## Dimension Reduction Techniques

for Efficiently Computing Distances in Massive Data

Workshop on Algorithms for Modern Massive Data Sets
June 22, 2006

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## Let's Begin with $\mathrm{AA}^{\top}$

The data matrix $\mathbf{A} \in \mathbb{R}^{n \times D}$ consists of $n$ rows (data points) in $\mathbb{R}^{D}, D$ dimensions (features or attributes).

$\mathrm{A}=$|  | $\mathrm{t}_{1}$ | $\mathrm{t}_{2}$ | $\mathrm{t}_{3}$ | $\mathrm{t}_{4}$ | $\cdots$ | $\mathrm{t}_{\mathrm{D}}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{u}_{1}$ | $*$ | $*$ | $*$ | $*$ | $\cdots$ | $*$ |
| $\mathrm{u}_{2}$ | $*$ | $*$ | $*$ | $*$ | $\cdots$ | $*$ |
| $\mathrm{u}_{3}$ | $*$ | $*$ | $*$ | $*$ | $\ldots$ | $*$ |
| $\mathbf{u}_{4}$ | $*$ | $*$ | $*$ | $*$ | $\cdots$ | $*$ |
| $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ |
| $\mathbf{u}_{\mathrm{n}}$ | $*$ | $*$ | $*$ | $*$ | $\cdots$ | $*$ |

What is the cost of computing $\mathbf{A A}^{\top}$ ?
What if $n=0.6$ million, $D=70$ million?
Why do we care about $\mathbf{A} \mathbf{A}^{\top}$ ?
$O\left(n^{2} D\right)$ A big deal ?
$n^{2} D=2.5 \times 10^{19}$. Take a while!
Useful for a lot of things.

- $\left[\mathbf{A A}^{\top}\right]_{1,2}=u_{1}^{\top} u_{2}=\sum_{j=1}^{D} u_{1, j} u_{2, j}$ is the inner product, an important measure of vector similarity.
- $\left[\mathbf{A A}^{\top}\right]$ is fundamental in distance-based clustering, support vector machine (SVM) kernels, information retrieval, and more.
- An example. Ravichandran et. al. (ACL 2005) found the top similar nouns for each of $n=655,495$ nouns, from a collection of $\mathrm{D}=70$ million Web pages. Brute-force $O\left(n^{2} D\right) \approx 10^{19}$ may take forever. They used random projections.

Other similarity or dissimilarity measures

- $l_{2}$ distance: $\left\|u_{1}-u_{2}\right\|_{2}^{2}=\sum_{j=1}^{D}\left(u_{1, j}-u_{2, j}\right)^{2}$.
- $l_{1}$ distance: $\left\|u_{1}-u_{2}\right\|_{1}=\sum_{j=1}^{D}\left|u_{1, j}-u_{2, j}\right|$
- Multi-way inner product: $\sum_{j=1}^{D} u_{1, j} u_{2, j} u_{3, j}$


## Let's Approximate $\mathrm{AA}^{\top}$ and Other Distances

Many reasons why approximation is a good idea.

- Exact computation could be practically infeasible.
- Often do not need exact answers. Distances are used by other tasks such as clustering, retrieval, and ranking, which introduce errors.
- An approximate solution may help finding the exact solution more efficiently. Example: Databases query optimization


## What Are Real Data Like?: Google Page Hits

|  | Query | Hits (Google) |
| :--- | :--- | ---: |
|  | A | $22,340,000,000$ |
| Function words | The | $20,980,000,000$ |
| Frequent words | Country | $2,290,000,000$ |
|  | Knuth | $5,530,000$ |
| Names | "John Nash" | $1,090,000$ |
|  | Kalevala | $1,330,000$ |
| Rare words | Griseofulvin | 423,000 |

- Term-by-document matrix ( $n$ by $D$ ) is huge, and highly sparse
- Approx $n=10^{7}$ (interesting) words/items
- Approx $D=10^{10}$ Web pages (indexed)
- Lots of large counts (even for so-called rare words)


## Outline of the Talk

- Two strategies (besides SVD) for dimension reduction:
- Sampling
- Sketching
- Normal random projections (for $l_{2}$ ).
- Cauchy random projections (for $l_{1}$ ). A case study on Microarray Data.
- Conditional Random Sampling (CRS), a new sketching algorithm for sparse data: Sampling + sketching
- Comparisons.


## Strategies for Dimension Reduction: Sampling and Sketching

Sampling: Randomly pick $k$ (out of $D$ ) columns from the data matrix $\mathbf{A}$.

$\mathbf{A} \in \mathbb{R}^{n \times D} \Longrightarrow \tilde{\mathbf{A}} \in \mathbb{R}^{n \times k}$ $\left(u_{1}^{\top} u_{2}=\sum_{j=1}^{D} u_{1, j} u_{2, j}\right) \approx\left(\tilde{u}_{1}^{\top} \tilde{u}_{2}=\sum_{j=1}^{k} \tilde{u}_{1, j} \tilde{u}_{2, j}\right) \times \frac{D}{k}$

- Pros: Simple, popular, generalizes beyond approximating distances
- Cons: No accuracy guarantee. Large errors for worst case (heavy-tailed distributions). Mostly "zeros" in sparse data.

Sketching: Scan the data; compute specific summary statistics; repeat $k$ times.

(Know everything about the margins: means, moments, \# of non-zeros)
Two well-known examples of sketching algorithms

- Random Projections
- Broder's min-wise sketches.

A new algorithm

- Conditional Random Sampling (CRS): sampling + sketching, a hybrid method


## Random Projections: A Brief Introduction

Let $\mathbf{B}=\mathbf{A R}, \quad \mathbf{A} \in \mathbb{R}^{n \times D}$ is the original data matrix. $\mathbf{R} \in \mathbb{R}^{D \times k}$ is the random projection matrix. $\mathbf{B} \in \mathbb{R}^{n \times k}$ is the projected data.


Estimate original distances from B. (Vempala 2004, Indyk FOCS00,01)

- For $l_{2}$ distance, use $\mathbf{R}$ with entries of i.i.d. Normal $N(0,1)$.
- For $l_{1}$ distance, use $\mathbf{R}$ with entries of i.i.d. Cauchy $C(0,1)$.

Computational cost: $O(n D k)$ for generating the sketch $\mathbf{B}$.
$O\left(n^{2} k\right)$ for computing all pairwise distances. $k \ll \min (n, D)$.
$O\left(n D k+n^{2} k\right)$ is a huge reduction, from $O\left(n^{2} D\right)$.

## Normal Random Projections: $l_{2}$ Distance Preserving Properties

Notation: $\mathbf{B}=\frac{1}{\sqrt{k}} \mathbf{A R}$, $\mathbf{R}=\left\{r_{j i}\right\} \in \mathbb{R}^{D \times k}, r_{j i}$ i.i.d. $N(0,1)$.

- $u_{1}, u_{2} \in \mathbb{R}^{D}$, first two rows in $\mathbf{A}$.
- $v_{1}, v_{2} \in \mathbb{R}^{k}$, first two rows in $\mathbf{B}$.
$\mathbf{B B}^{\top} \approx \mathbf{A} \mathbf{A}^{\top}$. In fact, $\mathrm{E}\left(\mathbf{B B}^{\top}\right)=\mathbf{A} \mathbf{A}^{\top}$, in the expectations.
Projected data $\left(v_{1, i}, v_{2, i}\right)(\mathrm{i}=1,2, \ldots, k)$ are i.i.d. samples of a bivariate normal

$$
\left[\begin{array}{c}
v_{1, i} \\
v_{2, i}
\end{array}\right] \sim N\left(\left[\begin{array}{l}
0 \\
0
\end{array}\right], \frac{1}{k}\left[\begin{array}{cc}
m_{1} & a \\
a & m_{2}
\end{array}\right]\right)
$$

Margins: $\quad m_{1}=\left\|u_{1}\right\|^{2}, \quad m_{2}=\left\|u_{2}\right\|^{2}$,
Inner Product: $\quad a=u_{1}^{\top} u_{2}$,
$l_{2}$ distance: $\quad d=\left\|u_{1}-u_{2}\right\|^{2}=m_{1}+m_{2}-2 a$.

$$
\left[\begin{array}{l}
v_{1, i} \\
v_{2, i}
\end{array}\right] \sim N\left(\left[\begin{array}{l}
0 \\
0
\end{array}\right], \frac{1}{k}\left[\begin{array}{cc}
m_{1} & a \\
a & m_{2}
\end{array}\right]\right)
$$

Linear estimators (sample distances are unbiased for original distances)

$$
\begin{array}{ll}
\hat{a}=v_{1}^{\top} v_{2}=\sum_{i=1}^{k} v_{1, i} v_{2, i}, & \mathrm{E}(\hat{a})=a \\
\hat{d}=\left\|v_{1}-v_{2}\right\|^{2}=\sum_{i=1}^{k}\left(v_{1, i}-v_{2, i}\right)^{2}, & \mathrm{E}(\hat{d})=d
\end{array}
$$

However
Marginal norms $m_{1}=\left\|u_{1}\right\|^{2}, m_{2}=\left\|u_{2}\right\|^{2}$ can be computed exactly $\mathbf{B B}^{\top} \approx \mathbf{A A}^{\top}$, but at least we can make the diagonals exact (easily).
And off-diagonals can be improved (a little bit more work)

## Margin-constrained Normal Random Projections

$$
\left[\begin{array}{l}
v_{1, i} \\
v_{2, i}
\end{array}\right] \sim N\left(\left[\begin{array}{l}
0 \\
0
\end{array}\right], \frac{1}{k}\left[\begin{array}{cc}
m_{1} & a \\
a & m_{2}
\end{array}\right]\right)
$$

Linear estimator and its variance

$$
\hat{a}=v_{1}^{\top} v_{2}, \quad \operatorname{Var}(\hat{a})=\frac{1}{k}\left(m_{1} m_{2}+a^{2}\right)
$$

If the margins $m_{1}$ and $m_{2}$ are known; a maximum likelihood estimator, $\hat{a}_{M L E}$, is the solution to a cubic equation:
$a^{3}-a^{2}\left(v_{1}^{\top} v_{2}\right)+a\left(-m_{1} m_{2}+m_{1}\left\|v_{2}\right\|^{2}+m_{2}\left\|v_{1}\right\|^{2}\right)-m_{1} m_{2} v_{1}^{\top} v_{2}=0$,
Consequently, an MLE for the distance $\hat{d}_{M L E}=m_{1}+m_{2}-2 \hat{a}_{M L E}$.

The (asymptotic) variance of the MLE:

$$
\operatorname{Var}\left(\hat{a}_{M L E}\right)=\frac{1}{k} \frac{\left(m_{1} m_{2}-a^{2}\right)^{2}}{m_{1} m_{2}+a^{2}} \leq \operatorname{Var}(\hat{a})=\frac{1}{k}\left(m_{1} m_{2}+a^{2}\right)
$$

Substantial improvement when the data are strongly correlated ( $a^{2} \approx m_{1} m_{2}$ ). But does not help when $a \approx 0$.

Next, Cauchy random projections for $l_{1} \ldots$

## Cauchy Random Projections for $l_{1}$

$$
\mathbf{B}=\mathbf{A R}, \quad \mathbf{R}=\left\{r_{j i}\right\} \in \mathbb{R}^{D \times k}, r_{j i} \text { i.i.d. } C(0,1) .
$$

- $u_{1}, u_{2} \in \mathbb{R}^{D}$, first two rows in $\mathbf{A}$.
- $v_{1}, v_{2} \in \mathbb{R}^{k}$, first two rows in $\mathbf{B}$.

The projected data are Cauchy distributed.
$v_{1, i}-v_{2, i}=\sum_{j=1}^{D}\left(u_{1, j}-u_{2, j}\right) r_{j i} \sim C\left(0, \sum_{j=1}^{D}\left|u_{1, j}-u_{2, j}\right|=d\right)$

Linear estimator fails! (Charikar et. al, FOCS03, JACM05)
$\hat{d}=\frac{1}{k} \sum_{i=1}^{k}\left|v_{1, i}-v_{2, i}\right|, \quad$ does not work. $\quad \mathrm{E}\left|v_{1, i}-v_{2, i}\right|=\infty$.

However, if only interested in approximating distances, then ...

## Cauchy Random Projections: Our Results

- Many applications (e.g., clustering, SVM kernels) only need the distances, linear or nonlinear estimators do not really matter.
- Statistically, we need to estimate the scale parameter of Cauchy, from $k$ i.i.d. samples of $C(0, d): v_{1, i}-v_{2, i}, i=1,2, \ldots, k$.

Two nonlinear estimators:

- A new unbiased estimator is derived, which exhibits exponential tail bounds; (hence an analog of JL bound for $l_{1}$ exists, in a sense.)
- The MLE is even better. A highly accurate approximation is proposed for the distribution of the MLE, which does not have closed-from distribution.


## Cauchy Random Projections: The Procedure

Estimation Method $\quad$ The original $l_{1}$ distance $d=\left|u_{1}-u_{2}\right|$ is estimated from the projected data, $v_{1, i}-v_{2, i}, i=1,2, \ldots, k$, by

$$
\hat{d}_{1}=\hat{d}\left(1-\frac{1}{k}\right)
$$

where $\hat{d}$ solves the nonlinear MLE equation

$$
-\frac{k}{d}+\sum_{i=1}^{k} \frac{2 d}{\left(v_{1, i}-v_{2, i}\right)^{2}+d^{2}}=0
$$

by iterative methods, starting with the following initial guess

$$
\hat{d}_{g m}=\cos ^{k}\left(\frac{\pi}{2 k}\right) \prod_{i=1}^{k}\left|v_{1, i}-v_{2, i}\right|^{\frac{1}{k}}
$$

## Cauchy Random Projections: An Unbiased Estimator

$$
\hat{d}_{g m}=\cos ^{k}\left(\frac{\pi}{2 k}\right) \prod_{i=1}^{k}\left|v_{1, i}-v_{2, i}\right|^{1 / k}, \quad k>1
$$

is unbiased, with the variance (valid when $k>2$ )

$$
\operatorname{Var}\left(\hat{d}_{g m}\right)=\frac{\pi^{2}}{4} \frac{d^{2}}{k}+O\left(\frac{1}{k^{2}}\right)
$$

The $\frac{\pi^{2}}{4 k} \approx \frac{2.5}{k}$ implies that $\hat{d}_{g m}$ is $80 \%$ efficient, as the MLE has variance in terms of $\frac{2.0}{k}$.

## Cauchy Random Projections: Tail Bounds

If we restrict that $0 \leq \epsilon<1$, the following exponential tail bounds hold:

$$
\begin{aligned}
& \operatorname{Pr}\left(\hat{d}_{g m} \geq(1+\epsilon) d\right) \leq \exp \left(-k \frac{\epsilon^{2}}{8(1+\epsilon)}\right) \\
& \operatorname{Pr}\left(\hat{d}_{g m} \leq(1-\epsilon) d\right) \leq \exp \left(-k \frac{\epsilon^{2}}{20}\right), \quad k>\frac{\pi^{2}}{4 \epsilon}
\end{aligned}
$$

An analog of the JL bound follows by restricting $\operatorname{Pr}\left(\left|\hat{d}_{g m}-d\right| \geq \epsilon d\right) \leq \xi / \nu$ with $\nu=\frac{n^{2}}{2}$, (e.g.,) $\xi=0.05$.

Comments

- These bounds are not tight. (we have more tight bounds)
- Without the restriction $\epsilon<1$, the exponential bounds do not exist.
- We prefer the exponential bounds of the MLE.


## Cauchy Random Projections: MLE

The maximum likelihood estimator $\hat{d}$ is the solution to

$$
-\frac{k}{d}+\sum_{i=1}^{k} \frac{2 d}{\left(v_{1, i}-v_{2, i}\right)^{2}+d^{2}}=0
$$

We suggest the bias-corrected version based on (Bartlett, Biometrika 53):

$$
\hat{d}_{1}=\hat{d}\left(1-\frac{1}{k}\right)
$$

What about the distribution?

- Need the distribution of $\hat{d}_{1}$ to select sample size $k$.
- The distribution of $\hat{d}_{1}$ can not be characterized exactly,
- We can at least study the asymptotic moments.


## Cauchy Random Projections: MLE Moments

The first four (asymptotic) moments of the $\hat{d}_{1}$ are

$$
\begin{aligned}
& \mathrm{E}\left(\hat{d}_{1}-d\right)=O\left(\frac{1}{k^{2}}\right) \\
& \operatorname{Var}\left(\hat{d}_{1}\right)=\frac{2 d^{2}}{k}+\frac{3 d^{2}}{k^{2}}+O\left(\frac{1}{k^{3}}\right) \\
& \mathrm{E}\left(\hat{d}_{1}-\mathrm{E}\left(\hat{d}_{1}\right)\right)^{3}=\frac{12 d^{3}}{k^{2}}+O\left(\frac{1}{k^{3}}\right) \\
& \mathrm{E}\left(\hat{d}_{1}-\mathrm{E}\left(\hat{d}_{1}\right)\right)^{4}=\frac{12 d^{4}}{k^{2}}+\frac{186 d^{4}}{k^{3}}+O\left(\frac{1}{k^{4}}\right)
\end{aligned}
$$

by carrying out the horrible algebra in (Shenton, JORSS 63).
Magic: They match the first four moments of an inverse Gaussian distribution, which has the same support as $\hat{d}_{1},[0, \infty]$.

## Cauchy Random Projections: Inverse Gaussian Approximation

Assume $\hat{d}_{1} \sim I G(\alpha, \beta)$, with $\alpha=\frac{1}{\frac{2}{k}+\frac{3}{k^{2}}}, \quad \beta=\frac{2 d}{k}+\frac{3 d}{k^{2}}$.
The moments

$$
\begin{aligned}
& \mathrm{E}\left(\hat{d}_{1}\right)=d, \quad \operatorname{Var}\left(\hat{d}_{1}\right)=\frac{2 d^{2}}{k}+\frac{3 d^{2}}{k^{2}} \\
& \mathrm{E}\left(\hat{d}_{1}-\mathrm{E}\left(\hat{d}_{1}\right)\right)^{3}=\frac{12 d^{3}}{k^{2}}+O\left(\frac{1}{k^{3}}\right) \\
& \mathrm{E}\left(\hat{d}_{1}-\mathrm{E}\left(\hat{d}_{1}\right)\right)^{4}=\frac{12 d^{4}}{k^{2}}+\frac{156 d^{4}}{k^{3}}+O\left(\frac{1}{k^{4}}\right)
\end{aligned}
$$

The exact (asymptotic) fourth moment of $\hat{d}_{1}=\frac{12 d^{4}}{k^{2}}+\frac{186 d^{4}}{k^{3}}+O\left(\frac{1}{k^{4}}\right)$

The density

$$
\operatorname{Pr}\left(\hat{d}_{1}=y\right)=\sqrt{\frac{\alpha d}{2 \pi}} y^{-\frac{3}{2}} \exp \left(-\frac{(y-d)^{2}}{2 y \beta}\right)
$$

The Chernoff bounds

$$
\begin{array}{ll}
\operatorname{Pr}\left(\hat{d}_{1} \geq(1+\epsilon) d\right) \leq \exp \left(-\frac{\alpha \epsilon^{2}}{2(1+\epsilon)}\right), & \epsilon \geq 0 \\
\operatorname{Pr}\left(\hat{d}_{1} \leq(1-\epsilon) d\right) \leq \exp \left(-\frac{\alpha \epsilon^{2}}{2(1-\epsilon)}\right), & 0 \leq \epsilon<1
\end{array}
$$

A symmetric bound

$$
\operatorname{Pr}\left(\left|\hat{d}_{1}-d\right| \geq \epsilon d\right) \leq 2 \exp \left(-\frac{\alpha \epsilon^{2}}{2(1+\epsilon)}\right), \quad 0 \leq \epsilon<1
$$

A JL-type of Bound (Derived by approximation, verified by simulations) A JL-type of bound follows by letting $\operatorname{Pr}\left(\left|\hat{d}_{1}-d\right|>\epsilon d\right) \leq \xi / \nu$,

$$
k \geq \frac{4.4(\log 2 \nu-\log \xi)}{\epsilon^{2} /(1+\epsilon)}
$$

This holds at least for $\xi / \nu \geq 10^{-10}$, verified by simulations.
(Why the $95 \%$ normal quantile $=1.645$ ?)

## Cauchy Random Projections: Simulations

Tail probability $\operatorname{Pr}\left(\left|\hat{d}_{1}-d\right|>\epsilon d\right)$


The inverse Gaussian approximation is remarkably accurate.

Tail bound

$$
\operatorname{Pr}\left(\left|\hat{d}_{1}-d\right|>\epsilon d\right) \leq \exp \left(-\frac{\alpha \epsilon^{2}}{2(1+\epsilon)}\right)+\exp \left(-\frac{\alpha \epsilon^{2}}{2(1-\epsilon)}\right), \quad 0 \leq \epsilon<1 .
$$



The inverse Gaussian Chernoff bound is reliable at least for $\xi / \nu \geq 10^{-10}$.

## A Case Study on Microarray Data

Harvard Dataset (PNAS 2001, thank Wing H. Wong): 176 specimen, 3 classes, 12600 genes.

Only 2 (out of 176) specimen were misclassified, by a 5 -nearest neighbor classifer using $l_{1}$ distances in 12600 dimensions.

Using Cauchy random projections and both nonlinear estimators, the dimension can be reduced from 12600 to 100, with little loss in accuracy.

Two error measures:

- Median (among $176 \times 175 / 2=15488$ pairs) absolute errors of estimated $l_{1}$ distances, normlized by original median $l_{1}$ distance.
- Number of misclassifications.

Left: Distance errors


Right: Misclassifications


- When $k=100$, relative absolute distance error about $10 \%$.
- When $k=100$, number of misclassifications $<5$.
- MLE is about $10 \%$ better than GM (unbiased estimator) in distance errors, as expected.
- MLE is about $5 \%-10 \%$ better than GM in misclassifications.


## Summary for Cauchy Random Projections

- Linear projections + linear estimators do not work well (impossibility results).
- Linear projections + nonlinear estimators are available and suffice for many applications (e.g., clustering, SVM kernels, information retrieval).
- Analog of JL bound in $l_{1}$ exists (in a sense), proved using an unbiased nonlinear estimator
- The MLE is even better. Highly accurate and convenient closed-form approximations of the tail bounds are practically useful.

So far so good...

## Limitations of Random Projections

- Designed for specific summary statistics ( $l_{1}$ or $l_{2}$ )
- Limited to two-way (pairwise) distances

What about sampling?

- Suitable for any norm and multi-way
- Most samples are zeros, in sparse data
- Possibly large errors in heavy-tailed data

Conditional Random Sampling (CRS): A sketch-based sampling algorithm.
Directly exploit data sparsity

## Conditional Random Sampling (CRS): A Global View



## Conditional Random Sampling (CRS): An Example

Random Sampling on Data Matrix $\mathbf{A}$ : If columns are random, first $D_{s}=10$ columns constitute a random sample.

$$
\begin{array}{c|cccccccccc:cccccc} 
& 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 \\
\hline \mathrm{u}_{1} & 0 & 3 & 0 & 2 & 0 & 1 & 0 & 0 & 1 & 2 & 1 & 0 & 1 & 0 & 2 & 0 \\
\mathrm{u}_{2} & 1 & 4 & 0 & 0 & 1 & 2 & 0 & 1 & 0 & 0 & 3 & 0 & 0 & 2 & 1 & 1
\end{array}
$$

Postings P: Only store non-zeros, "ID (Value)," sorted ascending by the IDs.

$$
\begin{array}{rllllllllll}
\mathrm{P}_{1}: & 2(3) & 4(2) & 6(1) & 9(1) & 10(2) & 11(1) & 13(1) & 15(2) \\
\mathrm{P}_{2}: & 1(1) & 2(4) & 5(1) & 6(2) & 8(1) & 11(3) & 14(2) & 15(1) & 16(1)
\end{array}
$$

Sketches K : A sketch, $\mathrm{K}_{i}$, of postings $\mathrm{P}_{i}$, is the first $k_{i}$ entries of $\mathrm{P}_{i}$. Suppose $k_{1}=5, k_{2}=6$.

$$
\begin{aligned}
& \mathrm{K}_{1}: \\
& \mathrm{K}_{2}: \\
& \hline
\end{aligned} 1(3)
$$

What if remove the entry $11(3) ? \ldots$ We get random samples.

Exclude all elements of sketches whose IDs are larger than

$$
\begin{aligned}
D_{s} & =\min \left(\max \left(\operatorname{ID}\left(\mathrm{K}_{1}\right)\right), \max \left(\operatorname{ID}\left(\mathrm{K}_{2}\right)\right)\right) \\
& =\min (10,11)=10,
\end{aligned}
$$

Obtain exactly the same samples as if directly sampled the first $D_{s}$ columns.

This converts sketches into random samples by conditioning on $D_{s}$, different pairwise (or group-wise), and not known beforehand.

For example, when estimating pairwise distances for all $n$ data points, we will have $\frac{n(n-1)}{2}$ different values of $D_{s}$.

Sketch size $k_{i}$ can be small, but the effective sample $D_{s}$ could be very large. The more sparse, the better.

## Conditional Random Sampling (CRS): Procedure

Our algorithm consists of the following steps:

- A random permutation on the data column IDs to ensure randomness.
- Construct sketches for all data points, i.e. finding $k_{i}$ entries with the smallest IDs after permutation. Need a linear scan (hence called sketches).
- Construct conditional random samples from sketches online pairwise (or group-wise). Compute $D_{s}$. Estimate the original space by scaling ( $\frac{D}{D_{s}}$ ) any sample distances. (We can do better than that...)

Take advantage of the margins for sharper estimates (MLE):

- In 0/1 data, numbers of non-zeros ( $f_{i}$, document frequency) are known. The MLE amounts to estimating two-way contingency tables with margin constraints. The solution is a cubic equation.
- In general real-valued data, $f_{i}$, marginal norms, marginal means are known. The MLE amounts to a cubic equation (assuming normality, works well).


## Variances: CRS V.S. Random Projections (RP)

$u_{1}, u_{2} \in \mathbf{R}^{D}$, Inner Product $a=u_{1}^{\top} u_{2}, \quad \hat{a}_{C R S}$ v.s. $\hat{a}_{R P}$ (not using margins).
$\operatorname{Var}\left(\hat{a}_{C R S}\right)=\frac{\max \left(f_{1}, f_{2}\right)}{D} \frac{1}{k}\left(D \sum_{j=1}^{D} u_{1, j}^{2} u_{2, j}^{2}-a^{2}\right)$
$\operatorname{Var}\left(\hat{a}_{R P}\right)=\frac{1}{k}\left(\sum_{j=1}^{D} u_{1, j}^{2} \sum_{j=1}^{D} u_{2, j}^{2}+a^{2}\right)$
Sparsity: $f_{1}$ and $f_{2}$ are numbers of non-zeros. Often $\frac{\max \left(f_{1}, f_{2}\right)}{D}<1 \%$
$D \sum_{j=1}^{D} u_{1, j}^{2} u_{2, j}^{2}>\sum_{j=1}^{D} u_{1, j}^{2} \sum_{j=1}^{D} u_{2, j}^{2}$ usually, $\gg$ in heavy-tailed data.

When $u_{1}$ and $u_{2}$ are independent, by law of large numbers
$D \sum_{j=1}^{D} u_{1, j}^{2} u_{2, j}^{2} \approx \sum_{j=1}^{D} u_{1, j}^{2} \sum_{j=1}^{D} u_{2, j}^{2}$,
then $\operatorname{Var}\left(\hat{a}_{C R S}\right)<\operatorname{Var}\left(\hat{a}_{R P}\right)$, even ignoring sparsity.
In boolean ( $0 / 1$ ) data ...

## CRS V.S. RP in Boolean Data

CRS are always better in boolean data. The ratio $\frac{\operatorname{Var(CRS)}}{\operatorname{Var}(\mathrm{RP})}$ is always $<1$, when both do not use marginal information.




$f_{1}$ and $f_{2}$ are the numbers of non-zeros in $u_{1}$ and $u_{2}$.

When both use margins, the ratio $\frac{\operatorname{Var(CRS)}}{\operatorname{Var}(\mathrm{RP})}$ is $<1$ almost always, unless $u_{1}$ and $u_{2}$ are almost identical.


## Empirical Evaluations of CRS and RP

Data (Each has total $\frac{n(n-1)}{2}$ pairs of distances)

|  | $n$ | $D$ | Sparsity | Kurtosis | Skewness |
| :--- | ---: | ---: | ---: | ---: | ---: |
| NSF | 100 | 5298 | $1.09 \%$ | 349.8 | 16.3 |
| NEWSGROUP | 100 | 5000 | $1.01 \%$ | 352.9 | 16.5 |
| COREL | 80 | 4096 | $4.82 \%$ | 765.9 | 24.7 |
| MSN (original) | 100 | 65536 | $3.65 \%$ | 4161.5 | 49.6 |
| MSN (square root) | 100 | 65536 | $3.65 \%$ | 175.3 | 10.7 |
| MSN (logarithmic) | 100 | 65536 | $3.65 \%$ | 111.8 | 9.5 |

- NEWSGROUP and NSF (thank Bingham and Dhillon): document distance
- COREL: Image histogram distance
- MSN : Word distance,
- Median sample kurtosis and skewness, (heavy-tailed, highly-skewed)

Variable sketch size for CRS
We could adjust sketch sizes according to data sparsity. Sample more from the more frequent ones.

Evaluation metric
Among the $\frac{n(n-1)}{2}$ pairs, the percentage for which CRS does better than random projections. Want $>0.5$

Results...

NSF Data: Conditional Random Sampling (CRS) is overwhelmingly better than Random Projections (RP).


Dashed: Fixed sample size, Solid: Variable sketch size

NEWSGROUP Data: CRS is overwhelmingly better than RP.


COREL Image Data: $\quad$ CRS are still better than RP for inner product and $l_{2}$ distance (using margins)


|  | $n$ | $D$ | Sparsity | Kurtosis | Skewness |
| :--- | ---: | ---: | ---: | ---: | ---: |
| NSF | 100 | 5298 | $1.09 \%$ | 349.8 | 16.3 |
| NEWSGROUP | 100 | 5000 | $1.01 \%$ | 352.9 | 16.5 |
| COREL | 80 | 4096 | $4.82 \%$ | 765.9 | 24.7 |
| MSN (original) | 100 | 65536 | $3.65 \%$ | 4161.5 | 49.6 |
| MSN (square root) | 100 | 65536 | $3.65 \%$ | 175.3 | 10.7 |
| MSN (logarithmic) | 100 | 65536 | $3.65 \%$ | 111.8 | 9.5 |

MSN Data (original): CRS do better than RP in inner product and $l_{2}$ distance (using margins)


MSN Data (square root): After transformation (as in practice), CRS do better than RP in inner product, $l_{1}$ and $l_{2}$ (using margins)


## Summary of the Empirical Comparisons

Conditional Random Sampling (CRS) v.s. Random Projections (RP)

- CRS are particularly well-suited for inner products.
- CRS are often comparable to Cauchy random projections for $l_{1}$ distances.
- Using the margins, CRS are also effectively for $l_{2}$ distances.
- Can adjust the sketch size according to the data sparsity, which in general improves the overall performance.
- Using a fixed sketch size, then the less freqent (but often more interesting) items are emphasized.


## Conclusions

- Too much data (although never enough)
- Compact data representations
- Accurate approximation algorithms (estimators)
- Dimension Reduction Techniques (in addition to SVD)
- Random sampling
- Sketching (e.g., normal and Cauchy random projections)
- Conditional Random Sampling (sampling + sketching)
- Improve normal random projection (for $l_{2}$ ) using margins by nonlinear MLE.
- Propose nonlinear estimators for Cauchy random projections for $l_{1}$.
- Conditional Random Sampling (CRS), for sparse data and 0/1 data
- Flexible (can adjust sample size according to sparsity)
- Good for estimating inner products
- Easy to take advantage of margins.


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