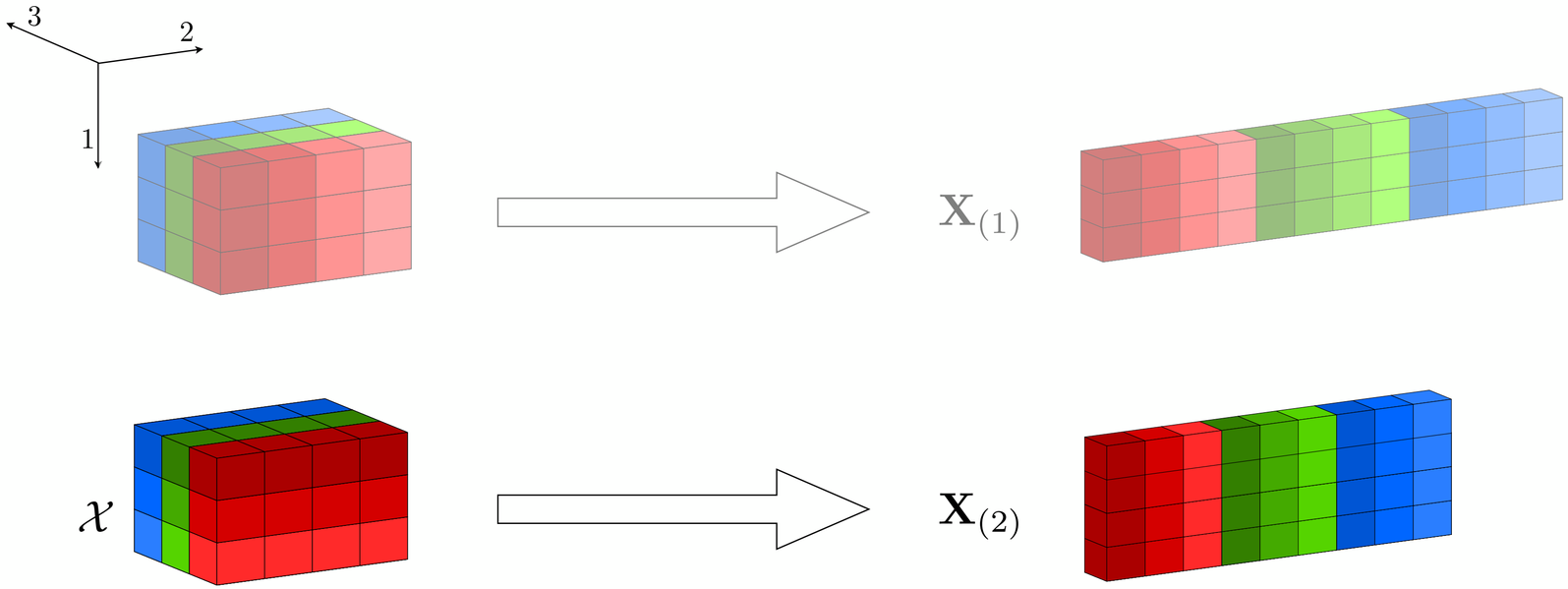

row fibers

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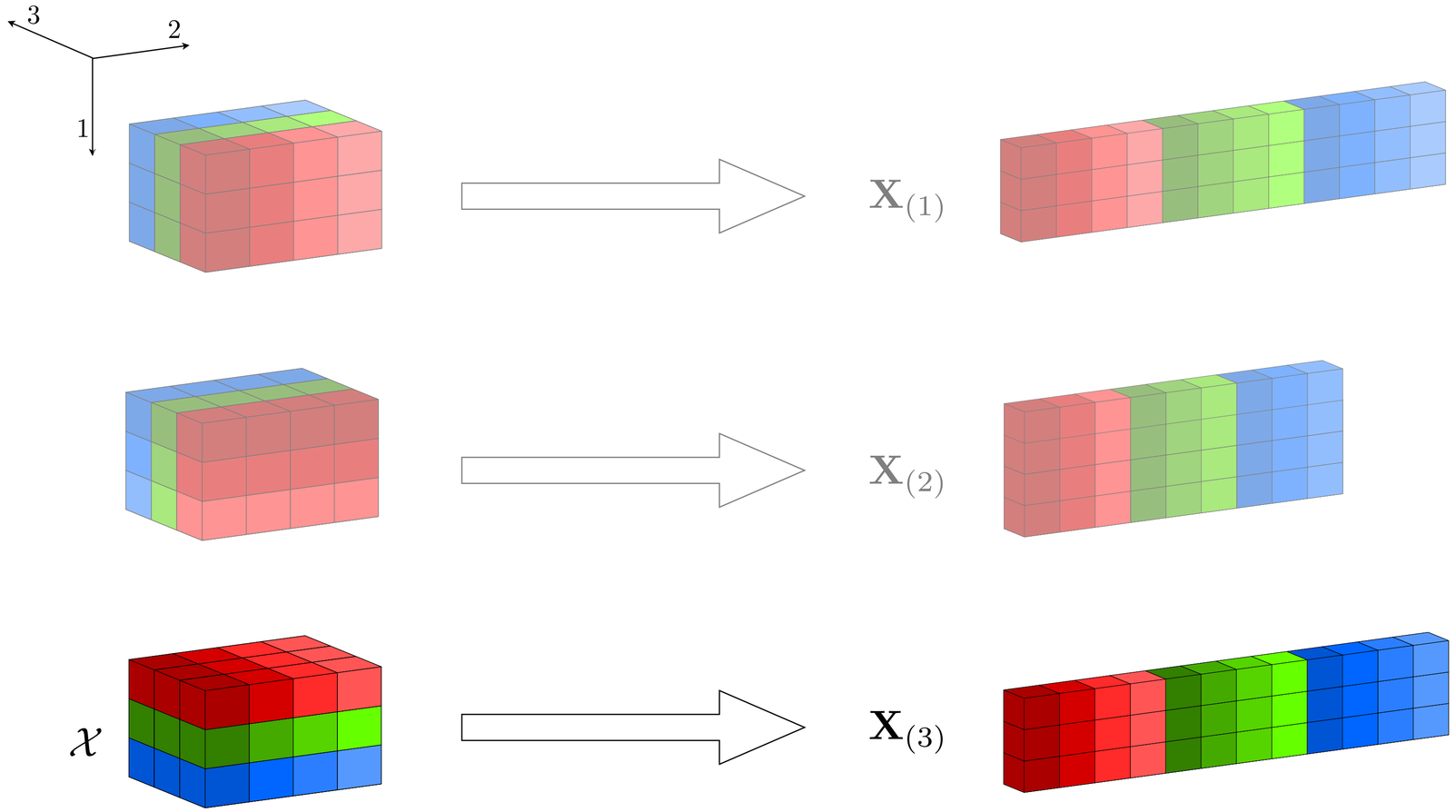


"tube" fibers

Tensor operations 2: tensor-times-matrix

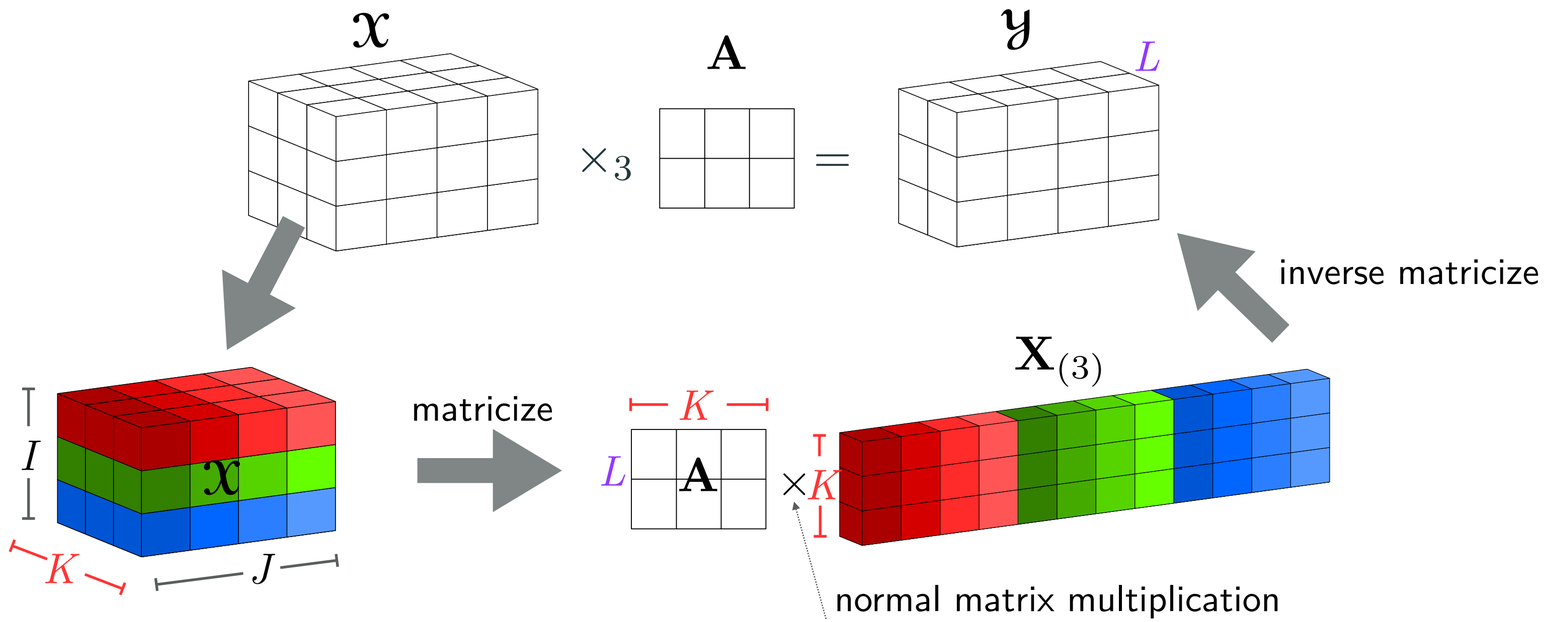
Example:

- Let $\mathcal{X} \in \mathbb{R}^{I \times J \times K}$ and $\mathbf{A} \in \mathbb{R}^{L \times K}$.
- We define $\mathcal{Y} \overset{\text{def}}{=} \mathcal{X} \times_3 \mathbf{A} \in \mathbb{R}^{I \times J \times L}$ elementwise by

$$y_{ijl} = \sum_{k=1}^{K} x_{ijk} a_{kl}.$$

- In matrix terms, $\mathbf{Y}_{(3)} = \mathbf{A}\mathbf{X}_{(3)}$.

Conveniently, order doesn't matter*
$\mathcal{X} \times_1 \mathbf{A_1} \times_2 \mathbf{A_2} = \mathcal{X} \times_2 \mathbf{A_2} \times_1 \mathbf{A_1}$

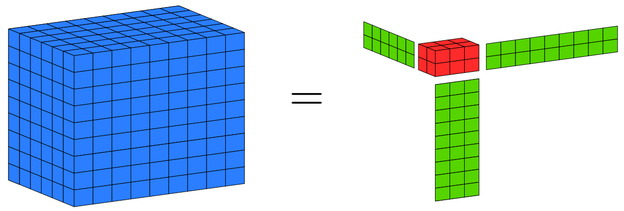


The Tucker decomposition

A Tucker decomposition of $\mathcal{X} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ is of the form

$$\mathcal{X} = \mathcal{G} \times_1 \mathbf{A}^{(1)} \times_2 \mathbf{A}^{(2)} \cdots \times_N \mathbf{A}^{(N)} =: [\![\mathcal{G}; \mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \ldots, \mathbf{A}^{(N)}]\!] \text{ (shorthand notation)}$$

where $\mathcal{G} \in \mathbb{R}^{R_1 \times R_2 \times \cdots \times R_N}$ and each $\mathbf{A}^{(n)} \in \mathbb{R}^{I_n \times R_n}$.

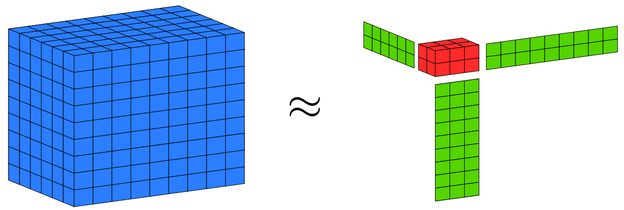


$\mathcal{G}$ is the *core tensor* and $\mathbf{A}^{(n)}$, $n = 1, 2, \ldots, N$, are *factor matrices*.

We say that $\mathcal{X}$ is a rank-$(R_1, R_2, \ldots, R_N)$ tensor.

Applications of the Tucker decomposition

- **Data compression.** Storing the red and green objects require less storage than the full blue tensor.
- **Data analysis.** Use rows of factor matrices as feature vectors—*unsupervised learning*.



Computing the Tucker decomposition

Given a data tensor $\mathcal{X} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$, we can find a decomposition $\mathcal{X} \approx [\![\mathcal{G}; \mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}]\!]$ by solving the optimization problem

$$\min_{\mathcal{G}, \mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}} \|\mathcal{X} - [\![\mathcal{G}; \mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \ldots, \mathbf{A}^{(N)}]\!]\|^2, \tag{4}$$

where $\mathcal{G} \in \mathbb{R}^{R_1 \times R_2 \times \cdots \times R_N}$ and $\mathbf{A}^{(n)} \in \mathbb{R}^{I_n \times R_n}$ for $n = 1, 2, \ldots, N$.

- Nonlinear!
- A common approach to this issue is to use *alternating least squares (ALS)*: Minimize with respect to each $\mathbf{A}^{(n)}$ and $\mathcal{G}$ one at a time. Repeat!
- With ALS, each subproblem is linear and easily solved.

i.e., Gauss-Siedel style

ALS same as *higher-order orthogonal iteration* (HOOI)
and if you do just one iteration, it's like *higher-order SVD* (HOSVD)

Computing the Tucker decomposition

The algorithm looks like this. Repeat the following until convergence:

Repeat until convergence

1. For $n = 1, \dots, N$, update (10)

$$\mathbf{A}^{(n)} = \underset{\mathbf{A} \in \mathbb{R}^{I_n \times R_n}}{\arg\min} \left\| \left(\bigotimes_{\substack{i=N \\ i \neq n}}^{1} \mathbf{A}^{(i)} \right) \mathbf{G}_{(n)}^{\top} \mathbf{A}^{\top} - \mathbf{X}_{(n)}^{\top} \right\|_F^2 . \quad (11)$$

2. Update $\mathcal{G} = \mathcal{X} \times_1 \mathbf{A}^{(1)\top} \times_2 \mathbf{A}^{(2)\top} \cdots \times_N \mathbf{A}^{(N)\top}$. (12)

$$= \underset{\mathcal{Z} \in \mathbb{R}^{R_1 \times \cdots \times R_N}}{\arg\min} \left\| \left(\bigotimes_{i=N}^{1} \mathbf{A}^{(i)} \right) \mathbf{z}_{(:)} - \mathbf{x}_{(:)} \right\|_2^2 .$$

(Line 12 follows if the factor matrices are orthogonalized)

Make extensive use of this identity:

$$\mathcal{Y} = \mathcal{X} \times_1 \mathbf{A}^{(1)} \times_2 \mathbf{A}^{(2)} \cdots \times_N \mathbf{A}^{(N)} \quad \Leftrightarrow$$

$$\mathbf{Y}_{(n)} = \mathbf{A}^{(n)} \mathbf{X}_{(n)} \left(\mathbf{A}^{(N)} \otimes \cdots \otimes \mathbf{A}^{(n+1)} \otimes \mathbf{A}^{(n-1)} \otimes \cdots \otimes \mathbf{A}^{(1)} \right)^{\top}$$

Computing the Tucker decomposition

The algorithm looks like this. Repeat the following until convergence:

1. For $n = 1, \ldots, N$, update (10)

$$\mathbf{A}^{(n)} = \underset{\mathbf{A} \in \mathbb{R}^{I_n \times R_n}}{\arg\min} \left\| \left(\bigotimes_{\substack{i=N \\ i \neq n}}^{1} \mathbf{A}^{(i)} \right) \mathbf{G}_{(n)}^{\top} \mathbf{A}^{\top} - \mathbf{X}_{(n)}^{\top} \right\|_F^2 . \quad (11)$$

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Issues when dealing with large, sparse tensors:

- The Kronecker product matrix is huge.
- The series of tensor-times-matrix products is very costly, and can require lots of additional memory when $\mathcal{X}$ is sparse.
- We address this problem by using *TensorSketch*.

Aside: *we initially thought that **solving** the least-squares problem would be an issue, and something to fix with sketching, but this is not exactly the case* → (partly because of many clever tricks due to orthogonality of A)

Our modified algorithm: Tucker-TS

We simply sketch each of these least-squares problems with TensorSketch operators $\mathbf{S}^{(n)}$, $n = 1, \ldots, N+1$, which are defined at the start of the algorithm:

Repeat until convergence

1. For $n = 1, \ldots, N$, update

$$\mathbf{A}^{(n)} = \underset{\mathbf{A} \in \mathbb{R}^{I_n \times R_n}}{\arg\min} \left\| \left(\mathbf{S}^{(n)} \bigotimes_{\substack{i=N \\ i \neq n}}^{1} \mathbf{A}^{(i)} \right) \mathbf{G}_{(n)}^{\top} \mathbf{A}^{\top} - \mathbf{S}^{(n)} \mathbf{X}_{(n)}^{\top} \right\|_F^2 . \tag{18}$$

(and orthogonalize)

2. Update

$$\mathcal{G} = \underset{\mathcal{Z} \in \mathbb{R}^{R_1 \times \cdots \times R_N}}{\arg\min} \left\| \left(\mathbf{S}^{(N+1)} \bigotimes_{i=N}^{1} \mathbf{A}^{(i)} \right) \mathbf{z}_{(:)} - \mathbf{S}^{(N+1)} \mathbf{x}_{(:)} \right\|_2^2 . \tag{19}$$

sketched once at very beginning

Tricks:

- don't draw new sketches each iteration
- the TensorSketches have CountSketches/hashes in common $\mathbf{S}^{(n)}, \mathbf{S}^{(n')}$ (each is leave-one-out)
- G update solved via conjugate gradient (CG) algo, and can prove it is well-conditioned
- advanced tricks and variants in the paper

Numerical experiment: sparse 3D tensor

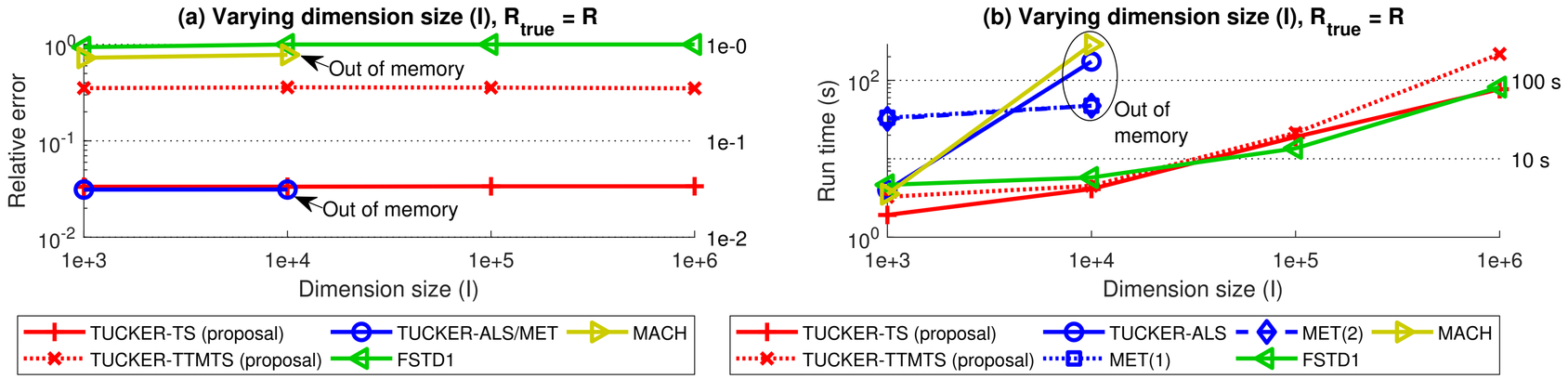


Figure 3: Relative error and run time for random sparse 3-way tensors with varying dimension size I and $\text{nnz}(\mathcal{Y}) \approx$ 1e+6. Both the true and target ranks are $(10, 10, 10)$.

Tucker-TS approximates least-squares like this:

$$\begin{aligned}\text{argmin}_x \frac{1}{2}\|Ax-b\|_2^2 &\approx \text{argmin}_x \frac{1}{2}\|\Phi(Ax-b)\|_2^2 \\ &= (A^\top \Phi^\top \Phi A)^{-1} A^\top \Phi^\top \Phi b\end{aligned}$$

Tucker-TTMTS approximates least-squares like this:

$$\begin{aligned}\text{argmin}_x \frac{1}{2}\|Ax-b\|_2^2 &= (A^\top A)^{-1} A^\top b \\ &\approx (A^\top A)^{-1} A^\top \Phi^\top \Phi b\end{aligned}$$

(and exploit orthogonality here)

Video

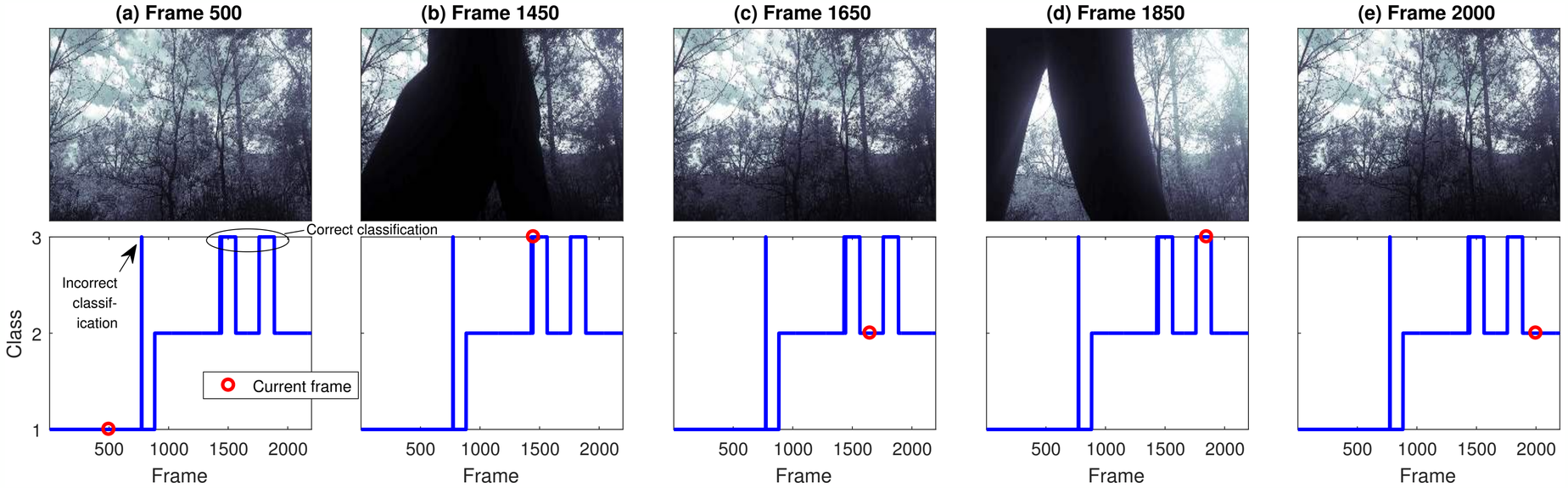


Figure 6: Five sample frames with their assigned classes. The frames (b) and (d) contain a disturbance.

38 GB video (can't all fit into RAM): 2,200 frames, each of size 1,080 by 1,980 pixels

Compute rank (10,10,10) factorization, 30 iterations max

Find 3 factor matrices — take the one corresponding to time and run k-means clustering

We load chunk-by-chunk and do the sketches (in one pass)

(used Tucker-TTMTS variant)

OUTLINE

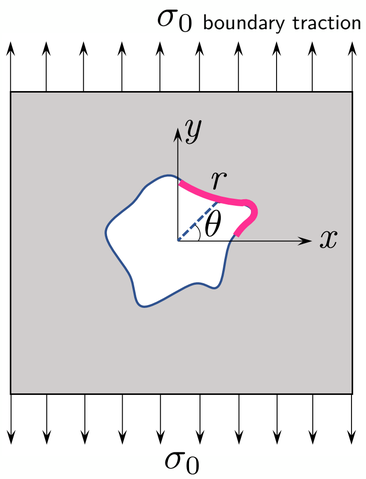
1. Randomized "sketches"
   a. Warmup: PCA
   b. Classical sketches
   c. Structured sketches
2. Applications
   a. Warmup: linear algebra
   b. K-means clustering
   c. Tensor factorizations
   d. Gradient-free optimization

Motivating Application: shape optimization

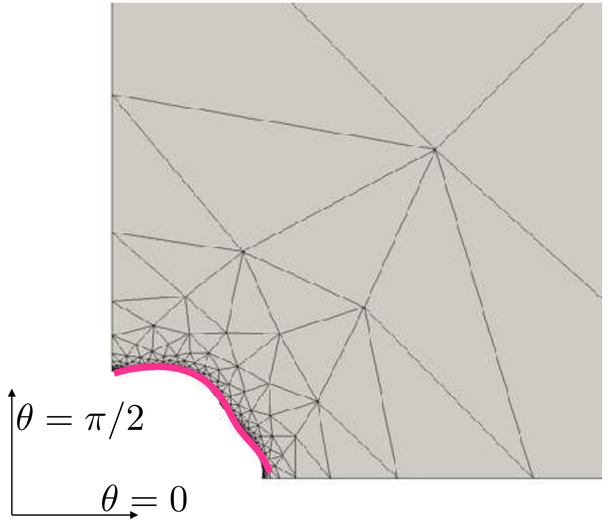
Forward problem: find vertical stress σ_y

linear elasticity PDE

(boundary conditions depend on shape of the hole)



conforming finite element mesh, used in FEniCS




Change in notation temporarily

Motivating Application: shape optimization

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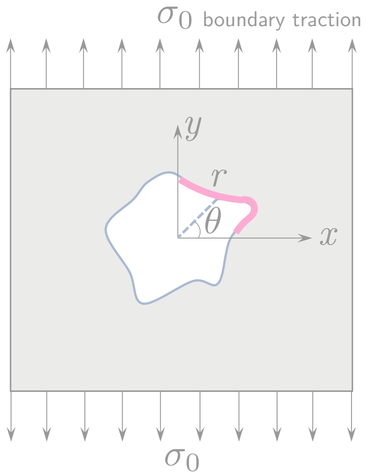

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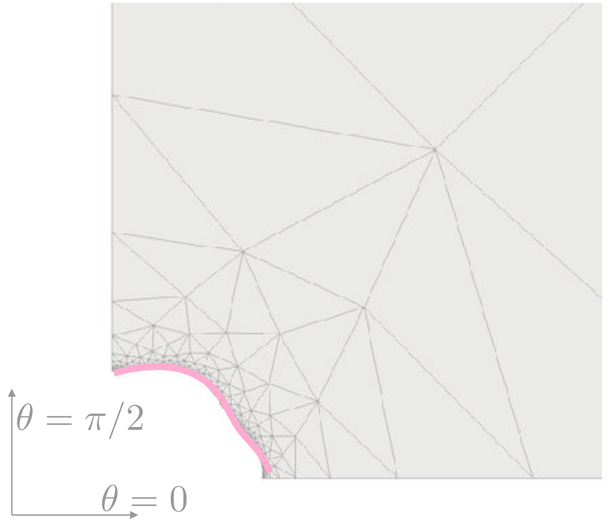

Inverse problem: what shape minimizes the vertical stress?

parameterize the shape of the hole as follows, which automatically enforces a constant area constraint

$$r(\theta) = \frac{1}{2\pi} + \delta \sum_{k=0}^{d/2-1} \frac{1}{\sqrt{2k+1}} \left(x_{2k+1} \sin((2k+1)\cdot\theta) + x_{2k+2} \cos((2k+1)\cdot\theta) \right)$$

optimization variable:

$x \in \mathbb{R}^d$

Generic PDE-constrained optimization

implicitly saying that u solves the PDE

$$\min_{u,x} \mathcal{L}(u) \quad \text{subject to} \quad \phi(u,x) = 0$$

Examples:

$\dot{u} = \Delta u,\ u(0) = h$ "x" is the initial condition

$\ddot{u} = c^2 \Delta u,\ u(0) = h$ "x" is a parameter

$\Delta u = 0,\ u(\Gamma) = h$ "x" is the boundary condition

$\mathcal{L}(u)$ is the loss which penalizes something like:

- deviation from observations
- drag
- mass
- cost of materials
- compliance

etc.

Generic PDE-constrained optimization

implicitly saying that u solves the PDE

$$\min_{u,x} \mathcal{L}(u) \quad \text{subject to} \quad \phi(u,x) = 0$$

$$\phi(u,x) = 0 \quad \Longrightarrow \quad u = u(x)$$

Rewrite: $\min_x f(x) \stackrel{\text{def}}{=} \mathcal{L}(u(x))$

... but finding the gradient is tricky:

$$\nabla f(x) = \frac{\partial \mathcal{L}}{\partial u} \cdot \frac{\partial u}{\partial x}$$

Why not just find gradients automatically?

✔ The **adjoint state method** and **reverse-mode automatic differentiation** can automatically calculate gradients in about the same time (~4x) as a function evaluation

- ... so if we can evaluate $f(x)$ numerically, we can find the gradient
- (this applies if $f : \mathbb{R}^d \to \mathbb{R}$; $f : \mathbb{R}^d \to \mathbb{R}^q$ with $q \gg 1$ is another story)

Note: we're assuming derivative exists, just hard to actually calculate

This is *not* non-smooth optimization

Why not just find gradients automatically?

✔ The **adjoint state method** and **reverse-mode automatic differentiation** can automatically calculate gradients in about the same time (~4x) as a function evaluation

✘ Requires specialized/restricted libraries/code (`dolfin-adjoint/FEniCS`, `autograd`)

`Jax, PyTorch, Tensorflow, …`

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✘ Adjoint state method requires a method to solve adjoint PDE

(and have to parallelize for HPC)

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- difficult to maintain in large code bases, e.g., 4D-var for weather codes

✘ Slow if used for intermediate calculations involving some $f : \mathbb{R}^d \to \mathbb{R}^q$

- e.g., seismic inversion with many observations

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✗ Possible memory explosion

- e.g., time-dependent problems. Check-pointing schemes somewhat helpful

Example: hyper-parameter optimization in deep learning

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✘ Assumes a computational structure

- inapplicable for physical observations (wind farms; *rollout* in AI)

Baseline Algorithms (for comparison)

$f : \mathbb{R}^d \to \mathbb{R}$

These days, often called "zeroth order" optimization

Algorithm Gradient Descent via Finite Differences

1: **for** $k = 1, 2, \ldots$ **do**
2: Estimate $g_k \approx \nabla f(x_k)$ ▷ Use finite differences
3: $x_{k+1} \leftarrow x_k - \eta_k g_k$ ▷ For appropriate step-size η_k

✔ ignoring finite-difference error, enjoys well-understood convergence

✘ requires $d+1$ function evaluations per iter.

Why not use traditional Derivative Free Optimization (DFO) methods?

Answer: most classical DFO methods don't scale well with dimension

Note: there are many other DFO methods... but we won't discuss in this talk

From heuristics to theoretically based, from local to global

- Heuristics: Nelder-Mead, genetic algorithms, particle swarm optimization
  - e.g., CMA-ES, Covariance matrix adaptation evolution strategy
- Simulated Annealing (typical as heuristic)
- Bayesian Optimization
  - Model is Gaussian Process, with acquisition function (exploration/exploitation tradeoff)
- DFO-TR (Trust-region)
  - Model is polynomial

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Algorithm Randomized Coordinate Descent (CD)

1: **for** $k = 1, 2, \ldots$ **do**
2: Choose $j \in \{1, 2, \ldots, d\}$ at random
3: $g_k = e_j e_j^T \nabla f(x_k)$
4: $x_{k+1} \leftarrow x_k - \eta_k g_k$ ▷ For appropriate step-size η_k (or exact minimization… depends on structure)

✔ just 1 function evaluation per iteration

✘ poor convergence properties, slow rates

Stochastic Subspace Descent

directional derivative $qq^T \nabla f(x_k) = \left(\lim_{h \to 0} \frac{f(x_k + h \cdot q) - f(x_k)}{h} \right) q$

Assume we can compute this!

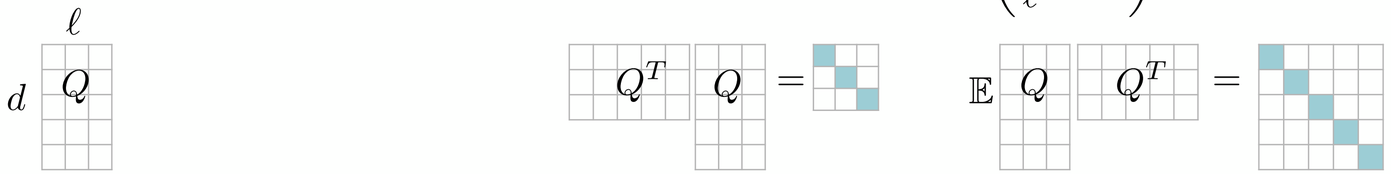
e.g.,

1) forward finite diff
2) forward-mode AD

Stochastic Subspace Descent

directional derivative $qq^T \nabla f(x_k) = \left(\lim_{h \to 0} \frac{f(x_k + h \cdot q) - f(x_k)}{h} \right) q$

$Q = [q_1, q_2, \ldots, q_\ell] \sim \text{Haar}(d \times \ell)$ $\quad Q^T Q = I_{\ell \times \ell}, \quad \mathbb{E}\left(\frac{d}{\ell} Q Q^T \right) = I_{d \times d}$



One benefit: in the limit $\ell = d$, $QQ^T = I_{d \times d}$, and so we'll recover the full gradient (for Gaussians, this is only true in expectation)

Stochastic Subspace Descent

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Algorithm "Stochastic Subspace Descent" (SSD)

1: **for** $k = 1, 2, \ldots$ **do**
2: Draw $Q \sim \text{Haar}(d \times \ell)$ or *any* generic SSD
3: $x_{k+1} \leftarrow x_k - \eta_k \frac{d}{\ell} Q Q^T \nabla f(x_k)$

Generic SSD $\boxed{Q^T Q = I_{\ell \times \ell}, \quad \mathbb{E}\left(\frac{d}{\ell} Q Q^T \right) = I_{d \times d}}$

Both **Haar** and **Coordinate Descent** methods are valid generic SSD

Stochastic Subspace Descent

directional derivative $qq^T \nabla f(x_k) = \left(\lim_{h \to 0} \frac{f(x_k + h \cdot q) - f(x_k)}{h} \right) q$

$Q = [q_1, q_2, \ldots, q_\ell] \sim \text{Haar}(d \times \ell)$ $\quad Q^T Q = I_{\ell \times \ell}, \quad \mathbb{E}\left(\frac{d}{\ell} Q Q^T \right) = I_{d \times d}$

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We call Q a "Haar" distributed r.v. (i.e., the Haar measure over orthogonal matrices), but really care about QQ^T which is a projection matrix (onto $\text{col}(Q)$).

We get Q via Gram-Schmidt (or appropriately modified `QR`) on a Gaussian G, and note $\text{col}(Q) = \text{col}(G)$ w.p. 1, so our update is equivalent to

$$x_{k+1} \leftarrow x_k - \eta_k \frac{d}{\ell} \mathcal{P}_{\text{col}(G)} \left(\nabla f(x_k) \right)$$

and hence the term "stochastic subspace".

First theory results (for *generic* SSD)

Theorem (Kozak, Becker, Tenorio, Doostan '20)

Assume: minimizer attained, gradient Lipschitz, stepsize η_k chosen appropriately.

constant L ← η_k ; $\eta = \frac{\ell}{d}\frac{1}{L}$

1. If f is **convex**,

$$\mathbb{E}f(x_k) - f^\star \leq 2\frac{d}{\ell}\frac{L}{k}R^2 = \mathcal{O}(k^{-1})$$

constant μ ← 2. If f is **not convex** but satisfies the **Polyak-Lojasiewicz** inequality,

$$\mathbb{E}f(x_k) - f^\star \leq \rho^k(f(x_0) - f^\star) = \mathcal{O}(\rho^k) \qquad \text{and} \qquad f(x_k) \xrightarrow{\text{a.s.}} f^\star$$

3. If f is **strongly convex**, statements of 2 above hold, and also

$$x_k \xrightarrow{\text{a.s.}} \operatorname{argmin}_x f(x)$$

4. If f is **not convex** (nor PL),

$$\min_{k' \in \{0,\ldots,k\}} \mathbb{E}\|\nabla f(x_{k'})\|^2 \leq \frac{d}{\ell}\frac{2L(f(x_0) - f^\star)}{k+1}$$

SSD is a special type of SGD, but results are much better than generic SGD analysis

$f^\star \stackrel{\text{def}}{=} \min_x f(x)$

$\rho = 1 - \frac{\mu}{L}\frac{\ell}{d}$

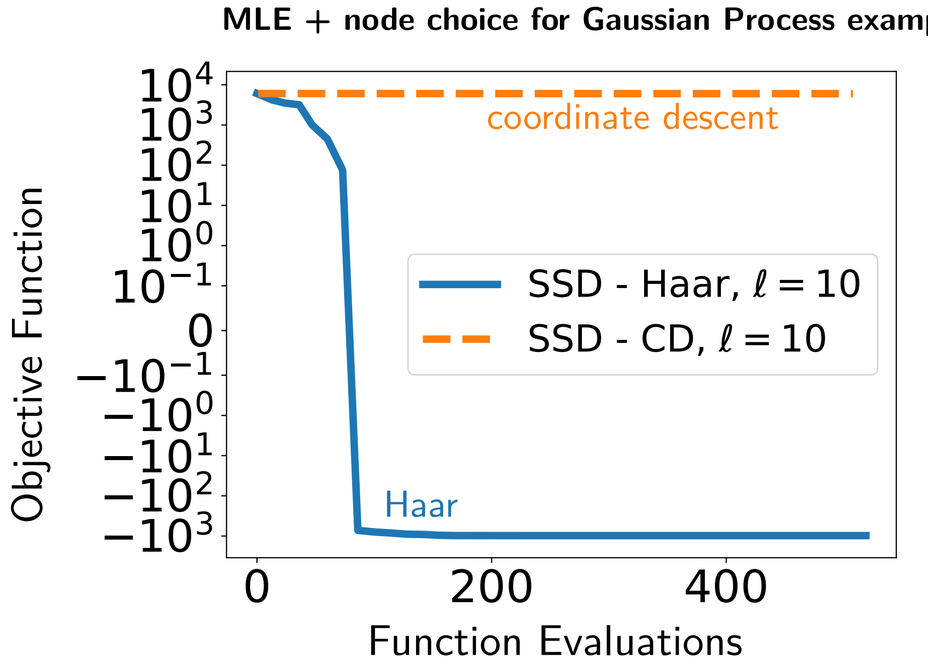
$d =$ ambient dimension

$\ell =$ # directional derivs

Generic SSD $\quad Q^TQ = I_{\ell\times\ell}, \quad \mathbb{E}\left(\frac{d}{\ell}QQ^T\right) = I_{d\times d}$

$\frac{d}{\ell} = 1$ is gradient descent

Numerical Results: better than expected

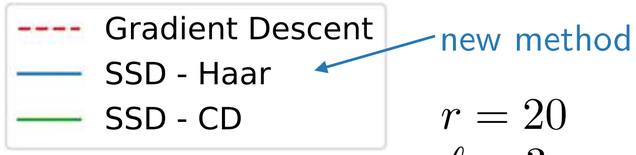


Observation: sometimes SSD (with Haar) drastically outperforms randomized coordinate descent (CD)

Generic SSD $\quad Q^T Q = I_{\ell \times \ell}, \quad \mathbb{E}\left(\frac{d}{\ell} Q Q^T\right) = I_{d \times d}$

Numerical Results: better than expected

Haar SSD drastically outperforms randomized coordinate descent (CD)

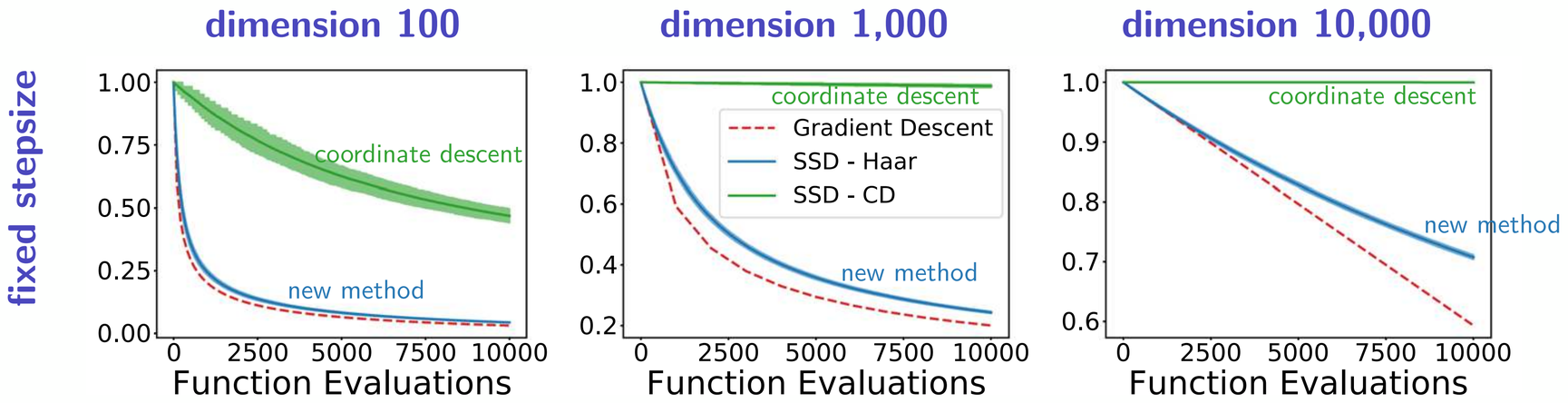


$r = 20$
$\ell = 3$

We can force it to happen by making a problem with low "intrinsic" dimension, e.g., Nesterov's "worst function in the world"

$$f_{\lambda,r}(\mathbf{x}) = \lambda((x_1^2 + \sum_{i=1}^{r-1} (x_i - x_{i+1})^2 + x_r^2)/2 - x_1)/4,$$

This has **intrinsic dimension** of r



Numerical Results: better than expected

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Gradient Descent
SSD - Haar
SSD - CD

new method

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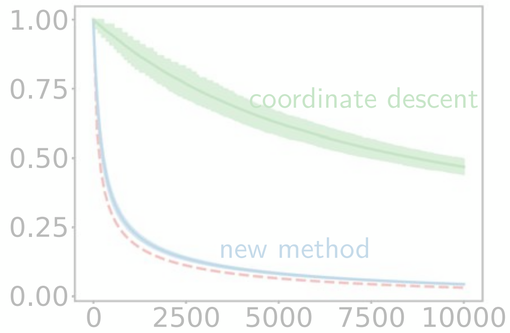
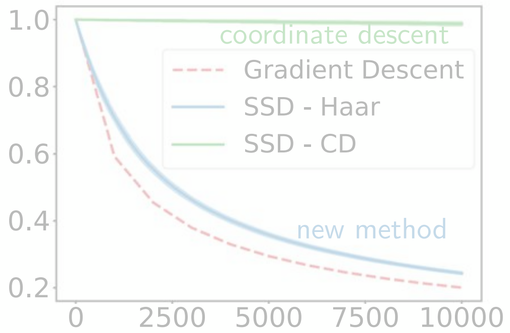
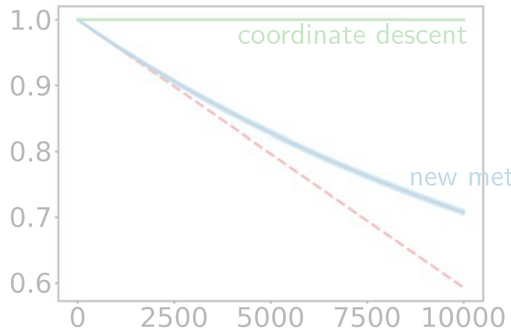
This has **intrinsic dimension** of r

dimension 100 | **dimension 1,000** | **dimension 10,000**

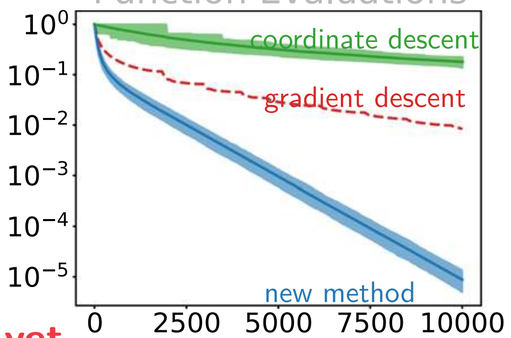
fixed stepsize

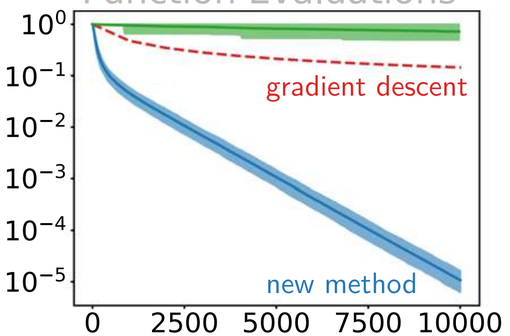


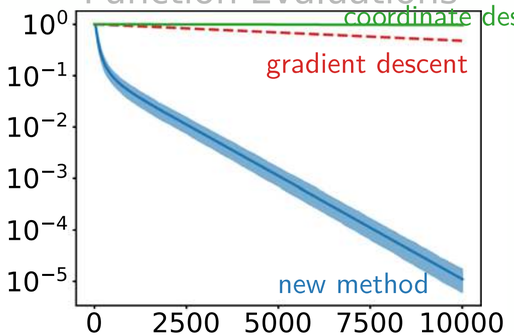




line search







no theory yet

Theory: explain better-than-expected results

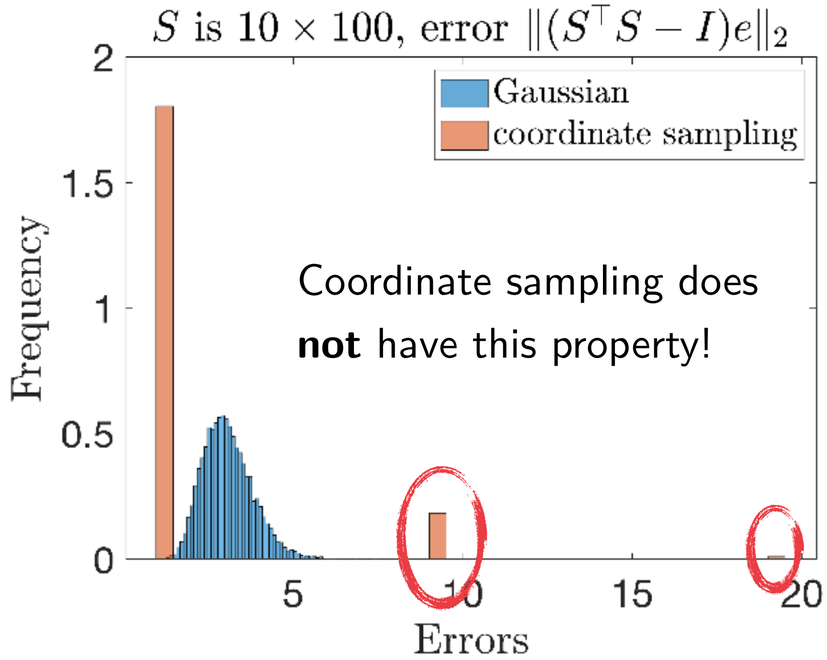
Previous theorem didn't actually rely on properties of Haar distribution, just generic Q:

$$Q^T Q = I_{\ell \times \ell}, \quad \mathbb{E}\left(\frac{d}{\ell} Q Q^T\right) = I_{d \times d}$$

Tighter analysis using concentration-of-measure:

Lemma 2 (Johnson-Lindenstrauss style embedding, from Kozak, Becker, Tenorio '19, Lemma 1)**.** $\forall \epsilon \in (0,1)$, *if* $\ell \gtrsim \epsilon^{-2}$, $Q \sim \text{Haar}(d \times \ell)$, *then* $\forall 0 \neq g \in \mathbb{R}^d$,

$$1 - \epsilon \leq \frac{d}{\ell} \frac{\|Q^T g\|^2}{\|g\|^2} \leq 1 + \epsilon \quad \textit{w/ prob. } \delta \geq 0.8$$



Recall...

$d =$ ambient dimension

$\ell =$ # directional derivs

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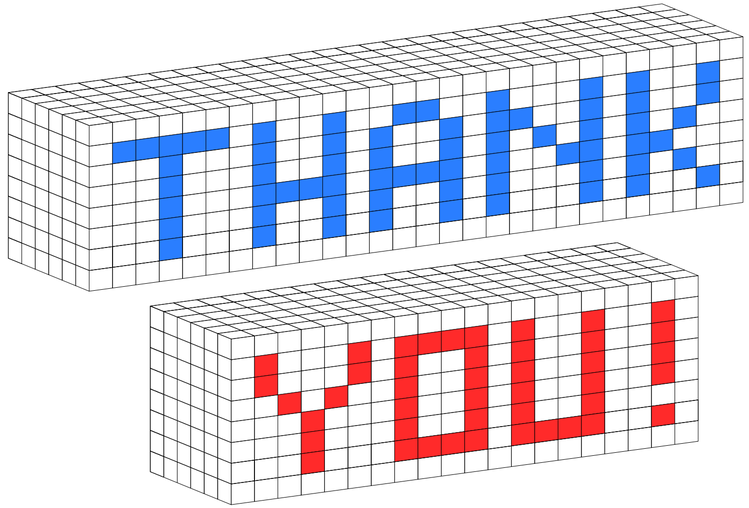
Theorem 3 (Kozak, Becker, Tenorio '19, Thm. 1)**.** *If f is strongly convex and ∇f is Lipschitz continuous, then for an appropriate stepsize η_k, the sequence (x_k) generated by SSD (with $Q \sim$ Haar), for $k > 100$, satisfies*

$$f(x_k) - f^\star \leq (1 + (1-\epsilon)\rho)^{k/2} (f(x_0) - f^\star) \quad \textit{with probability } \geq 0.998,$$

where $\rho < 1$ depends on ℓ, d and the Lipschitz and strong convexity parameters.

due to possibility of failure of JL

error in JL embedding

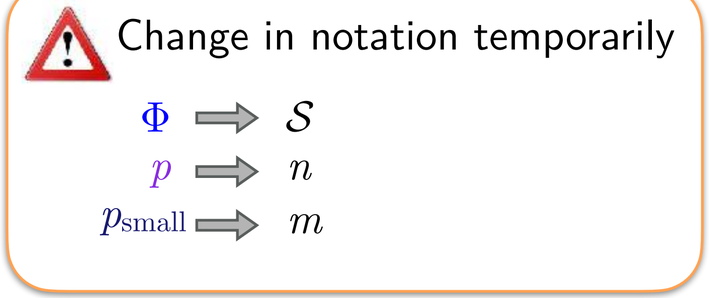


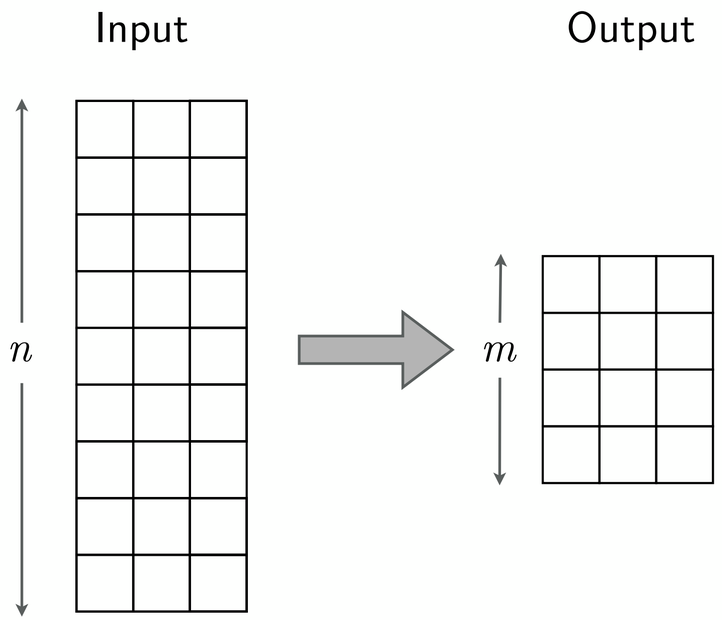
Papers and code available at https://amath.colorado.edu/faculty/becker/

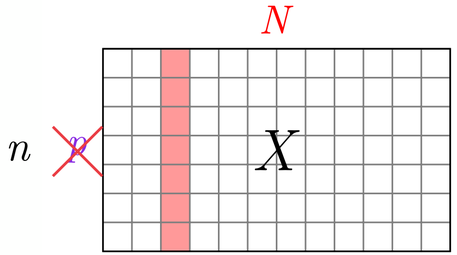
Method 7: CountSketch

Introduced in Charikar et al. (2004), more analysis in, e.g., Clarkson and Woodruff (2017)

$\mathcal{S} : \mathbb{R}^n \to \mathbb{R}^m$ linear operator







Method 7: CountSketch

$\mathcal{S} : \mathbb{R}^n \to \mathbb{R}^m$ linear operator

Notation: $[n] = (0, 1, \ldots, n-1)$

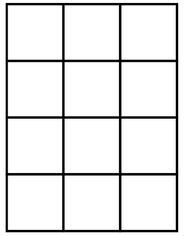
(use 0-based indexing)

Step 1:

Multiply by random sign*

$s : [n] \to \{\pm 1\}$
(uniform)

+1	+1	+1
+1	+1	+1
−1	−1	−1
+1	+1	+1
−1	−1	−1
−1	−1	−1
−1	−1	−1
+1	+1	+1
−1	−1	−1



* technically doesn't have to be fully random, but must be 2-wise independent

$$s(i) \perp s(j) \quad \text{if } i \neq j$$

Method 7: CountSketch

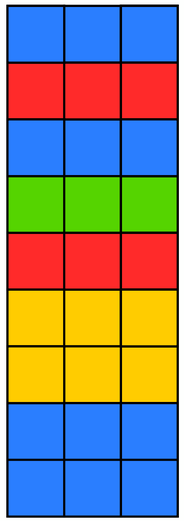
$\mathcal{S} : \mathbb{R}^n \to \mathbb{R}^m$ linear operator

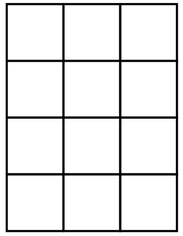
Step 2:

Assign an output row to every input row (randomly or with a hash function)

$h : [n] \to [m]$

(uniform)





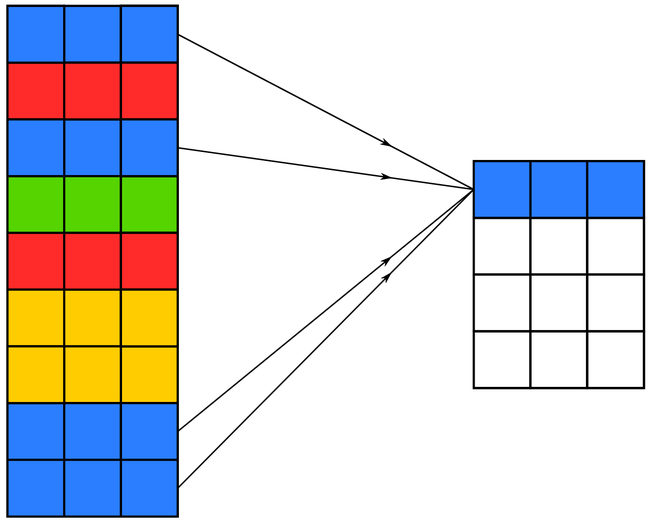
Again, don't need *all* of $h[i]$ to be independent, only pairwise independent (but easy enough to make them all independent)

Method 7: CountSketch

$\mathcal{S} : \mathbb{R}^n \to \mathbb{R}^m$ linear operator

Step 3:

Each output row is the sum of corresponding input rows



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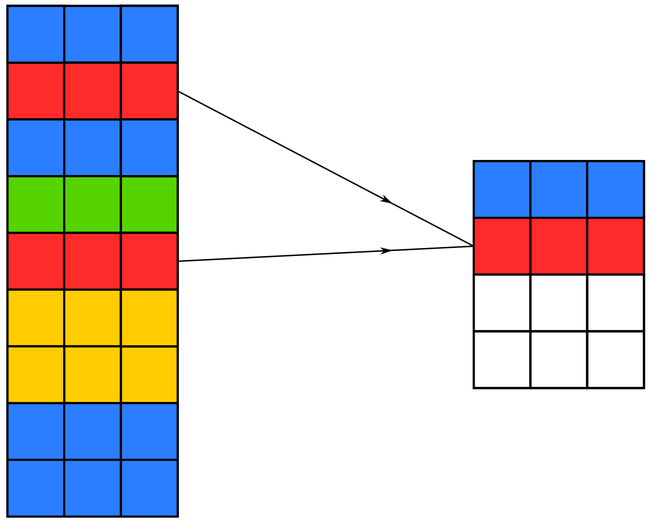

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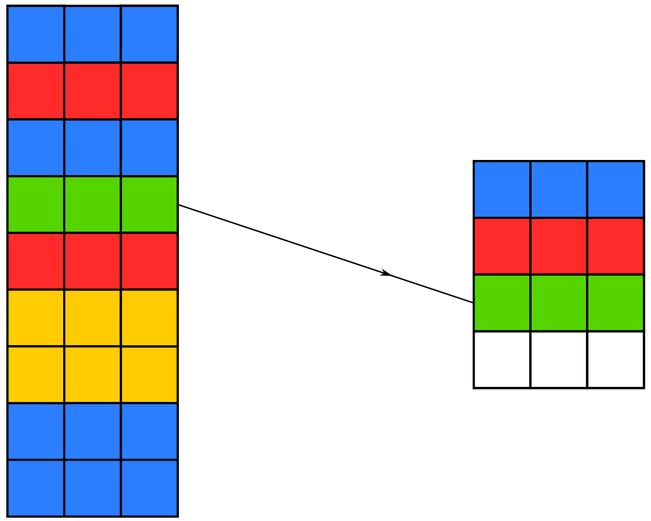

Method 7: CountSketch

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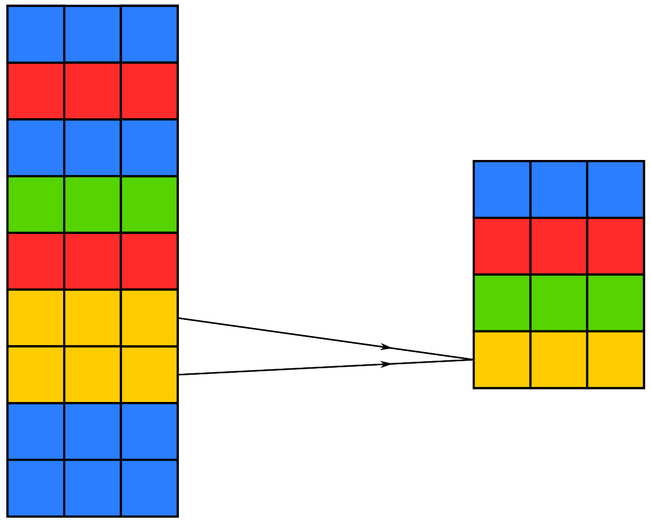

Method 7: CountSketch

$\mathcal{S} : \mathbb{R}^n \to \mathbb{R}^m$ linear operator

Complexity analysis: every input element is touched once

... so linear complexity

(and can exploit sparsity)

Method 7: CountSketch

$\mathcal{S} : \mathbb{R}^n \to \mathbb{R}^m$ linear operator

A formula for the output:

$$\boldsymbol{u} = \mathcal{S}(\boldsymbol{v}),\ u_i = \sum_{j|h(j)=i} s(j) v_j$$

$$s : [n] \to \{\pm 1\}$$
$$h : [n] \to [m] \quad \text{hash}$$

... and note that the following polynomial has the output as its coefficients:

$$p(x) \stackrel{\text{def}}{=} \sum_{j \in [n]} s(j) \cdot v_j \cdot x^{h(j)} = \sum_{i \in [m]} x^i \underbrace{\left(\sum_{j|h(j)=i} s(j) v_j \right)}_{u_i} = \sum_{i \in [m]} u_i \cdot x^i$$

(this will be key shortly...)

Method 8: TensorSketch

Introduced in Pagh (2013), more analysis in, e.g., Diao, Zong, Sun, Woodruff (2018)

TensorSketch is just CountSketch when the input can be written as a tensor product (for a special choice of the hash and sign functions)

Change in notation temporarily

$\Phi \Rightarrow \mathcal{S}$

$p \Rightarrow n$

$p_{\text{small}} \Rightarrow m$

$$\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^m$$

$$\boldsymbol{v} = \boldsymbol{v}^{(1)} \otimes \boldsymbol{v}^{(2)} \qquad \text{where size is} \qquad n = n^{(1)} \cdot n^{(2)}$$

Not (yet!) related to tensors

TensorSketch

Introduced in Pagh (2013), more analysis in, e.g., Diao, Zong, Sun, Woodruff (2018)

TensorSketch is just CountSketch when the input can be written as a tensor product (for a special choice of the hash and sign functions)

$$\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^m$$

$$\boldsymbol{v} = \boldsymbol{v}^{(1)} \otimes \boldsymbol{v}^{(2)} \qquad \text{where size is} \qquad n = n^{(1)} \cdot n^{(2)}$$

Kronecker/tensor product

$$\boldsymbol{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}, \ \boldsymbol{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \quad \boldsymbol{a} \otimes \boldsymbol{b} = \begin{bmatrix} a_1\boldsymbol{b} \\ a_2\boldsymbol{b} \\ a_3\boldsymbol{b} \end{bmatrix} = \begin{bmatrix} a_1b_1 \\ a_1b_2 \\ a_1b_3 \\ a_2b_1 \\ a_2b_2 \\ a_2b_3 \\ a_3b_1 \\ a_3b_2 \\ a_3b_3 \end{bmatrix}$$

TensorSketch

Introduced in Pagh (2013), more analysis in, e.g., Diao, Zong, Sun, Woodruff (2018)

TensorSketch is just CountSketch when the input can be written as a tensor product (for a special choice of the hash and sign functions)

$$\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^m$$

$$\boldsymbol{v} = \boldsymbol{v}^{(1)} \otimes \boldsymbol{v}^{(2)} \qquad \text{where size is} \qquad n = n^{(1)} \cdot n^{(2)}$$

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$$\boldsymbol{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}, \ \boldsymbol{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \qquad \boldsymbol{a} \otimes \boldsymbol{b} = \begin{bmatrix} a_1 \boldsymbol{b} \\ a_2 \boldsymbol{b} \\ a_3 \boldsymbol{b} \end{bmatrix} = \begin{bmatrix} a_1 b_1 \\ a_1 b_2 \\ a_1 b_3 \\ a_2 b_1 \\ a_2 b_2 \\ a_2 b_3 \\ a_3 b_1 \\ a_3 b_2 \\ a_3 b_3 \end{bmatrix}$$

another equivalent definition:

$$\boldsymbol{a} \otimes \boldsymbol{b} = \mathrm{vec}_{\mathrm{col}} \left(\boldsymbol{b} \boldsymbol{a}^T \right)$$

$$\boldsymbol{b} \boldsymbol{a}^T = \begin{bmatrix} b_1 a_1 & b_1 a_2 & b_1 a_3 \\ b_2 a_1 & b_2 a_2 & b_2 a_3 \\ b_3 a_1 & b_3 a_2 & b_3 a_3 \end{bmatrix} = \begin{bmatrix} a_1 b_1 & a_2 b_1 & a_3 b_1 \\ a_1 b_2 & a_2 b_2 & a_3 b_2 \\ a_1 b_3 & a_2 b_3 & a_3 b_3 \end{bmatrix}$$

$$\mathrm{vec} : [n^{(1)}] \times [n^{(2)}] \to [n^{(1)} \cdot n^{(2)}]$$
$$\mathrm{vec}^{-1} = \mathrm{mat} : [n^{(1)} \cdot n^{(2)}] \to [n^{(1)}] \times [n^{(2)}]$$

more generally,

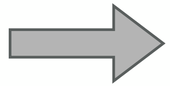
$$(\boldsymbol{A} \otimes \boldsymbol{B}) \, \mathrm{vec}_{\mathrm{col}} (\boldsymbol{X}) = \mathrm{vec}_{\mathrm{col}} \left(\boldsymbol{B} \boldsymbol{X} \boldsymbol{A}^T \right)$$

TensorSketch

Pick hash functions in a decomposable way:

Input has structure $\boldsymbol{v} = \boldsymbol{v}^{(1)} \otimes \boldsymbol{v}^{(2)}$ with sizes $n = n^{(1)} \cdot n^{(2)}$

build small hash functions: $h^{(1)} : [n^{(1)}] \to [m]$, $h^{(2)} : [n^{(2)}] \to [m]$



$$h : [n] \to [m]$$

$$h(j_1, j_2) = h^{(1)}(j_1) + h^{(2)}(j_2) \mod m$$

(we're being loose about how we write the input, since we can use the mat/vec bijection as needed)

Fact: as long as $h^{(i)}$ is fully independent (or at least 3-wise independent), then h is 2-wise independent

TensorSketch

Pick hash functions in a decomposable way:

Input has structure $\boldsymbol{v} = \boldsymbol{v}^{(1)} \otimes \boldsymbol{v}^{(2)}$ with sizes $n = n^{(1)} \cdot n^{(2)}$

build small hash functions: $h^{(1)} : [n^{(1)}] \to [m]$, $h^{(2)} : [n^{(2)}] \to [m]$

$$h : [n] \to [m]$$

$$h(j_1, j_2) = h^{(1)}(j_1) + h^{(2)}(j_2) \mod m$$

Fact: h is 2-wise independent

(we're being loose about how we write the input, since we can use the mat/vec bijection as needed)

same trick for sign functions: $s^{(1)} : [n^{(1)}] \to \{\pm 1\}$, $s^{(2)} : [n^{(2)}] \to \{\pm 1\}$

$$s : [n] \to \{\pm 1\}$$

$$s(j_1, j_2) = s^{(1)}(j_1) \cdot s^{(2)}(j_2)$$

still pairwise independent, as needed for theory!

TensorSketch

what's the point? Huge computational speedup.

$$h^{(1)} : [n^{(1)}] \to [m]$$
$$h^{(2)} : [n^{(2)}] \to [m]$$

$$p^{(1)}(x) \stackrel{\text{def}}{=} \sum_{j \in [n^{(1)}]} s^{(1)}(j) \cdot v_j^{(1)} \cdot x^{h^{(1)}(j)} = \sum_{i \in [m]} u_i^{(1)} \cdot x^i$$
$$p^{(2)}(x) \stackrel{\text{def}}{=} \sum_{j \in [n^{(2)}]} s^{(2)}(j) \cdot v_j^{(2)} \cdot x^{h^{(2)}(j)} = \sum_{i \in [m]} u_i^{(2)} \cdot x^i$$

Let's compute this: $p^{(1)}(x) \cdot p^{(2)}(x) \mod x^m - 1$

TensorSketch

what's the point? Huge computational speedup.

$$p^{(1)}(x) \cdot p^{(2)}(x) = \left(\sum_{j_1 \in [n^{(1)}]} s^{(1)}(j_1) \cdot v_{j_1}^{(1)} \cdot x^{h^{(1)}(j_1)} \right) \cdot \left(\sum_{j_2 \in [n^{(2)}]} s^{(2)}(j_2) \cdot v_{j_2}^{(2)} \cdot x^{h^{(2)}(j_2)} \right)$$

TensorSketch

what's the point? Huge computational speedup.

$$p^{(1)}(x) \cdot p^{(2)}(x) = \left(\sum_{j_1 \in [n^{(1)}]} s^{(1)}(j_1) \cdot v_{j_1}^{(1)} \cdot x^{h^{(1)}(j_1)} \right) \cdot \left(\sum_{j_2 \in [n^{(2)}]} s^{(2)}(j_2) \cdot v_{j_2}^{(2)} \cdot x^{h^{(2)}(j_2)} \right)$$

$$= \sum_{j_1 \in [n^{(1)}], j_2 \in [n^{(2)}]} s^{(1)}(j_1) \cdot s^{(2)}(j_2) \cdot v_{j_1}^{(1)} \cdot v_{j_2}^{(2)} \cdot x^{h^{(1)}(j_1)} \cdot x^{h^{(2)}(j_2)}$$

TensorSketch

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$$p^{(1)}(x) \cdot p^{(2)}(x) = \left(\sum_{j_1 \in [n^{(1)}]} s^{(1)}(j_1) \cdot v_{j_1}^{(1)} \cdot x^{h^{(1)}(j_1)} \right) \cdot \left(\sum_{j_2 \in [n^{(2)}]} s^{(2)}(j_2) \cdot v_{j_2}^{(2)} \cdot x^{h^{(2)}(j_2)} \right)$$

$$= \sum_{j_1 \in [n^{(1)}], j_2 \in [n^{(2)}]} s^{(1)}(j_1) \cdot s^{(2)}(j_2) \cdot v_{j_1}^{(1)} \cdot v_{j_2}^{(2)} \cdot x^{h^{(1)}(j_1)} \cdot x^{h^{(2)}(j_2)}$$

$$= \sum_{j_1 \in [n^{(1)}], j_2 \in [n^{(2)}]} \mathcal{S}(j_1, j_2) \cdot v_{j_1 j_2} \cdot x^{h^{(1)}(j_1) h^{(2)}(j_2)}$$

because input has tensor product structure

because of how we defined our sketch

TensorSketch

what's the point? Huge computational speedup.

$$p^{(1)}(x) \cdot p^{(2)}(x) = \left(\sum_{j_1 \in [n^{(1)}]} s^{(1)}(j_1) \cdot v^{(1)}_{j_1} \cdot x^{h^{(1)}(j_1)} \right) \cdot \left(\sum_{j_2 \in [n^{(2)}]} s^{(2)}(j_2) \cdot v^{(2)}_{j_2} \cdot x^{h^{(2)}(j_2)} \right)$$

$$= \sum_{j_1 \in [n^{(1)}], j_2 \in [n^{(2)}]} s^{(1)}(j_1) \cdot s^{(2)}(j_2) \cdot v^{(1)}_{j_1} \cdot v^{(2)}_{j_2} \cdot x^{h^{(1)}(j_1)} \cdot x^{h^{(2)}(j_2)}$$

$$= \sum_{j_1 \in [n^{(1)}], j_2 \in [n^{(2)}]} \mathcal{S}(j_1, j_2) \cdot v_{j_1 j_2} \cdot x^{h^{(1)}(j_1) h^{(2)}(j_2)}$$

$$\equiv \sum_{j_1 \in [n^{(1)}], j_2 \in [n^{(2)}]} \mathcal{S}(j_1, j_2) \cdot v_{j_1 j_2} \cdot x^{h(j_1, j_2)} \mod x^m - 1$$

$$x^{k\ell} = x^{dm + (k\ell \mod m)} = x^{dm + (k\ell \mod m)} = (x^m)^d x^{k\ell \mod m} \equiv x^{k\ell \mod m} \mod x^m - 1$$

Recall $x^m \equiv 1 \mod x^m - 1$

TensorSketch

what's the point? Huge computational speedup.

$$p^{(1)}(x) \cdot p^{(2)}(x) = \left(\sum_{j_1 \in [n^{(1)}]} s^{(1)}(j_1) \cdot v_{j_1}^{(1)} \cdot x^{h^{(1)}(j_1)} \right) \cdot \left(\sum_{j_2 \in [n^{(2)}]} s^{(2)}(j_2) \cdot v_{j_2}^{(2)} \cdot x^{h^{(2)}(j_2)} \right)$$

$$= \sum_{j_1 \in [n^{(1)}], j_2 \in [n^{(2)}]} s^{(1)}(j_1) \cdot s^{(2)}(j_2) \cdot v_{j_1}^{(1)} \cdot v_{j_2}^{(2)} \cdot x^{h^{(1)}(j_1)} \cdot x^{h^{(2)}(j_2)}$$

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$$\equiv \sum_{j_1 \in [n^{(1)}], j_2 \in [n^{(2)}]} \mathcal{S}(j_1, j_2) \cdot v_{j_1 j_2} \cdot x^{h(j_1, j_2)} \mod x^m - 1$$

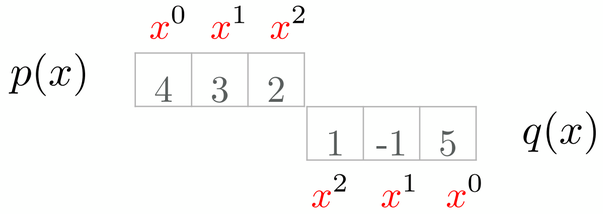
$$= p(x)$$

coefficients are the output of the CountSketch!

TensorSketch

How to multiply polynomials?

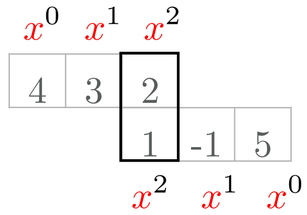
$$\underset{p(x)}{(2x^2 + 3x + 4)} \cdot \underset{q(x)}{(x^2 - x + 5)}$$



TensorSketch

How to multiply polynomials?

$$\left(2x^2 + 3x + 4\right) \cdot \left(x^2 - x + 5\right)$$



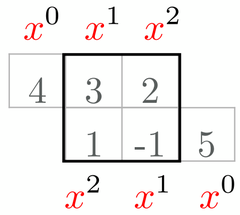
$$= 2x^4$$

$$2 \cdot 1$$

TensorSketch

How to multiply polynomials?

$$\left(2x^2 + 3x + 4\right) \cdot \left(x^2 - x + 5\right)$$



$$= 2x^4 + x^3$$

$$3 \cdot 1 + 2 \cdot (-1) = 1$$

TensorSketch

How to multiply polynomials?

$$(2x^2 + 3x + 4) \cdot (x^2 - x + 5)$$

x^0	x^1	x^2
4	3	2
1	-1	5
x^2	x^1	x^0

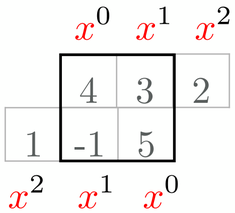
$$= 2x^4 + x^3 + 11x^2$$

$$4 \cdot 1 + 3 \cdot (-1) + 2 \cdot 5 = 11$$

TensorSketch

How to multiply polynomials?

$$\left(2x^2 + 3x + 4\right) \cdot \left(x^2 - x + 5\right)$$



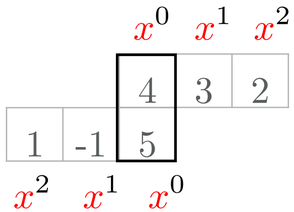
$$= 2x^4 + x^3 + 11x^2 + 11x$$

$$4 \cdot (-1) + 3 \cdot 5 = 11$$

TensorSketch

How to multiply polynomials?

$$\left(2x^2 + 3x + 4\right) \cdot \left(x^2 - x + 5\right)$$



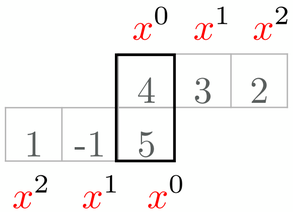
$$= 2x^4 + x^3 + 11x^2 + 11x + 20$$

$$4 \cdot 5 = 20$$

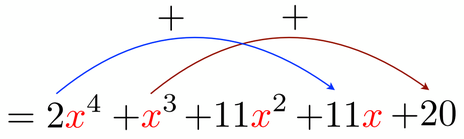
TensorSketch

How to multiply polynomials?

$$(2x^2 + 3x + 4) \cdot (x^2 - x + 5)$$



$$4 \cdot 5 = 20$$



$$\equiv 11x^2 + 13x + 21 \mod x^3 - 1$$

... this is circular convolution!

TensorSketch: complexity analysis

Convolution Theorem (for circular convolutions $*$)

pointwise multiplication

$$\mathcal{F}(g * h) = \mathcal{F}(g)\mathcal{F}(h) \quad \text{i.e.} \quad g * h = \mathcal{F}^{-1}\Big(\mathcal{F}(g)\mathcal{F}(h)\Big)$$

Discrete Fourier Transform (implemented via FFT)

TensorSketch: complexity analysis

Convolution Theorem (for circular convolutions $*$)

$$\mathcal{F}(g * h) = \mathcal{F}(g)\mathcal{F}(h) \quad \text{i.e.} \quad g * h = \mathcal{F}^{-1}\Big(\mathcal{F}(g)\mathcal{F}(h)\Big)$$

Complexity:

$\mathcal{T} : \mathbb{R}^n \to \mathbb{R}^m$

$n = n^{(1)} \cdot n^{(2)}$

CountSketch applied as TensorSketch: $\mathcal{O}(n^{(1)} + n^{(2)} + m \log m)$ vs CountSketch applied naively: $\mathcal{O}(n^{(1)} n^{(2)})$ vs generic dense matrix multiply: $\mathcal{O}(n^{(1)} n^{(2)} m)$

small CountSketches

polynomial multiplication via FFTs

Savings grow as we have more tensor products

If $n = n^{(1)} n^{(2)} \cdots n^{(q)}$

$$\mathcal{O}(n^{(1)} + n^{(2)} + \ldots + n^{(q)} + m \log m) \quad \text{vs} \quad \mathcal{O}(n^{(1)} n^{(2)} \cdots n^{(q)})$$