Randomized Algorithms in Data Mining: a Linear Algebraic Approach

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> To access my web page: Google drineas

Why linear algebra?

Data are represented by matrices (or tensors)

Numerous modern datasets are in matrix form.

Data in the form of tensors (multi-mode arrays) have become very common in the data mining and information retrieval literature in the last few years.

<u>Goal</u>

Learn a model for the underlying "physical" system generating the data.

<u>Toolbox</u>

Linear algebra (and numerical analysis) provide the fundamental mathematical and algorithmic tools to deal with matrix and tensor computations.

Tool: matrix decompositions

Matrix decompositions

(e.g., SVD, QR, SDD, CX and CUR, NMF, etc.)

- They use the relationships between the available data in order to identify components of the underlying physical system generating the data.
- Some assumptions on the relationships between the underlying components are necessary.
- Very active area of research; some matrix decompositions are more than one century old, whereas others are very recent.

Randomized algorithms

<u>**Randomization and sampling</u>** allow us to design provably accurate algorithms for problems that are:</u>

> Massive

(e.g., matrices so large that can not be stored at all, or can only be stored in slow, secondary memory devices)

Computationally expensive or NP-hard

(e.g., combinatorial optimization problems such as the Column Subset Selection Problem and the related CX factorization)

Randomized algorithms & Linear Algebra

Randomized algorithms

• By (carefully) sampling rows/columns/entries of a matrix, we can construct new matrices (that have smaller dimensions or are sparse) and have bounded distance (in terms of some matrix norm) from the original matrix (with some failure probability).

• By preprocessing the matrix using random projections (*), we can sample rows/columns/ entries(?) much less carefully (uniformly at random) and still get nice bounds (with some failure probability).

(*) Alternatively, we can assume that the matrix is "well-behaved" and thus uniform sampling will work.

Randomized algorithms & Linear Algebra

Randomized algorithms

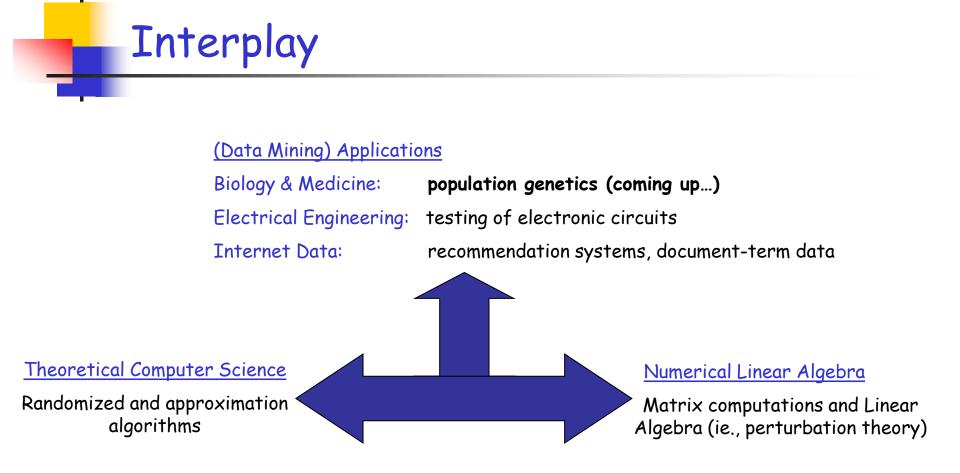
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• By preprocessing the matrix using random projections, we can sample rows/columns/ entries(?) much less carefully (uniformly at random) and still get nice bounds (with some failure probability).

Matrix perturbation theory

• The resulting smaller/sparser matrices behave similarly (in terms of singular values and singular vectors) to the original matrices thanks to the norm bounds.

In this talk, I will illustrate some applications of the above ideas.



Human genetics

Single Nucleotide Polymorphisms: the most common type of genetic variation in the genome across different individuals.

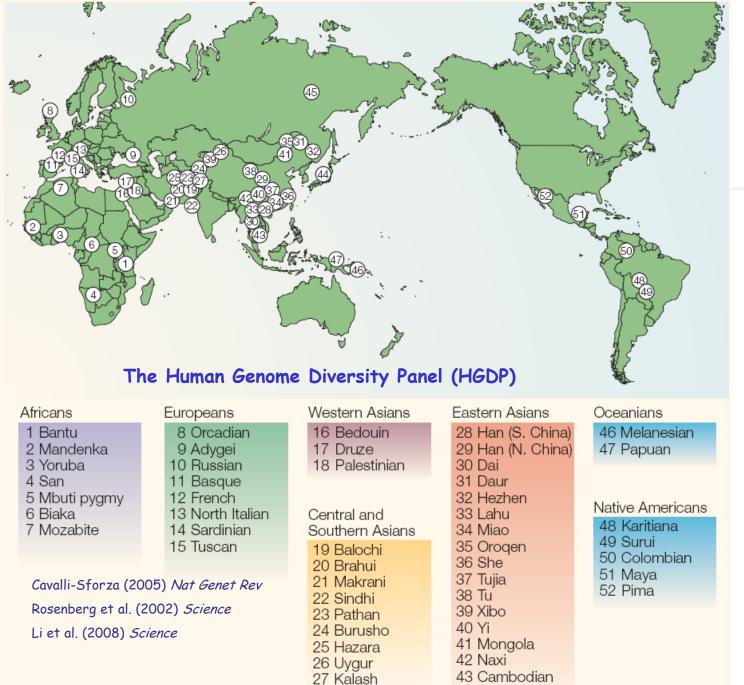
They are known locations at the human genome where two alternate nucleotide bases (alleles) are observed (out of A, C, G, T).

SNPs

individuals

... AG CT GT GG CT CC CC CC AG AG AG AG AG AG AA CT AA GG GG CC GG AG CG AC CC AA CC AA GG TT AG CT CG CG CG AT CT CT AG CT AG GG GT GA AG GG TT TT GG TT CC CC CC CG GA AG AG AG AA AG AG AG CT AA GG GG CC GG AA GG AA CC AA CC AA GG TT AG CT CG CG CG AT CT CT AG CT AG GG GT GA AG GG TT TT GG TT CC CC CC CG GA AG AG AG AA AG CT AA GG GG CC AG AG CG AC CC AA CC AA GG TT AG CT CG CG CG AT CT CT AG CT AG GT GA AG GG TT TT GG TT CC CC CC CC GG AA AG AG AG AA CC GG AA CC CA AG GC AC CC AA CC AA GG TT AG CT CG CG CG AT CT CT AG CT AG GT GT GA AG GG TT TT GG TT CC CC CC CC GG AA AG AG AG AA CC GG AA CC CC AG GG CC AC CC AA CG AA GG TT AG CT CG CG CG AT CT CT AG CT AG GT GT GA AG GG TT TT GG TT CC CC CC CC GG AA GG GG GG AA CT AA GG GG CT GG AA CC AC CG AA CC AA GG TT AG CT CG CG CG AT CT CT AG CT AG GT TGG AA GG TT TT GG TT CC CC CC CG GC AG AG AG AG AG AA CT AA GG GG CT GG AG CC CC CG AA CC AA GT TT AG CT CG CG CG AT CT CT AG CT AG GT TGG AA GG TT TT GG TT CC CC CC CG GC AA AG AG AG AG AA CT AA GG GG CT GG AG CC CC CG AA CC AA GT TT AG CT CG CG CG AT CT CT AG CT AG GT TGG AA GG TT TT GG TT CC CC CC CG GC AA AG AG AG AG AA TT AA GG GG CT GG AG CC CC CG AA CC AA GT TT AG CT CG CG CG AT CT CT AG CT AG GT TT GG AA GG TT TT GG TT CC CC CC CC GG AA AG AG AG AA TT AA GG GG CC AG AG CC AA CC AA CG AA GT TT AG TT GG GG GG TT TT CC GG TT GG AT ...

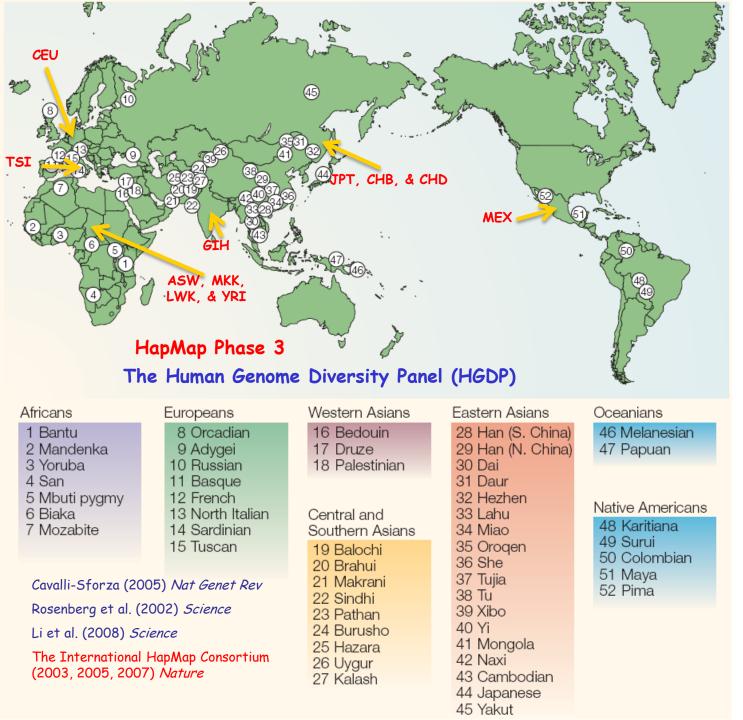
Matrices including thousands of individuals and hundreds of thousands if SNPs are available.



44 Japanese 45 Yakut

<u>HGDP data</u>

- 1,033 samples
- 7 geographic regions
- 52 populations

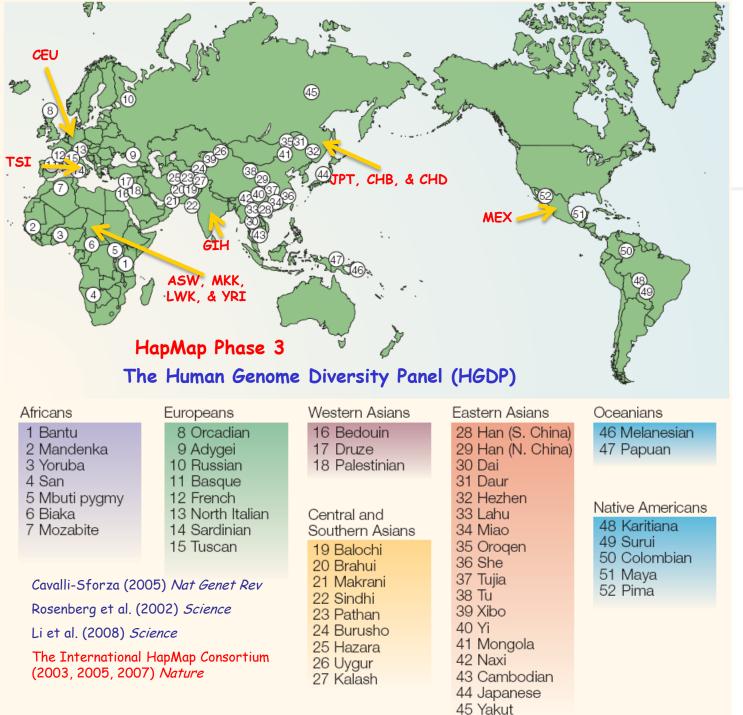


HGDP data

- 1,033 samples
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- 52 populations

HapMap Phase 3 data

- 1,207 samples
- 11 populations



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We will apply SVD/PCA on the (joint) HGDP and HapMap Phase 3 data.

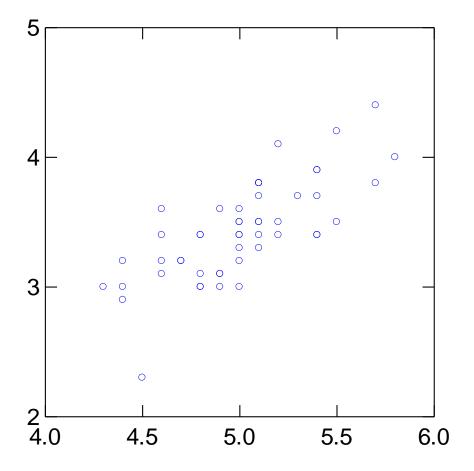
Matrix dimensions:

2,240 subjects (rows) 447,143 SNPs (columns)

Dense matrix:

over one billion entries

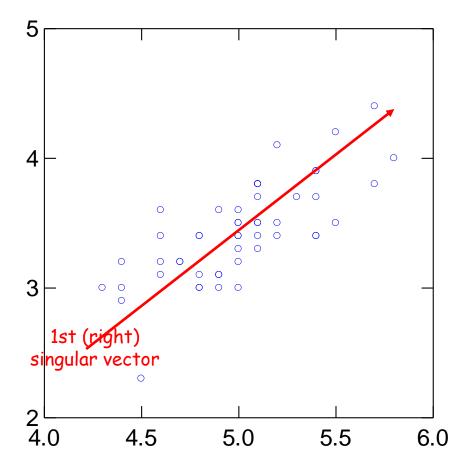
The Singular Value Decomposition (SVD)



Let the blue circles represent *m* data points in a 2-D Euclidean space.

Then, the SVD of the *m-by-2* matrix of the data will return ...

The Singular Value Decomposition (SVD)



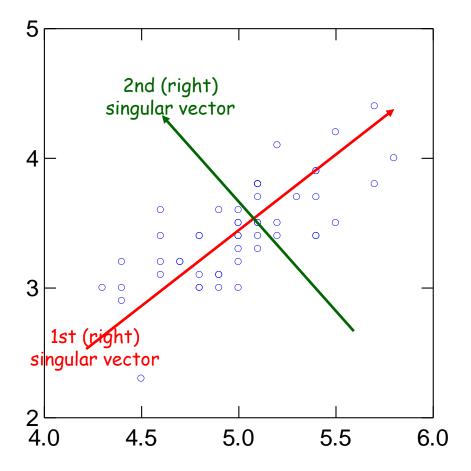
Let the blue circles represent *m* data points in a 2-D Euclidean space.

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1st (right) singular vector:

direction of maximal variance,

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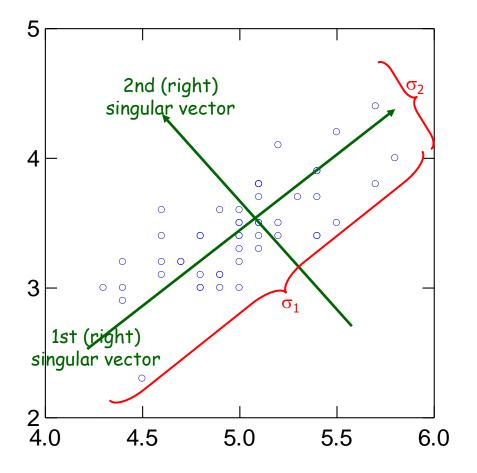
<u>1st (right) singular vector:</u>

direction of maximal variance,

2nd (right) singular vector:

direction of maximal variance, after removing the projection of the data along the first singular vector.

Singular values



 σ_1 : measures how much of the data variance is explained by the first singular vector.

 σ_2 : measures how much of the data variance is explained by the second singular vector.

Principal Components Analysis (PCA) is done via the computation of the Singular Value Decomposition (SVD) of a (mean-centered) covariance matrix.

Typically, a small constant number (say k) of the top singular vectors and values are kept.

SVD: formal definition

$$\left(\begin{array}{c} A \\ m \times n \end{array} \right) = \left(\begin{array}{c} U \\ m \times \rho \end{array} \right) \cdot \left(\begin{array}{c} \Sigma \\ \rho \times \rho \end{array} \right) \cdot \left(\begin{array}{c} V \\ \rho \times n \end{array} \right)^{T}$$

 ρ : rank of A

U (V): orthogonal matrix containing the left (right) singular vectors of A.

 Σ : diagonal matrix containing the singular values of A.

SVD: formal definition

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 $\rho : \textbf{rank of A}$

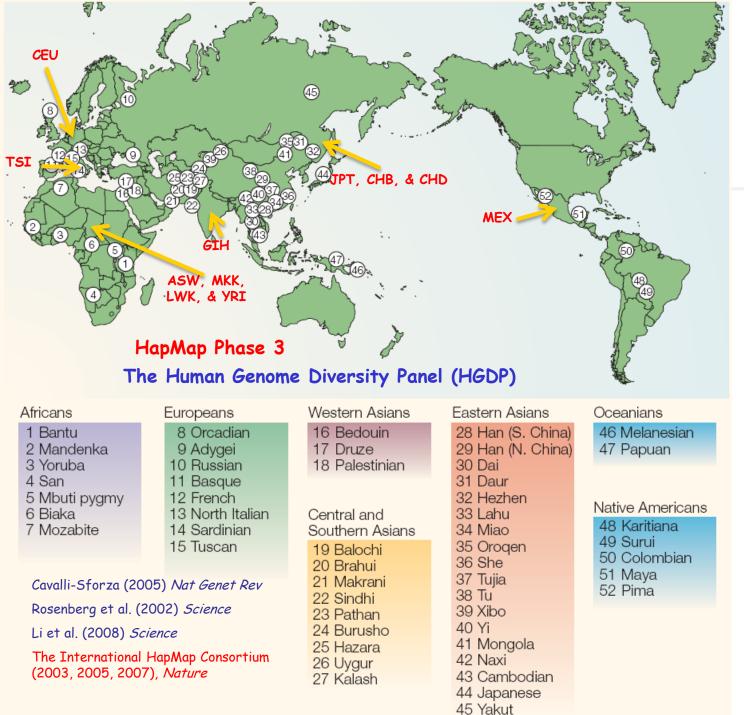
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 Σ : diagonal matrix containing the singular values of A.

Let σ_1 , σ_2 , ... , σ_ρ be the entries of $\Sigma.$

Computing the SVD takes $O(\min\{mn^2, m^2n\})$ time.

The top k left/right singular vectors/values can be computed faster using iterative methods.



HGDP data

- 1,033 samples
- 7 geographic regions
- 52 populations

HapMap Phase 3 data

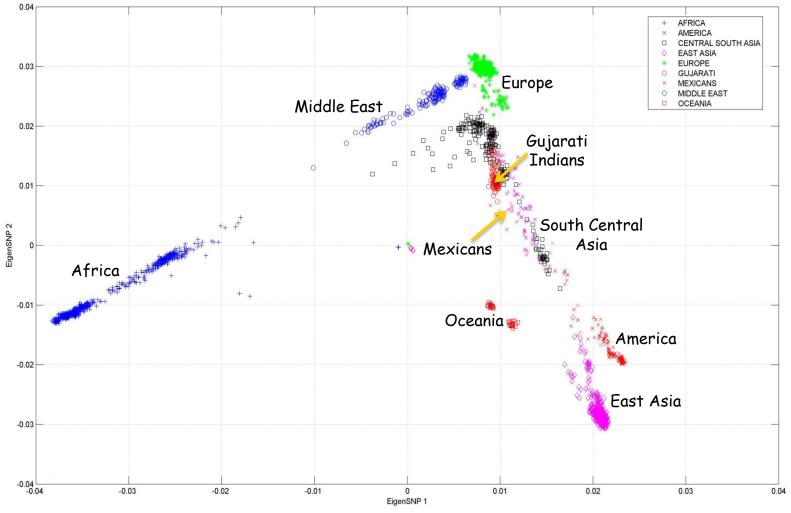
- 1,207 samples
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Matrix dimensions:

2,240 subjects (rows) 447,143 SNPs (columns)

SVD/PCA returns...

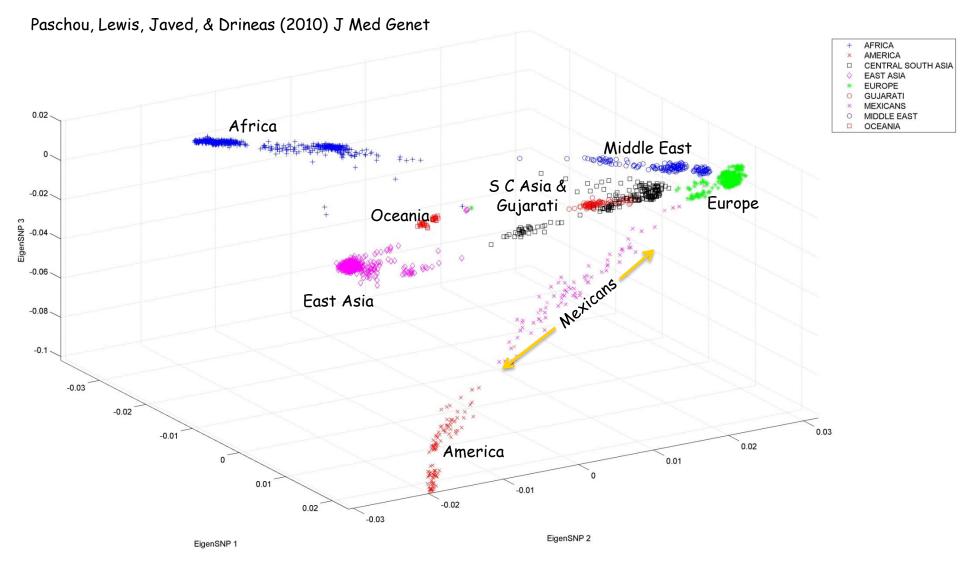
Paschou, Lewis, Javed, & Drineas (2010) J Med Genet



• Top two Principal Components (PCs or eigenSNPs)

(Lin and Altman (2005) Am J Hum Genet)

- The figure renders visual support to the "out-of-Africa" hypothesis.
- Mexican population seems out of place: we move to the top three PCs.



Not altogether satisfactory: the principal components are linear combinations of all SNPs, and - of course - can not be assayed!

Can we find **actual SNPs** that capture the information in the singular vectors? Formally: spanning the same subspace.



• Computing large SVDs: computational time

- In commodity hardware (e.g., a 4GB RAM, dual-core laptop), using MatLab 7.0 (R14), the computation of the SVD of the dense 2,240-by-447,143 matrix A <u>takes about 12 minutes</u>.
- Computing this SVD is not a one-liner, since we can not load the whole matrix in RAM (runs out-of-memory in MatLab).
- We compute the eigendecomposition of AA^{T} .
- In a similar experiment, we computed **1,200 SVDs** on matrices of dimensions (approx.) 1,200-by-450,000 (roughly speaking a full leave-one-out cross-validation experiment). (Drineas, Lewis, & Paschou (2010) PLoS ONE)
- Obviously, running time is a concern.
- We need efficient, easy to implement, methods.

Issues (cont'd)

- \cdot Selecting good columns that "capture the structure" of the top PCs
 - Combinatorial optimization problem; hard even for small matrices.
 - Often called the Column Subset Selection Problem (CSSP).
 - Not clear that such columns even exist.

Issues (cont'd)

\cdot Selecting good columns that "capture the structure" of the top PCs

- Combinatorial optimization problem; hard even for small matrices.
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- Not clear that such columns even exist.

Such datasets will only continue to increase in size:

In collaboration with K. Kidd's lab (Yale University, Department of Genetics) we are now analyzing:

- 4,000 samples from over 100 populations
- genotyped on over 500,000 SNPs.

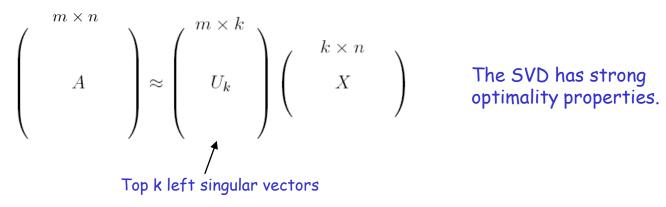
Our perspective

The two issues are connected

• There exist "good" columns in any matrix that contain information about the top principal components.

- We can identify such columns via a simple statistic: the leverage scores.
- This does not immediately imply faster algorithms for the SVD, but, combined with random projections, it does!

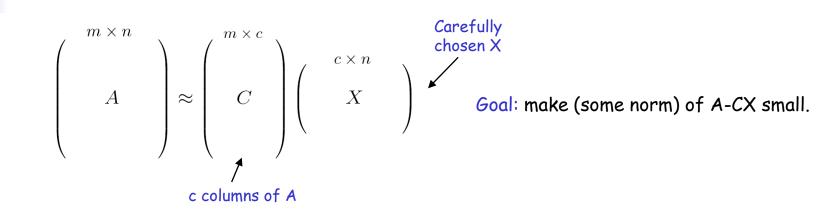




- > It is easy to see that X = $U_k^T A$.
- SVD has strong optimality properties.
- > The columns of U_k are linear combinations of up to all columns of A.

The CX decomposition

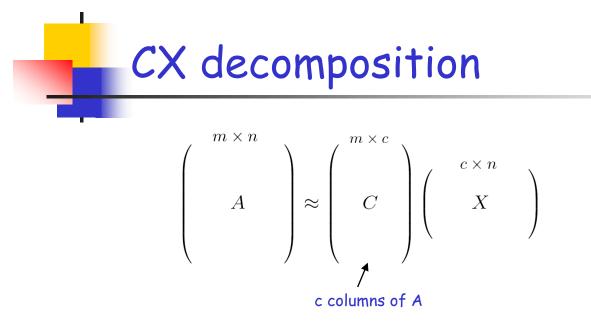
Drineas, Mahoney, & Muthukrishnan (2008) SIAM J Mat Anal Appl Mahoney & Drineas (2009) PNAS



Why?

If A is an subject-SNP matrix, then selecting representative columns is equivalent to selecting representative SNPs to capture the same structure as the top eigenSNPs.

We want c as small as possible!



Easy to prove that optimal $X = C^{+}A$. (C^{+} is the Moore-Penrose pseudoinverse of C.) Thus, the challenging part is to find good columns (SNPs) of A to include in C.

From a mathematical perspective, this is a hard combinatorial problem, closely related to the so-called Column Subset Selection Problem (CSSP).

The CSSP has been heavily studied in Numerical Linear Algebra.

A much simpler statistic

(Frieze, Kannan, & Vempala FOCS 1998, Drineas, Frieze, Kannan, Vempala & Vinay SODA '99, Drineas, Kannan, & Mahoney SICOMP '06)

<u>Algorithm</u>: given an m-by-n matrix A, let $A^{(i)}$ be the i-th column of A.

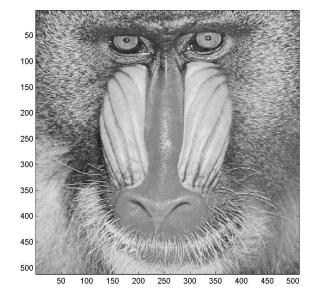
• Sample s columns of A in i.i.d. trials (with replacement), where in each trial

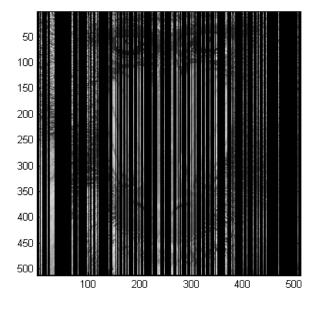
$$\Pr\left[\text{picking the } i\text{-th column}\right] = \frac{\left\|A^{(i)}\right\|_{2}^{2}}{\left\|A\right\|_{F}^{2}}$$

• Form the m-by-s matrix C by including $A^{(i)}$ as a column of C.

Error bound:
$$\mathbf{E} \left[\|A - CC^+A\|_F^2 \right] \le \|A - A_k\|_F^2 + \sqrt{\frac{4k}{s}} \|A\|_F^2$$

Approximating singular vectors





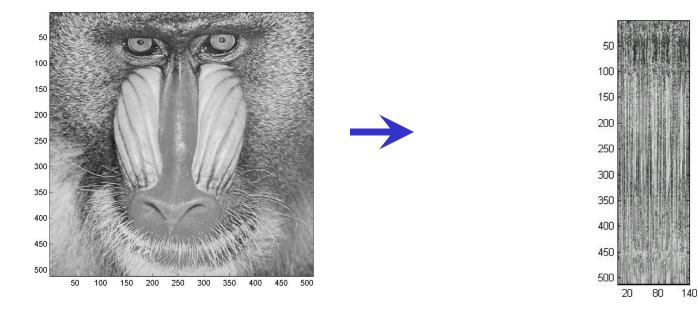
Original matrix

Sampling (s=140 columns)

- 1. Sample s (=140) columns of the original matrix A and form a 512-by-c matrix C.
- 2. Project A on CC^+ and show that $A-CC^+A$ is "small".

(C^+ is the pseudoinverse of C)

Approximating singular vectors



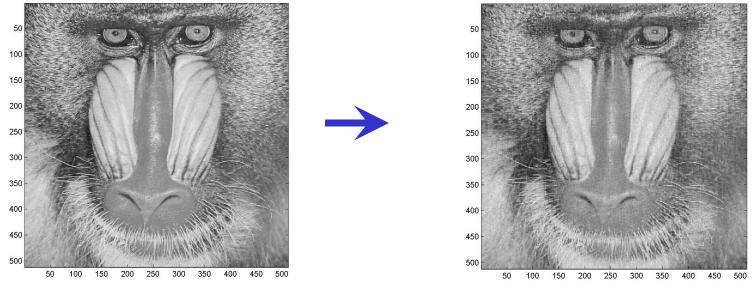
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Approximating singular vectors (cont'd)



Α

CC⁺A

<u>**Remark 1:**</u> Selecting the columns in this setting is trivial and can be implemented in a couple of (sequential) passes over the input matrix.

<u>Remark 2</u>: The proof is based on matrix perturbation theory and a probabilistic argument to bound $AA^{T} - \hat{C}\hat{C}^{T}$ (where \hat{C} is a rescaled C).

Is this a good bound?

$$\mathbf{E}\left[\left\|A - CC^{+}A\right\|_{F}^{2}\right] \leq \left\|A - A_{k}\right\|_{F}^{2} + \sqrt{\frac{4k}{s}} \left\|A\right\|_{F}^{2}$$

<u>Problem 1</u>: If s = n, we still do not get zero error.

That's because of sampling with replacement.

(We know how to analyze uniform sampling without replacement, but we have no bounds on nonuniform sampling without replacement.)

<u>Problem 2:</u> If A had rank exactly k, we would like a column selection procedure that drives the error down to zero when s=k.

This can be done deterministically simply by selecting k linearly independent columns.

<u>Problem 3:</u> If A had numerical rank k, we would like a bound that depends on the norm of $A - A_k$ and not on the norm of A.

A lot of prior work in the Numerical Linear Algebra community for the **spectral norm case** when s=k; the resulting bounds depend (roughly) on $(k(n-k))^{1/2}||A-A_k||_2$



Given an m-by-n matrix A, there exists an $O(mn^2)$ algorithm that picks

at most O((k/ ϵ^2) log (k/ ϵ)) columns of A

such that with probability at least .9

$$\left\| A - CC^{\dagger}A \right\|_{F} \le (1+\epsilon) \left\| A - A_{k} \right\|_{F}$$

The algorithm

- <u>Input:</u> m-by-n matrix A,
 - $0 < \epsilon < .5$, the desired accuracy
- <u>Output:</u> C, the matrix consisting of the selected columns

Sampling algorithm

- Compute probabilities p_j summing to 1.
- Let c = O($(k/\epsilon^2) \log (k/\epsilon)$).

• In c i.i.d. trials pick columns of A, where in each trial the j-th column of A is picked with probability p_j .

• Let C be the matrix consisting of the chosen columns.

Subspace sampling (Frobenius norm)

 $V_{\rm k}\!\!:$ orthogonal matrix containing the top k right singular vectors of A.

 Σ_k : diagonal matrix containing the top k singular values of A.

Remark: The rows of V_k^{T} are orthonormal vectors, but its columns $(V_k^{T})^{(i)}$ are not.

Subspace sampling (Frobenius norm)

$$\begin{pmatrix} A_k \\ m \times n \end{pmatrix} = \begin{pmatrix} U_k \\ m \times k \end{pmatrix} \cdot \begin{pmatrix} \Sigma_k \end{pmatrix} \cdot \begin{pmatrix} V_k^T \\ K \end{pmatrix}$$

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Subspace sampling in O(mn²) time

$$p_{j} = \frac{\left\| \left(V_{k}^{T} \right)^{(j)} \right\|_{2}^{2}}{k}$$
Normalization s.t. the p_{j} sum up to 1

Subspace sampling (Frobenius norm)

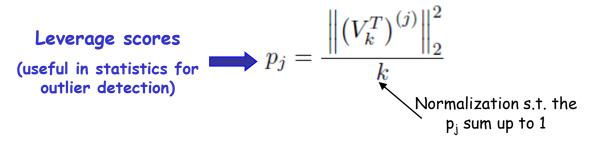
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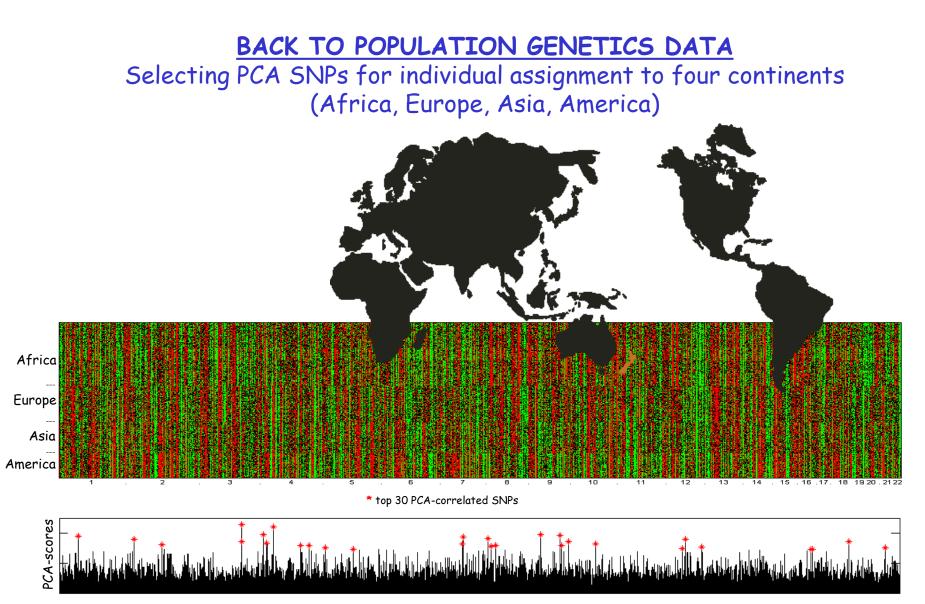
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<u>Subspace sampling</u> in O(mn²) time

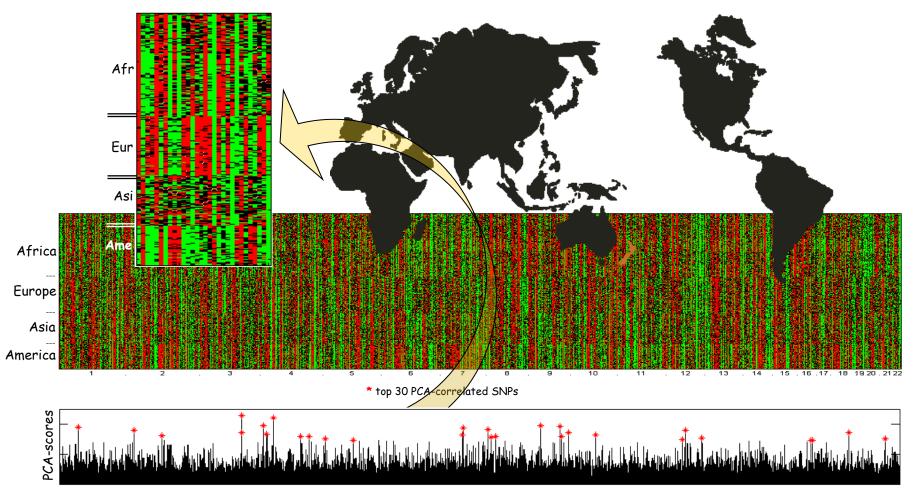




SNPs by chromosomal order

Paschou et al (2007; 2008) PLoS Genetics Paschou et al (2010) J Med Genet Drineas et al (2010) PLoS One

Selecting PCA SNPs for individual assignment to four continents (Africa, Europe, Asia, America)



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Approximating leverage scores

<u>Can we approximate the leverage scores fast?</u>

<u>Theorem</u>: Given any m-by-n matrix A with m > n, we can approximate its leverage scores with relative error accuracy in

O(mn log m) time,

as opposed to the - trivial - $O(mn^2)$ time.

(Drineas, Mahoney, Magdon-Ismail, & Woodruff ICML '12)

Selecting fewer columns

Problem

How many columns do we need to include in the matrix ${\cal C}$ in order to get relative-error approximations ?

<u>Recall</u>: with $O((k/\epsilon^2) \log (k/\epsilon))$ columns, we get (subject to a failure probability)

$$\left\| A - CC^{\dagger}A \right\|_{F} \le (1+\epsilon) \left\| A - A_{k} \right\|_{F}$$

Deshpande & Rademacher (FOCS '10): with exactly k columns, we get

$$\left|A - CC^{\dagger}A\right\|_{F} \le \sqrt{k} \left\|A - A_{k}\right\|_{F}$$

What about the range between k and O(k log(k))?

Selecting fewer columns (cont'd)

(Boutsidis, Drineas, & Magdon-Ismail, FOCS 2011)

Question:

What about the range between k and O(k log(k))?

Answer:

A relative-error bound is possible by selecting $s=3k/\epsilon$ columns!

Technical breakthrough;

A combination of sampling strategies with a novel approach on column selection, inspired by the work of Batson, Spielman, & Srivastava (STOC '09) on graph sparsifiers.

- The running time is $O((mnk+nk^3)\epsilon^{-1})$.
- Simplicity is gone ...

Lower bounds and alternative approaches

Deshpande & Vempala, RANDOM 2006

A relative-error approximation necessitates at least k/ϵ columns.

<u>Guruswami & Sinop, SODA 2012</u>

Alternative approaches, based on volume sampling, guarantee

(r+1)/(r+1-k) relative error bounds.

This bound is asymptotically optimal (up to lower order terms).

The proposed deterministic algorithm runs in $O(rnm^3 \log m)$ time, while the randomized algorithm runs in $O(rnm^2)$ time and achieves the bound in expectation.

Guruswami & Sinop, FOCS 2011

Applications of column-based reconstruction in Quadratic Integer Programming.

Random projections: the JL lemma

For every set S of m points in \mathbb{R}^n and every $\epsilon > 0$, there exists a mapping $f : \mathbb{R}^n \to \mathbb{R}^s$, where $s = O(\log m/\epsilon^2)$, such that for all points $u \in S$,

 $(1-\epsilon) \|u\|_2 \le \|f(u)\|_2 \le (1+\epsilon) \|u\|_2$

holds with probability at least $1 - 1/m^2$.

Johnson & Lindenstrauss (1984)

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Johnson & Lindenstrauss (1984)

- We can represent S by an m-by-n matrix A, whose rows correspond to points.
- We can represent all f(u) by an m-by-s \tilde{A} .
- The "mapping" corresponds to the construction of an n-by-s matrix R and computing

 $\widetilde{A} = AR$

(The original JL lemma was proven by projecting the points of S to a random k-dimensional subspace.)

Different constructions for R

- Frankl & Maehara (1988): random orthogonal matrix
- DasGupta & Gupta (1999): matrix with entries from N(0,1), normalized
- Indyk & Motwani (1998): matrix with entries from N(0,1)
- Achlioptas (2003): matrix with entries in {-1,0,+1}
- Alon (2003): optimal dependency on n, and almost optimal dependency on ϵ

Construct an n-by-s matrix R such that:

$$R_{ij} = \sqrt{3} \times \begin{cases} +1 & \text{,w.p. } 1/6 \\ 0 & \text{,w.p. } 2/3 \\ -1 & \text{,w.p. } 1/6 \end{cases}$$

Return:
$$\tilde{A} = \frac{1}{\sqrt{s}} AR \in \mathbb{R}^{m \times s}$$

 $O(mns) = O(mn \log n / \epsilon^2)$ time computation

Fast JL transform Ailon & Chazelle (2006) FOCS, Matousek (2006)

 $P \in \mathbb{R}^{s \times n}$ $s = O\left(\log m/\epsilon^2\right)$

$$P_{ij} = \sqrt{q} \times \begin{cases} +1 & \text{,w.p. } q/2 \\ 0 & \text{,w.p. } 1-q \\ -1 & \text{,w.p. } q/2 \end{cases}$$

 $H \in \mathbb{R}^{n \times n}$

Normalized Hadamard-Walsh transform matrix (if n is not a power of 2, add all-zero columns to A)

 $D \in \mathbb{R}^{n \times n}$ Diagonal matrix with D_{ii} set to +1 or -1 w.p. $\frac{1}{2}$. $R = (PHD)^T \in \mathbb{R}^{n \times s} \longrightarrow \tilde{A} = \frac{1}{\sqrt{s}}AR$



Applying PHD on a vector u in \mathbb{R}^n is fast, since:

- Du : O(n), since D is diagonal,
- H(Du) : O(n log n), using the Hadamard-Walsh algorithm,

• $P(H(Du)) : O(\log^3 m/\epsilon^2)$, since P has on average $O(\log^2 n)$ non-zeros per row (in expectation).

Back to approximating singular vectors

(Drineas, Mahoney, Muthukrishnan, & Sarlos Num Math 2011)

Let A by an m-by-n matrix whose SVD is:

Apply the (HD) part of the (PHD) transform to A.

$$A = U\Sigma V^T \in \mathbb{R}^{m \times n}$$

$$ADH = U\Sigma\left(\underbrace{V^T DH}_{}\right) \in \mathbb{R}^{m \times n}$$

orthogonal matrix

Observations:

- 1. The left singular vectors of ADH span the same space as the left singular vectors of A.
- The matrix ADH has (up to log n factors) uniform leverage scores.
 (Thanks to V^THD having bounded entries the proof closely follows JL-type proofs.)
- 3. We can approximate the left singular vectors of ADH (and thus the left singular vectors of A) by uniformly sampling columns of ADH.

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orthogonal matrix

Observations:

1. The left singular vectors of ADH span the same space as the left singular vectors of A.

The matrix ADH has (up to log n factors) uniform leverage scores. (Thanks to V^THD having bounded entries - the proof closely follows JL-type proofs.)

- 3. We can approximate the left singular vectors of ADH (and thus the left singular vectors of A) by uniformly sampling columns of ADH.
- 4. The orthonormality of HD and a version of our relative-error Frobenius norm bound (involving approximately optimal sampling probabilities) suffice to show that (w.h.p.)

$$\left\| A - \tilde{C}\tilde{C}^{\dagger}A \right\|_{F} \le (1+\epsilon) \left\| A - A_{k} \right\|_{F}$$

Uniform sample of $s = O\left(\frac{k}{\epsilon^2} \log^{c_0} \frac{n}{\epsilon}\right)$ columns of ADH



Let A by an m-by-n matrix whose SVD is:

Apply the (HD) part of the (PHD) transform to A.

$$A = U\Sigma V^T \in \mathbb{R}^{m \times n} \qquad ADH = U\Sigma \left(\underbrace{V^T DH}_{\text{orthogonal matrix}} \right) \in \mathbb{R}^{m \times n}$$

Running time:

- <u>Trivial analysis</u>: first, uniformly sample s columns of DH and then compute their product with A. Takes O(mns) = O(mnk polylog(n)) time, already better than full SVD.
- Less trivial analysis: take advantage of the fact that H is a Hadamard-Walsh matrix Improves the running time O(mn polylog(n) + mk²polylog(n)).



- <u>Randomization and sampling</u> can be used to solve problems that are massive and/or computationally expensive.
- <u>By (carefully) sampling rows/columns/entries of a matrix</u>, we can construct new sparse/smaller matrices that behave like the original matrix.
 - Can entry-wise sampling be made competitive to column-sampling in terms of accuracy and speed? See Achlioptas and McSherry (2001) STOC, (2007) JACM.
 - We improved/generalized/simplified it .
 - See Nguyen, Drineas, & Tran (2011), Drineas & Zouzias (2010).
 - Exact reconstruction possible using uniform sampling for constant-rank matrices that satisfy certain (strong) assumptions.
 - See Candes & Recht (2008), Candes & Tao (2009), Recht (2009).
- <u>By preprocessing the matrix using random projections</u>, we can sample rows/ columns much less carefully (even uniformly at random) and still get nice "behavior".



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