Recent Advances in Dimensionality Reduction with Provable Guarantees

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July 12, 2018

General setup

We have high-dimensional data, e.g.

- Machine learning. Database of e-mails featurized as high-dimensional vectors; we want to learn a spam classifier.
- ▶ Bioinformatics. Motif discovery in DNA sequences.
- Computational geometry. Fingerprint matching in a large database.
- ▶ Data mining. Clustering similar featurized objects.
- Compression and fast image acquisition. Compressed sensing.
- Large-scale linear algebra. Low-rank approximation or regression on a huge matrix.

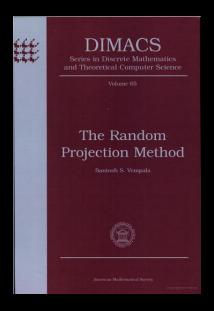
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Can we reduce dimensionality of the data in a pre-processing step, in a way that doesn't disrupt downstream applications?

- ▶ Faster running times (lower dimension = faster algorithms)
- Save space
- ▶ Minimize communication for distributed applications



Random projection method: pick some random linear map, $x \mapsto \Pi x$, and apply Π to input as a pre-processing step

Other dimensionality reduction methods?

- Principal component analysis (PCA)
- Kernel PCA
- Multidimensional scaling
- ISOMAP
- ► Hessian Eigenmaps
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Random projection is orthogonal to, and **complements**, other dimensionality reduction methods. Its purpose is to make other algorithms more efficient, not be the data analysis algorithm. (will say more soon)

Cornerstone dim. reduction/random projections result

JL lemma [Johnson, Lindenstrauss '84]

For every $X \subset \ell_2$ of size n, there is an embedding $f: X \to \ell_2^m$ for $m = O(\varepsilon^{-2} \log n)$ with distortion $1 + \varepsilon$. That is, for each $x, y \in X$,

$$|(1-\varepsilon)||x-y||_2^2 \le ||f(x)-f(y)||_2^2 \le (1+\varepsilon)||x-y||_2^2$$

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Summary: For any n vectors in arbitrary dimension, can map to $O(\log n)$ dim. while approximately preserving Euclidean geometry.

How to prove the JL lemma

Distributional JL (DJL) lemma

Lemma (DJL lemma [Johnson, Lindenstrauss '84])

For any $0 < \varepsilon, \delta < 1/2$ and $d \ge 1$ there exists a distribution $\mathcal{D}_{\varepsilon,\delta}$ on $\mathbb{R}^{m \times d}$ for $m = O(\varepsilon^{-2} \log(1/\delta))$ such that for any $z \in \mathbb{R}^d$

$$\mathop{\mathbb{P}}_{\Pi \sim \mathcal{D}_{\varepsilon, \delta}} \left(\|\Pi z\|_2^2 \notin [(1-\varepsilon)\|z\|_2^2, (1+\varepsilon)\|z\|_2^2] \right) < \delta.$$

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Proof of JL: Set $\delta=1/n^2$ in DJL and z as the difference vector of some pair of points. Union bound over the $\binom{n}{2}$ pairs. Thus the map $f:X\to\ell_2^m$ can be linear: $f(x)=\Pi x$.

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First proof of DJL in [JL'84] took $\mathcal{D}_{\varepsilon,\delta}$ as (scaled) orthogonal projection onto a random m-dimensional subspace.

- What about other, non-Euclidean norms?
- ▶ How fast can we apply the map $x \mapsto \Pi x$?
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(Formal) Theorem [Johnson-Naor'10]. Suppose Z is a normed space satisfying the following property: for every n points $x_1,\ldots,x_n\in Z$ there is a linear subspace $F\subset Z$ of dimension $O(\log n)$ and a linear map $L:Z\to F$ such that $\|x_i-x_j\|\leq \|L(x_i)-L(x_j)\|\leq O(1)\cdot \|x_i-x_j\|$ for all $1\leq i,j\leq n$. Then every k-dimensional subspace of Z embeds into Euclidean space with distortion $2^{2^{O(\log^* k)}}$.

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A lower bound is also shown, that the $2^{2^{O(\log^* k)}}$ term must be $\omega(1)$ (specifically $2^{\Omega(\alpha(k))}$).

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The DJL distribution over Π

Older proofs

- ► [Johnson-Lindenstrauss, 1984], [Frankl-Maehara, 1988]: Random rotation, then projection onto first *m* coordinates.
- ► [Indyk-Motwani, 1998], [Dasgupta-Gupta, 2003]: Random matrix with independent Gaussian entries.
- ► [Achlioptas, 2001]: Independent ±1 entries.
- ► [Clarkson-Woodruff, 2009]: $O(\log(1/\delta))$ -wise independent ± 1 entries.
- ► [Arriaga-Vempala, 1999], [Matousek, 2008]: Independent entries having mean 0, variance 1/m, and subGaussian tails

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Downside: Performing embedding is dense matrix-vector multiplication, $O(m \cdot ||x||_0)$ time

Fast JL Transforms

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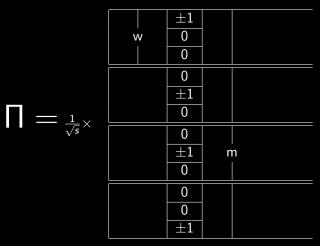
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- ➤ Several follow-up works with technical improvements: [Ailon-Liberty'08], [Ailon-Liberty'11], [Krahmer-Ward'11], [Rudelson-Vershynin'08], [Cheraghchi-Guruswami-Velingker'13], [N.-Price-Wootters'14], [Bourgain'14], [Haviv-Regev'16]

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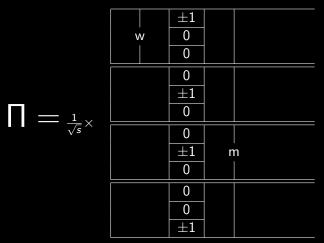
Downside: Slow to embed sparse vectors: running time is $\Omega(\min\{m \cdot ||x||_0, d \log d\})$.

CountSketch [Charikar-Chen-FarachColton'02]



- ▶ partition *m* rows into *s* blocks of size $w = \frac{m}{s}$ each
- \blacktriangleright each column has exactly one $\frac{\pm 1}{\sqrt{s}}$ per block in random location

CountSketch [Charikar-Chen-FarachColton'02]



- ▶ **Note:** can map $x \mapsto \Pi x$ in time $O(s \cdot ||x||_0)$.
- ► [Kane-N.'14] shows $m = O(\varepsilon^{-2} \log n)$, $s = O(\varepsilon m)$ suffices. [N.-Nguyễn'13] shows for this m, such s is almost necessary.
- ► See also [Bourgain-Dirksen-N.'15].

Sparse JL transforms

s=#non-zero entries per column in embedding matrix (so embedding time is $s\cdot \|x\|_0$)

reference	value of <i>s</i>	type
[JL84], [FM88], [IM98],	$mpprox 4arepsilon^{-2}\log(1/\delta)$	dense
[Achlioptas01]	<i>m</i> /3	sparse
		Bernoulli
[WDALS09]	no proof	hashing
[DKS10]	$ ilde{O}(arepsilon^{-1}\log^3(1/\delta))$	hashing
[KN10a]*, [BOR10]*	$ ilde{O}(arepsilon^{-1}\log^2(1/\delta))$	"
[KN14]	$O(arepsilon^{-1}\log(1/\delta))$	CountSketch

^{*} see also recent improvements by [Dahlgaard-Knudsen-Thorup'17], [Freksen-Kamma-Larsen'18].

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Theorem (Jayram-Woodruff, 2011; Kane-Meka-N., 2011) For DJL, $m = \min\{d, \Theta(\varepsilon^{-2} \log(1/\delta))\}$ is optimal.

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(easy direction of "Yao's minimax principle")

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Then show that if \mathcal{F} is the uniform distribution on the sphere and m < d/2, then the probability any fixed $\Pi \in \mathbb{R}^{m \times d}$ fails to preserve x is $\exp(-O(\varepsilon^2 m + 1)) \Longrightarrow m = \Omega(\varepsilon^{-2} \log(1/\delta))$ to succeed.

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JL lower bound

Theorem ([Larsen, Nelson '17])

For any integers $d, n \geq 2$ and any $\frac{1}{(\min\{n,d\})^{0.4999}} < \varepsilon < 1$, there exists a set $X \subset \ell_2^d$, |X| = n, such that any embedding $f: X \to \ell_2^m$ with distortion at most $1 + \varepsilon$ must have

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- ▶ Can always achieve m = n 1: translate so one vector is 0. Then all vectors live in (n 1)-dimensional subspace.

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- **Can always achieve** m = d: f is the identity map.
- ▶ Can always achieve m = n 1: translate so one vector is 0. Then all vectors live in (n 1)-dimensional subspace.
- ▶ So can only hope JL optimal for $\varepsilon^{-2} \log n \le \min\{n, d\}$, can view theorem assumption as $\varepsilon^{-2} \log n \ll \min\{n, d\}^{0.999}$.

over time

Lower bound techniques

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- **Encoding argument.** $m = \Omega(\frac{1}{\epsilon^2} \log n)$ [Larsen, Nelson '17]

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JL is optimal even against non-linear maps

We define a large collection \mathcal{X} of *n*-sized sets $X \subset \mathbb{R}^d$ s.t. if all $X \in \mathcal{X}$ can be embedded into dimension $\leq 10^{-10} \cdot \varepsilon^{-2} \log_2 n$, then there is an encoding of elements of \mathcal{X} into $< \log_2 |\mathcal{X}|$ bits (i.e. an injection from \mathcal{X} to $\{0,1\}^t$ for $t < \log_2 |\mathcal{X}|$). **Contradiction.**

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Encoding procedure based on very simple metric entropy $\/$ convex geometry argument.

OPEN: later [Alon-Klartag'17] showed lower bound of $\Omega(\min\{n, d, \varepsilon^{-2} \log(\varepsilon^2 n)\})$ for full range of ε . Is there a matching

upper bound for $\varepsilon \to 1/\sqrt{n}$?

Some natural questions

(this talk: and some recent answers)

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Total number of bits:

$$O(\log d + \log(1/\delta)(\log\log(1/\delta) + \log(1/\varepsilon))).$$

OPEN: $O(\log d + \log(1/\delta))$?

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Application-specific

k-means: given k and $x_1, \ldots, x_n \in \mathbb{R}^d$, find y_1, \ldots, y_k minimizing

$$\sum_{i=1}^{n} \min_{1 \le j \le k} \|x_i - y_j\|_2^2$$

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Clustering induces a k-partition \mathcal{P} on [n], so want to find best $\mathcal{P} = (P_1, \dots, P_k)$. For fixed \mathcal{P} , best choice of y_i is centroid of P_i .

$$cost(\mathcal{P}) = \sum_{j=1}^{k} \sum_{i \in P_j} \|x_i - \frac{\sum_{t \in P_j} x_t}{|P_j|}\|_2^2$$

$$j=1 \ i \in P_j$$

$$= \sum_{i=1}^k \frac{1}{|P_j|} \sum_{i < i' \in P_i} \|x_i - x_{i'}\|_2^2.$$

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$$= \sum_{i=1}^{k} \frac{1}{|P_j|} \sum_{i < i' \in P_i} \|x_i - x_{i'}\|_2^2.$$

Thus JL embedding f preserves $cost(\mathcal{P})$ for all \mathcal{P} , so can optimize over f(X) ($X = \{x_i\}_{i=1}^n$). Can reduce to dimension $O(\varepsilon^{-2} \log n)$.

[Boutsidis-Zouzias-Mahoney-Drineas'11]: can reformulate k-means as a constrained low-rank approximation problem



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 $Q = \{X_{\mathcal{P}}X_{\mathcal{P}}^{\mathsf{T}} : \mathcal{P} \text{ a } k\text{-partition}\}, \text{ constrained low-rank approx!: }$ want $Q_{opt} = argmin_{Q \in \mathcal{Q}} \|A - QA\|_F^2$,

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Evidence "k" may be log k: [CEMMP'15] shows $O(\log k)$ dimensions suffice for O(1)-approximation. (just can't get down to $1 + \varepsilon$).

Instance-wise bounds

Suppose we have $T \subset S^{d-1}$ and want matrix $\Pi \in \mathbb{R}^{m \times d}$ such that

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- ▶ Gordon showed result for Π having i.i.d. gaussian entries. But what about other Π ?

Dimensionality reduction beyond worst-case analysis

Using Π other than i.i.d. gaussian entries:

► [Klartag-Mendelson'05], [Mendelson-Pajor-TomczakJaegermann'07], [Dirksen'16] i.i.d. subgaussian entries suffice (e.g. $\pm 1/\sqrt{m}$).

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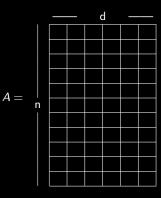
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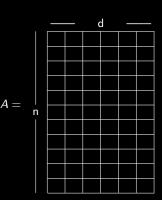
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- [Oymak-Recht-Soltanokotabi'17] Fast JL Transform of Ailon-Chazelle works with similar number of rows, up to log d factors.

More dimensionality reduction: large matrices

Subspace embeddings [Sarlós'06]



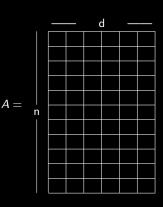
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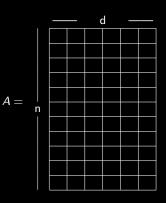
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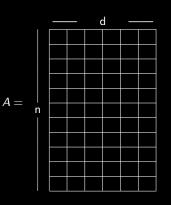


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- Also applications to clustering [BZMD'11], [CEMMP'15], [CNW'16]
 PCA, and many other problems; see

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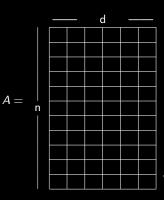
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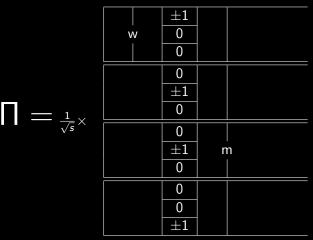
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What Π to use?

E.g. regression want to compute ΠX quickly.

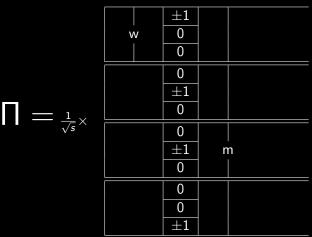


CountSketch [Charikar-Chen-FarachColton'02] (it's me again)



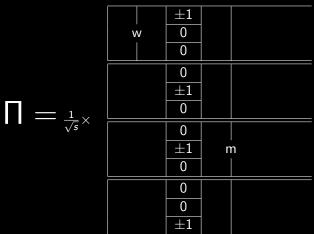
► Analyzed for approx. matrix mult, then regression and PCA, in [Kane-N.'12], [Clarkson-Woodruff'13], [Meng-Mahoney'13], [N.-Nguyễn'13], [BDN'15], [Cohen'16]

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- Leads to algorithms with runtime \approx the sparsity of X

Open problems

- ▶ Instance-wise optimality for ℓ₂ dimensionality reduction?
 What's the right m in terms of X itself? Bicriteria results?
- ▶ JL map that can be applied to x in time $\tilde{O}(m + \|x\|_0)$? $\|\cdot\|_0$ denotes support size
- ► Explicit DJL distribution with seed length $O(\log \frac{d}{\delta})$?
- ▶ Rasmus Pagh: Las Vegas algorithm for computing a JL map for set of n points faster than repeated random projections then checking?