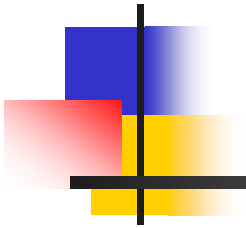


CUR Matrix Decompositions for Improved Data Analysis

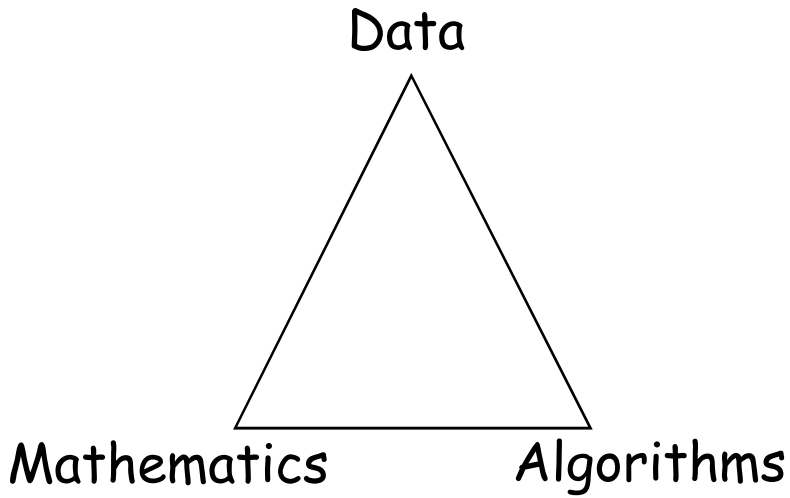
Michael W. Mahoney

Yahoo Research
http://www.cs.yale.edu/homes/mmahoney

(Joint work with P. Drineas, R. Kannan, S. Muthukrishnan,
and P. Paschou, K. Kidd, M. Maggioni)

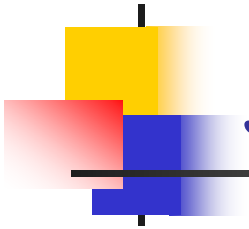
Workshop on Algorithms for Modern Massive Datasets, June 2006

Modeling data as matrices



Matrices often arise with data:

- n objects ("documents," genomes, images, web pages),
- each with m features,
- may be represented by an m x n matrix A.



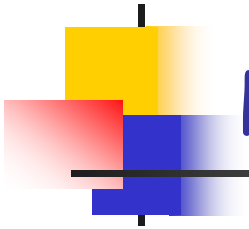
SVD and low-rank approximations

Basic SVD Theorem: Let A be an m x n matrix with rank ρ.

- Can express *any* matrix A as $A = U \Sigma V^T$.
- Truncate SVD of A: $A_k = U_k \Sigma_k V_k^T$, get "best" rank-k approximation.

Properties of truncated SVD:

- Used in data analysis via Principal Components Analysis (PCA) .
- Gives a very particular structure (think: rotate-rescale-rotate).
- Problematic w.r.t. sparsity, nonnegativity, interpretability, etc.



Problems with SVD/Eigen-Analysis

Problems arise: since structure in the data is *not* respected by mathematical operations on the data:

- Sparsity - is destroyed by orthogonalization.
- Non-negativity - is a convex and not linear algebraic notion.
- Interpretability - what does a linear combination of 6000 genes "mean."
- Reification - maximum variance directions are just that.

Question: Do there exist "better" low-rank matrix approximations.

- "better" structural properties for certain applications.
- "better" at respecting relevant structure.
- "better" for interpretability and informing intuition.

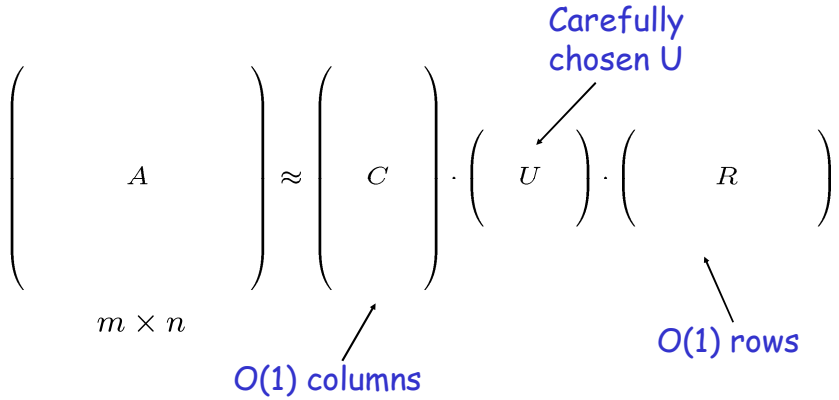
CX and CUR matrix decompositions

Recall: Matrices are about their rows and columns.

Recall: Low-rank matrices have redundancy in their rows and columns.

Def: A **CX matrix decomposition** is a low-rank approximation *explicitly expressed* in terms of a small number of columns of the original matrix A (e.g., $P_C A = CC^+A$).

Def: A **CUR matrix decomposition** is a low-rank approximation *explicitly expressed* in terms of a small number of columns and rows of the original matrix A.



Two CUR Theorems

Additive-Error Theorem: [DKM04]

In O(m+n) space and time after two passes over the data, use *"column/row-norm sampling"* to find $O(k/\varepsilon^2)$ columns and rows s.t.:

$$||A-CUR||_{2,F} < ||A-A_k||_{2,F} + \varepsilon||A||_F$$

Relative-Error Theorem: [DMM06]

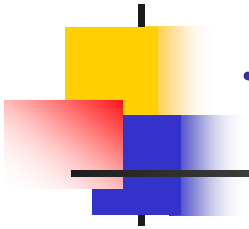
In $O(SVD(A_k))$ space and time, use *"subspace-sampling"* to find $O(k \log(k)/\varepsilon^2)$ columns and rows s.t.:

$$||A-CUR||_F < (1+\varepsilon)||A-A_k||_F$$

$$\begin{pmatrix} \quad A \quad \end{pmatrix} \approx \begin{pmatrix} \quad C \quad \end{pmatrix} \cdot \begin{pmatrix} \quad U \quad \end{pmatrix} \cdot \begin{pmatrix} \quad R \quad \end{pmatrix}$$

Previous CUR-type decompositions

Goreinov, Tyrtyshnikov, & Zamarashkin (LAA '97, …)	C: columns that span max volume U: W^+ R: rows that span max volume	Existential result Error bounds depend on $\|\|W^+\|\|_2$ Spectral norm bounds!
Berry, Stewart, & Pulatova (Num. Math. '99, TR '04, …)	C: variant of the QR algorithm R: variant of the QR algorithm U: minimizes $\|\|A-CUR\|\|_F$	No a priori bounds A must be known to construct U. Solid experimental performance
Williams & Seeger (NIPS '01, …)	C: uniformly at random U: W^+ R: uniformly at random	Experimental evaluation A is assumed PSD Connections to Nystrom method
Drineas, Kannan & Mahoney (TR '04, SICOMP '06)	C: w.r.t. column lengths U: in linear/constant time R: w.r.t. row lengths	"Sketching" massive matrices Provable, a priori, bounds Explicit dependency on $A - A_k$
Drineas, Mahoney, & Muthukrishnan (TR '06)	C: depends on singular vectors of A. U: (almost) W^+ R: depends on singular vectors of C	$(1+\varepsilon)$ approximation to $A - A_k$ Computable in low polynomial time (Suffices to compute SVD(A_k))



Three CUR Data Applications

Human Genetics: DNA SNP Data
- Biological Goal: Evaluate intra- and inter-population tag-SNP transferability.

Medical Imaging: Hyperspectral Image Data
- Medical Goal: Compress the data, without sacrificing classification quality.

Recommendation Systems: Customer Preference Data
- Business Goal: Reconstruct the data, to make high-quality recommendations.

CUR Data Application: Human Genetics

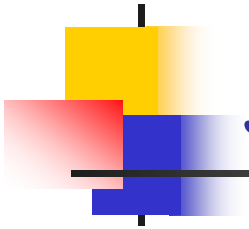
(Joint work with P. Paschou and K. Kidd's lab at Yale University)

Recall, "the" human genome:

- 30,000 – 40,000 genes
- 3 billion base pairs
- The functionality of 97% of the genome is unknown.
- BUT: individual differences (polymorphic variation) at ≈ 1 b.p. per thousand.

SNPs (Single Nucleotide Polymorphisms):

- The most common type of genetic polymorphic variation.
- They are known locations at the human genome where two (out of A, C, G, T) alternate nucleotide bases (alleles) are observed.



SNP Biology

SNPs carry redundant information:

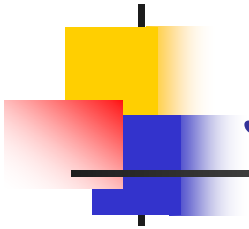
- Human genome is organized into block-like structure.
- Strong, but nontrivial, intra-block correlations.
- Can focus only on "tagging SNPs," or tSNPs.

Different patterns of SNP frequencies/correlations in different populations (e.g., European, Asian, African, etc.):

- Can track population histories and disease genes.
- Effective markers for genomic research.

International HapMap Project:

- Create a haplotype map of human genetic variability.
- Map all 10,000,000 SNPs for 270 individuals from 4 different populations.



SNP Pharmacology

Disease association studies:

- Locate causative genes for common complex disorders (e.g., diabetes, heart disease).
- Identify association between affection status and known SNPs.
- Don't need: knowledge of function of the genes or etiology of the disorder.
- Investigate candidate genes in physical proximity with associated SNPs.

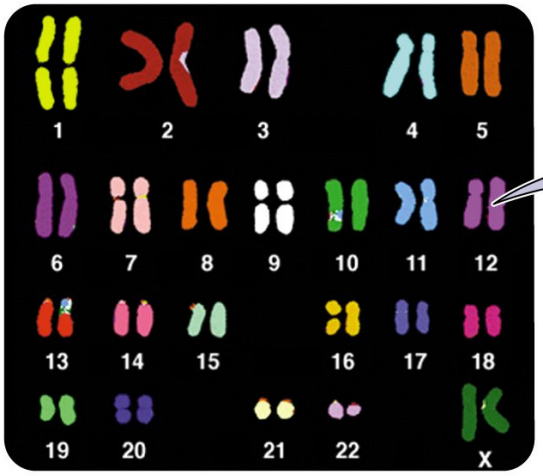
Develop the "next generation" of drugs:

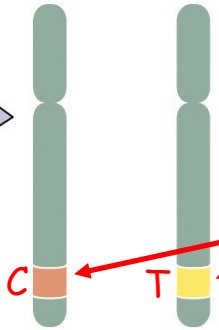
- "*population-specific*," eventually "*genome-specific*," not just "*disease-specific*".

Funding:

- HapMap project (~$100,000,000 from NIH, etc.).
- Funding also from pharmaceutical companies, NSF, the DOJ*, etc.

*Is it possible to identify the ethnicity of a suspect from his DNA?





Two copies of a chromosome
(father, mother)

Focus at a specific locus and assay the observed alleles.

SNP: exactly two alternate alleles appear.

An individual could be:

- Heterozygotic (in our study, CT = TC)

SNPs

individuals

… AG CT GT GG CT CC CC CC CC 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 CC GG AA AG AG AG AA CT AA GG GG CC GG AA GG AA CC AA CC AA GG TT AA TT GG GG GG TT TT CC GG TT GG GG TT GG AA …

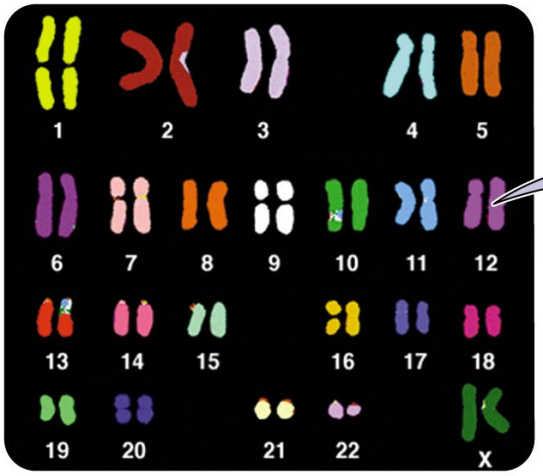
… GG TT TT GG TT CC CC CC CC GG AA AG AG AG AA AG CT AA GG GG CC AG AG CG AC CC AA CC AA GG TT AG **CT** GG CG CG AT CT CT AG CT AG GG GT GA AG …

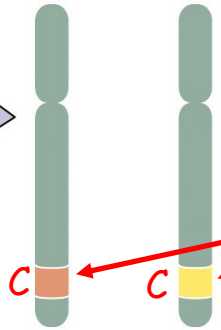
… GG TT TT GG TT CC CC CC CC GG AA AG AG AG AA CC GG AA CC CC AG GG CC AC CC AA CG AA GG TT AG CT CG CG CG AT CT CT AG CT AG GT GT GA AG …

… 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 GG CC CG CG CG AT CT CT AG CT AG GG TT GG AA …

… GG TT TT GG TT CC CC CG CC 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 GG 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 CG AA CC AA CG AA GG TT AA TT GG GG GG TT TT CC GG TT GG GT TT GG AA …





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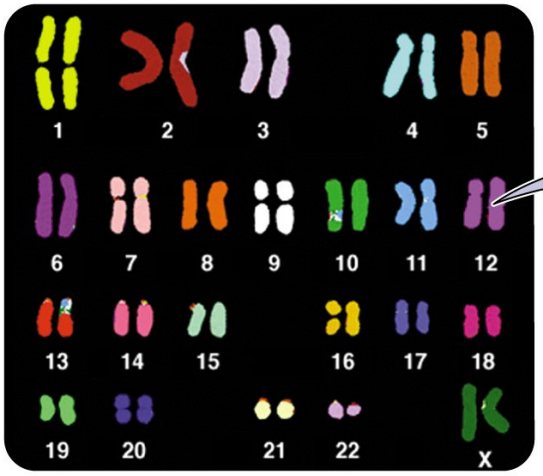
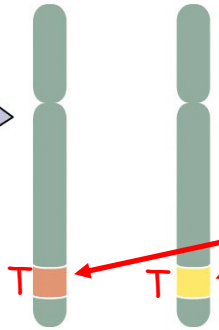
- Homozygotic at the first allele, e.g., C

SNPs

individuals

… AG CT GT GG CT CC CC CC CC 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 CC GG AA AG AG AG AA CT AA GG GG CC GG AA GG AA CC AA CC AA GG TT AA TT GG GG GG TT TT CC GG TT GG GG TT GG AA …
… GG TT TT GG TT CC CC CC CC GG AA 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 GG 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 GG **CC** CG CC CG AT CT CT AG CT AG GG TT GG AA …
… GG TT TT GG TT CC CC CG CC 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 GG 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 CG AA CC AA CG AA GG TT AA TT GG GG GG TT TT CC GG TT GG GT TT GG AA …





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- Homozygotic at the first allele, e.g., C
- Homozygotic at the second allele, e.g., T

SNPs

individuals

… AG CT GT GG CT CC CC CC CC 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 CC GG AA AG AG AG AA CT AA GG GG CC GG AA GG AA CC AA CC AA GG TT AA TT GG GG GG TT TT CC GG TT GG GG TT GG AA …

… GG TT TT GG TT CC CC CC CC GG AA 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 GG 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 GG CC CG CG CG AT CT CT AG CT AG GG TT GG AA …

… GG TT TT GG TT CC CC CG CC 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 GG 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 CG AA CC AA CG AA GG TT AA **TT** G GG GG TT TT CC GG TT GG GT TT GG AA …

Encoding the SNP data ...

... as an m x n matrix *A*:

- Exactly two "known" nucleotides (out of *A*,*G*,*C*,*T*) appear in each column.
- Two alleles might be both equal to the first one (+1), both equal to the second one (-1), or different (0).

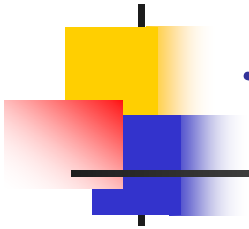
SNPs

individuals

```
 0  0  0  1  0 -1  1  1  1  0  0  0  0  0  1  0  1 -1 -1  1 -1  0  0  0  1  1  1  1 -1 -1  0  0  0  0  0  0  0  0  0  0  1  0  0  0
-1 -1 -1  1 -1 -1  1  1  1 -1  1  0  0  0  1  0  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 -1  1
-1 -1 -1  1 -1 -1  1  1  1 -1  1  0  0  1  0  0  1 -1 -1  1  0  0  0  0  1  1  1  1 -1 -1  0  0  0  0  0  0  0  0  0  0  1  0  0  0
-1 -1 -1  1 -1 -1  1  1  1 -1  1  0  0  0  1  1 -1  1  1  1  0 -1  1  0  1  1  0  1 -1 -1  0  0  0  0  0  0  0  0  0  0  0  0  0  0
-1 -1 -1  1 -1 -1  1  1  1 -1  1 -1 -1 -1  1  0  1 -1 -1  0 -1  1  1  0  0  1  1  1 -1 -1 -1  1  0  0  0  0  0  0  0  0  1 -1 -1  1
-1 -1 -1  1 -1 -1  1  0  1  0  0  0  0  0  1  0  1 -1 -1  0 -1  0  1 -1  0  1  1  1 -1 -1  0  0  0  0  0  0  0  0  0  0  1 -1 -1  1
-1 -1 -1  1 -1 -1  1  1  1 -1  1  0  0  0  1 -1  1 -1 -1  1  0  0  0  1  1  1  0  1 -1 -1  1 -1 -1 -1 -1 -1 -1  1 -1 -1 -1  0 -1 -1  1
```

Notes:

- Redundancy in rows and columns <=> Redundancy in SNPs and people.
- SVD has been used (Lin and Altman),
- but, then must *get actual-SNPs/people from eigen-SNPs/people*.



The SNP data we considered

Yale dataset

- Samples from 2000 individuals from 38 different populations.
- Four genomic regions (PAH, SORCS3, HOXB,17q25), a total of ≈ 250 SNPs.

HapMap dataset

- Samples from 270 individuals from 4 different populations (YRI, CEU, CHB, JPT)
- Four genomic regions (PAH, SORCS3, HOXB,17q25), a total of ≈ 1336 SNPs.

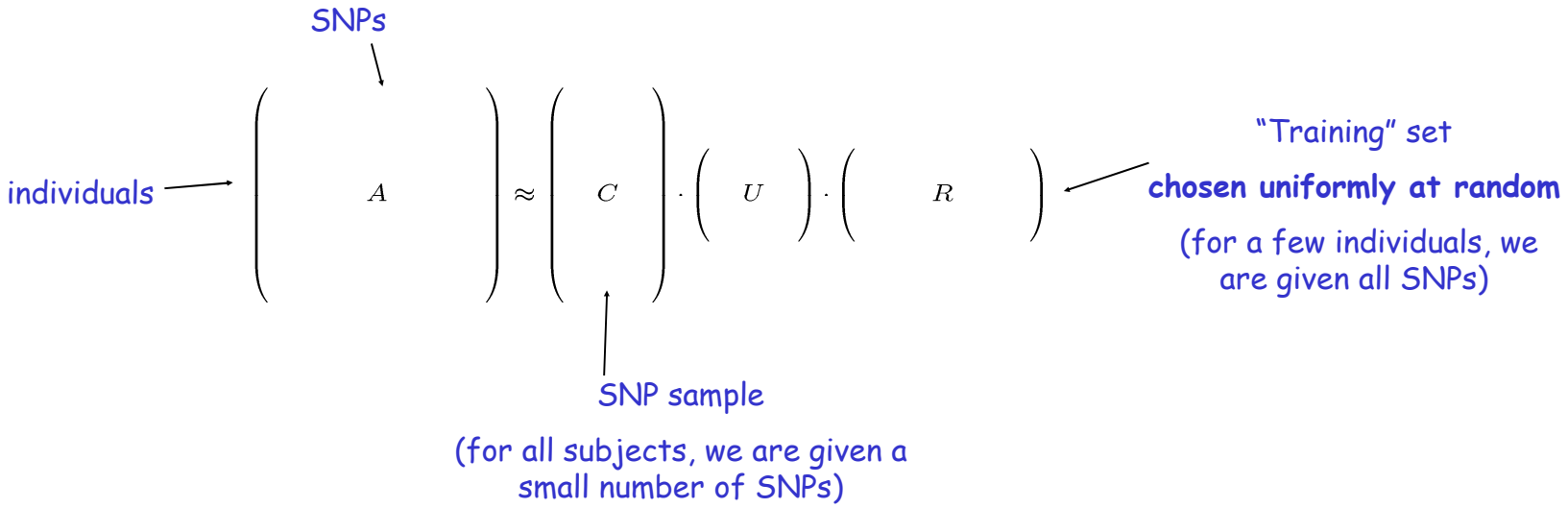

N > 50
N: 25 ~ 50
Finns
Kom
Zyrian
Khanty
Irish
Danes
Chuvash
Russians
Jews, Ashkenazi
Adygei
Druze
Samaritans
Yakut
European, Mixed
African Americans
Pima, Arizona
Cheyenne
Chinese,
Han
Hakka
Japanese
Chinese, Taiwan
Cambodians
Atayal
Ami
Pima, Mexico
Maya
Jews, Yemenite
Hausa
Yoruba
Biaka
Jews, Ethiopian
Ibo
Mbuti
Chagga
Micronesians
Nasioi
Ticuna
Surui
Karitiana
Africa
Europe
NW Siberia
NE Siberia
Oceania
SW Asia
E Asia
N America
S America

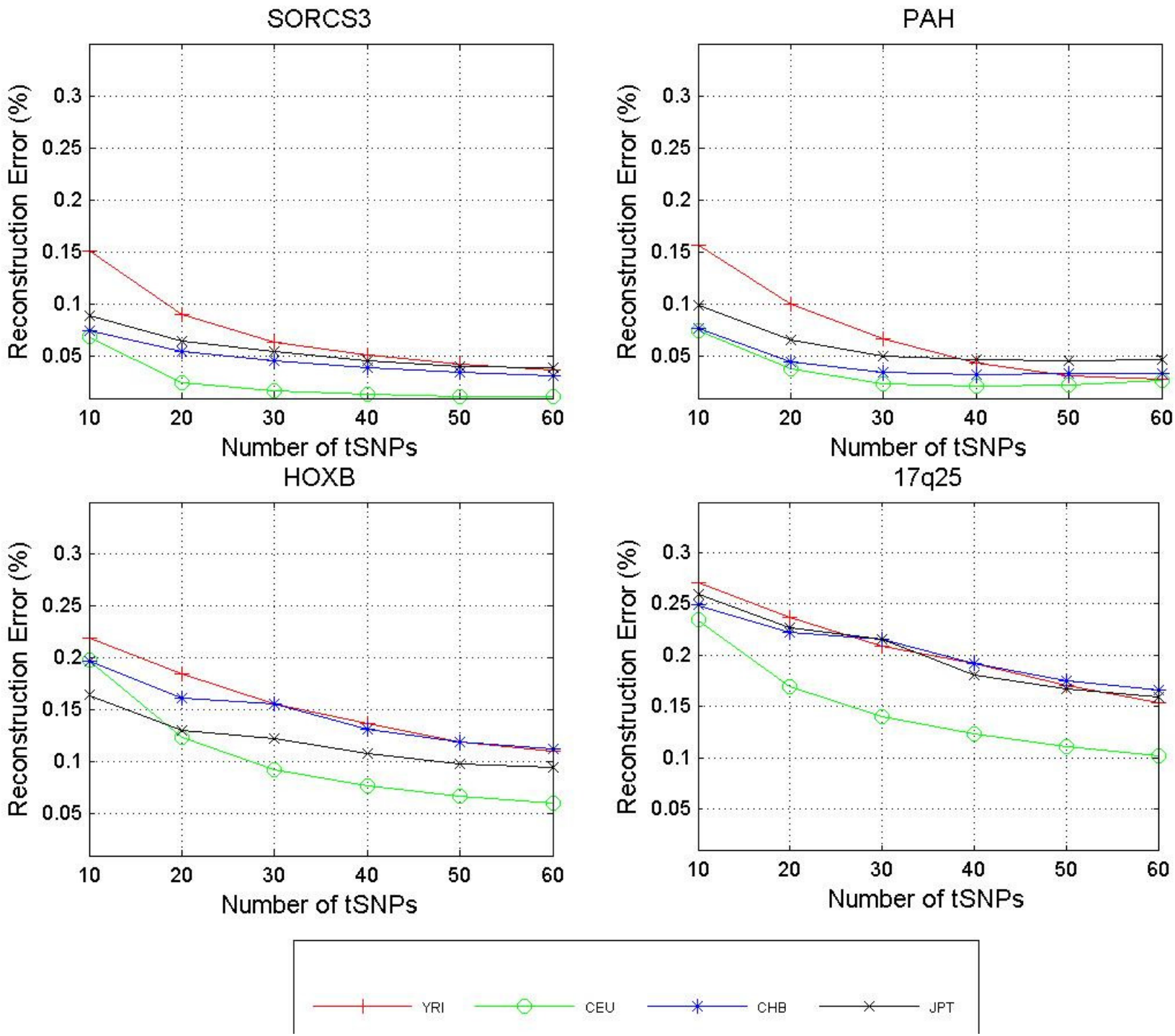
Predicting SNPs within a population

Split each population: training and test sets.

Goal: Given SNP information for all individuals in the training set AND for a small number of SNPs for all individuals (tagging-SNPs), *predict all unassayed SNPs*.

Note: Tagging-SNPs are selected using *only* the training set.



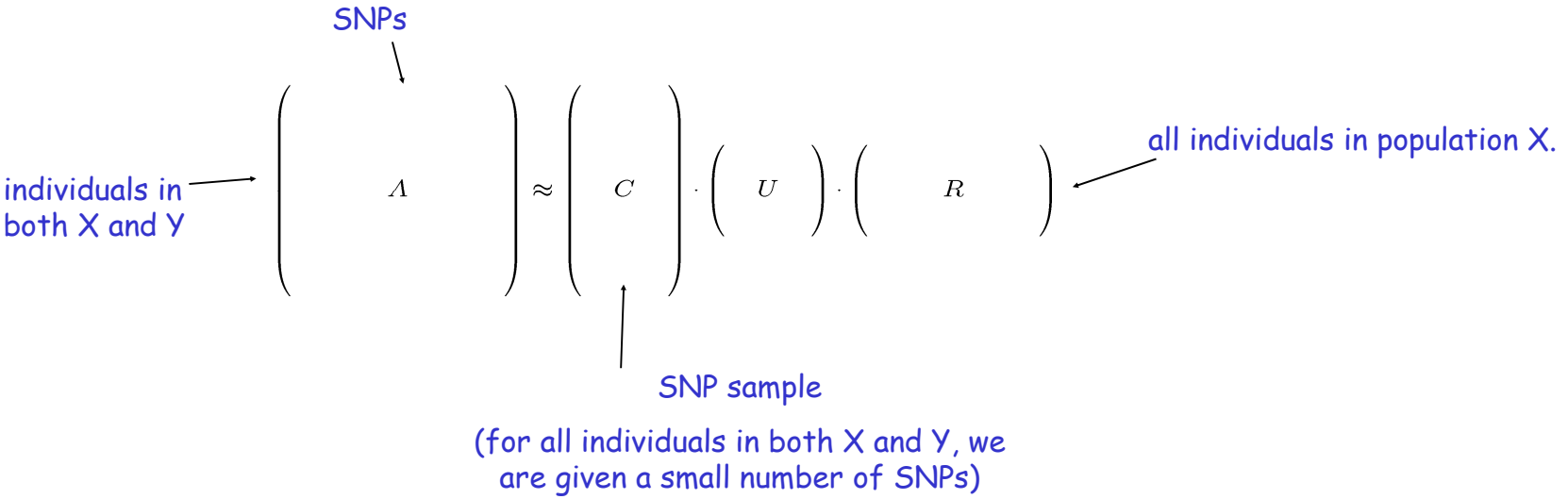

SORCS3
PAH
HOXB
17q25
Reconstruction Error (%)
Number of tSNPs
0.3
0.25
0.2
0.15
0.1
0.05
10
20
30
40
50
60
YRI
CEU
CHB
JPT

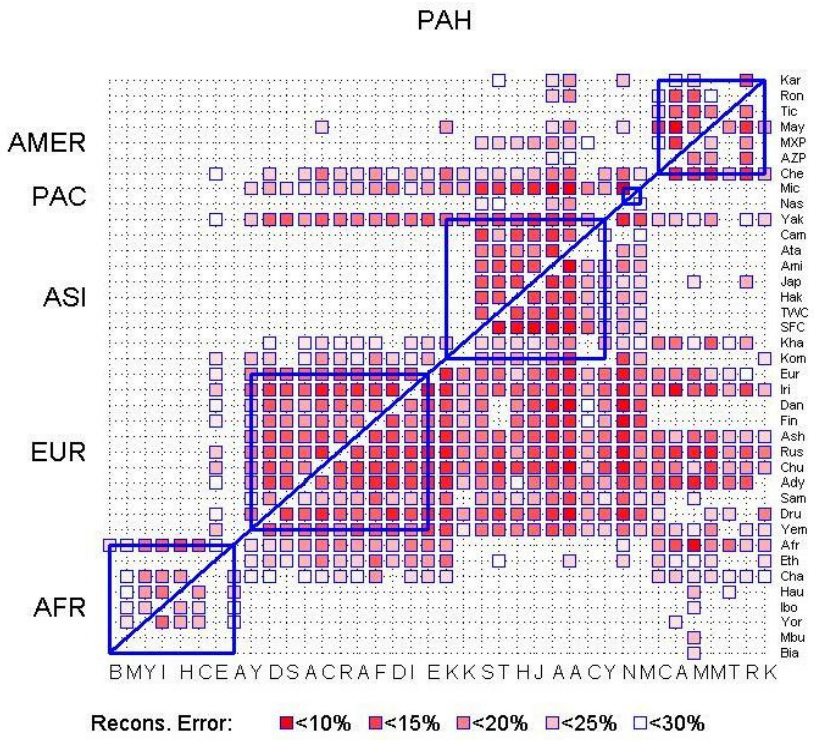
Predicting SNPs across populations

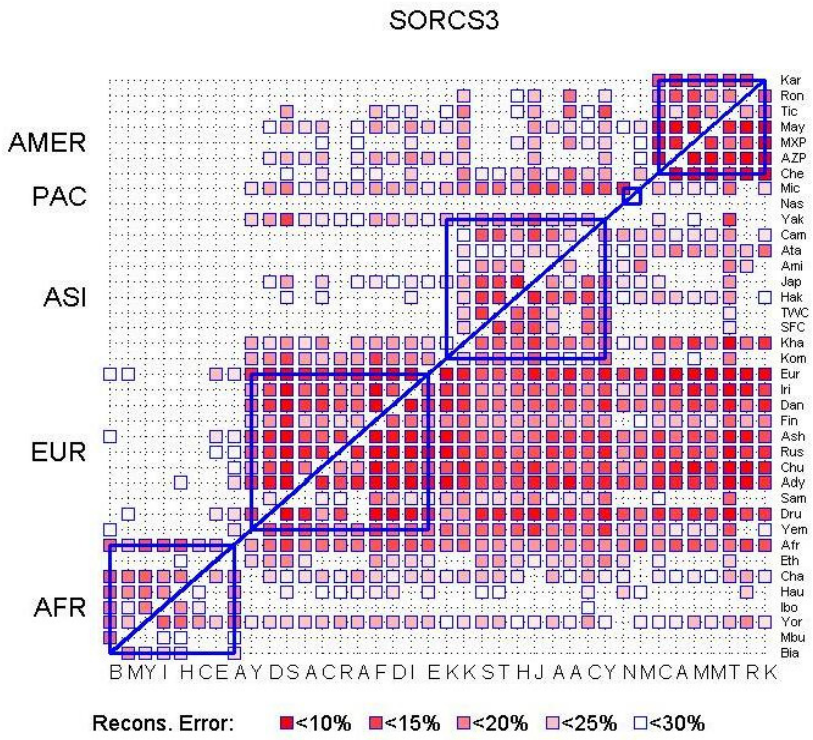
Goal: Given all SNPs information for all individuals in population X AND a small number of tagging-SNPs for population Y, *predict all unassayed SNPs for all individuals of Y.*

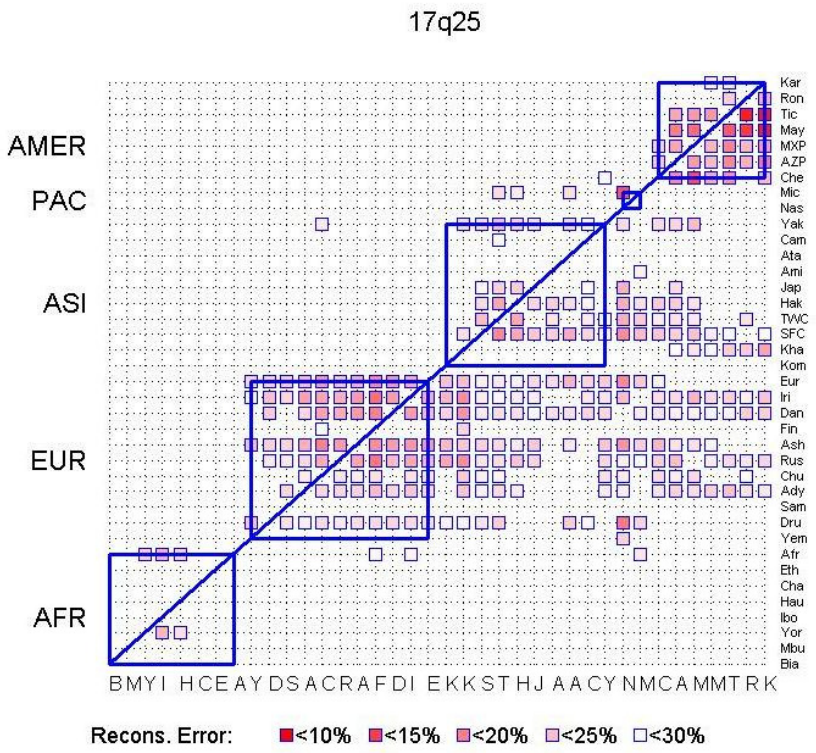
Note: Tagging-SNPs are selected using *only* the population X.

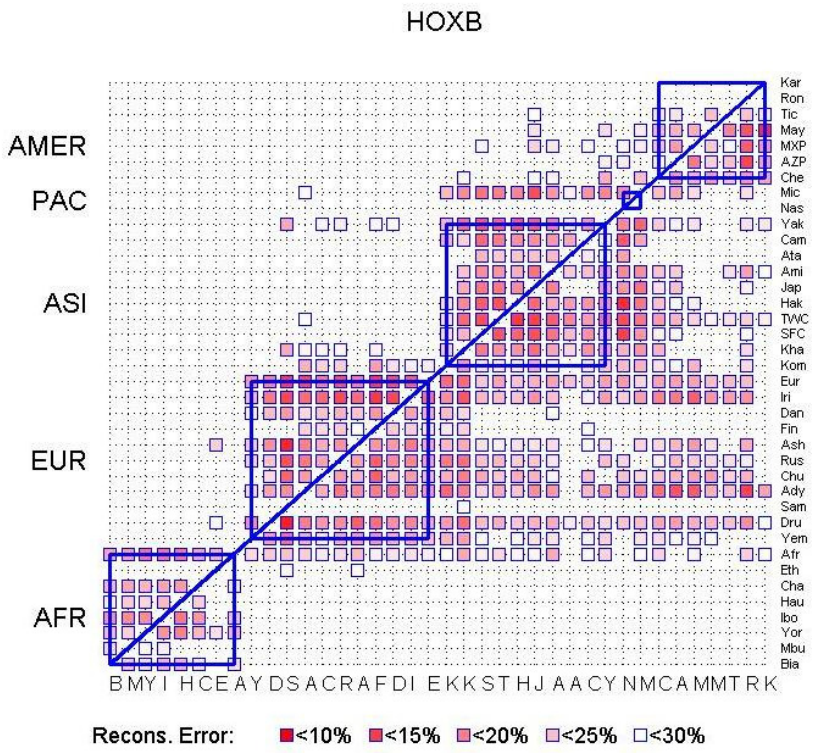
(Training set: individuals in X; Test set: individuals in Y; A: contains all individuals in both X and Y.)




PAH
AMER
PAC
ASI
EUR
AFR
Kar
Ron
Tic
May
MXP
AZP
Che
Mic
Nas
Yak
Cam
Ata
Ami
Jap
Hak
TWC
SFC
Kha
Kom
Eur
Iri
Dan
Fin
Ash
Rus
Chu
Ady
Sam
Dru
Yem
Afr
Eth
Cha
Hau
Ibo
Yor
Mbu
Bia
B M Y I H C E A Y D S A C R A F D I E K K S T H J A A C Y N M C A M M T R K
Recons. Error: <10% <15% <20% <25% <30%


SORCS3
AMER
PAC
ASI
EUR
AFR
Kar
Ron
Tic
May
MXP
AZP
Che
Mic
Nas
Yak
Cam
Ata
Ami
Jap
Hak
TWC
SFC
Kha
Kom
Eur
Iri
Dan
Fin
Ash
Rus
Chu
Ady
Sam
Dru
Yem
Afr
Eth
Cha
Hau
Ibo
Yor
Mbu
Bia
B M Y I H C E A Y D S A C R A F D I E K K S T H J A A C Y N M C A M M T R K
Recons. Error: <10% <15% <20% <25% <30%


17q25
AMER
PAC
ASI
EUR
AFR
Kar
Ron
Tic
May
MXP
AZP
Che
Mic
Nas
Yak
Cam
Ata
Ami
Jap
Hak
TWC
SFC
Kha
Kom
Eur
Iri
Dan
Fin
Ash
Rus
Chu
Ady
Sam
Dru
Yem
Afr
Eth
Cha
Hau
Ibo
Yor
Mbu
Bia
B M Y I H C E A Y D S A C R A F D I E K K S T H J A A C Y N M C A M M T R K
Recons. Error: <10% <15% <20% <25% <30%

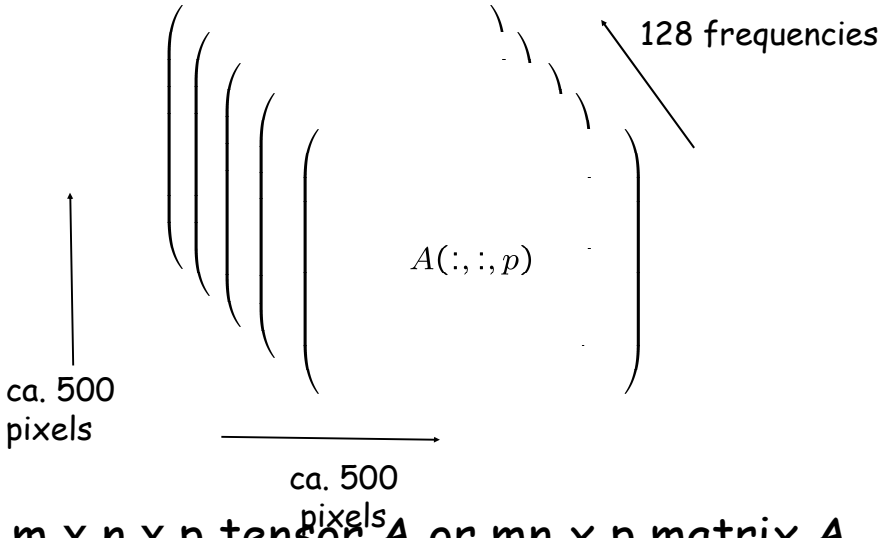

HOXB
AMER
PAC
ASI
EUR
AFR
Kar
Ron
Tic
May
MXP
AZP
Che
Mic
Nas
Yak
Cam
Ata
Ami
Jap
Hak
TWC
SFC
Kha
Kom
Eur
Iri
Dan
Fin
Ash
Rus
Chu
Ady
Sam
Dru
Yem
Afr
Eth
Cha
Hau
Ibo
Yor
Mbu
Bia
B M Y I H C E A Y D S A C R A F D I E K K S T H J A A C Y N M C A M M T R K
Recons. Error: <10% <15% <20% <25% <30%

CUR Data Application: Hyperspectral Image Analysis

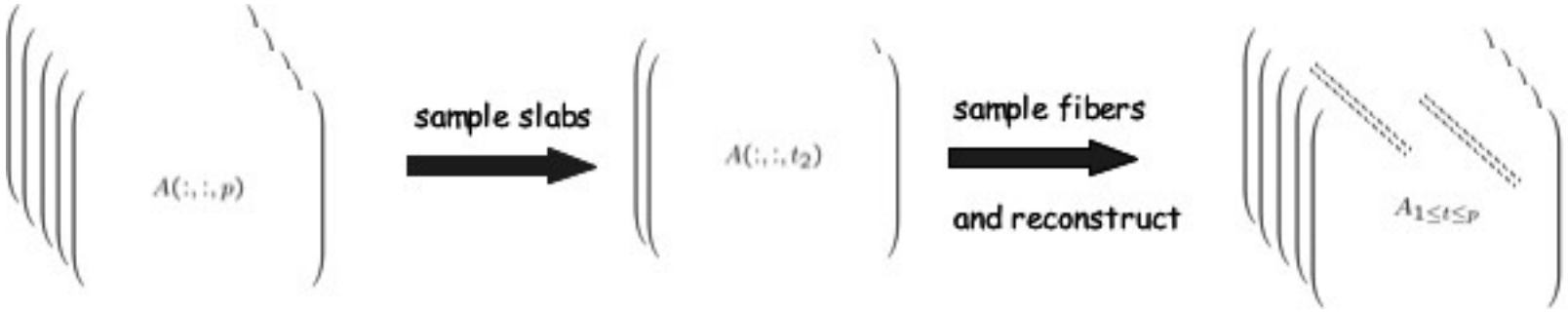
(Joint work with M. Maggioni and R. Coifman lab at Yale University)

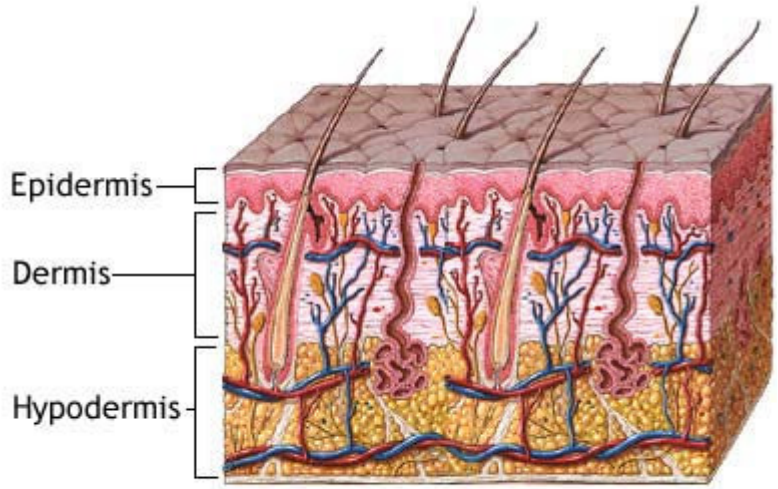
The Data: Images of a single object (e.g., earth or colon cells) at many consecutive frequencies.

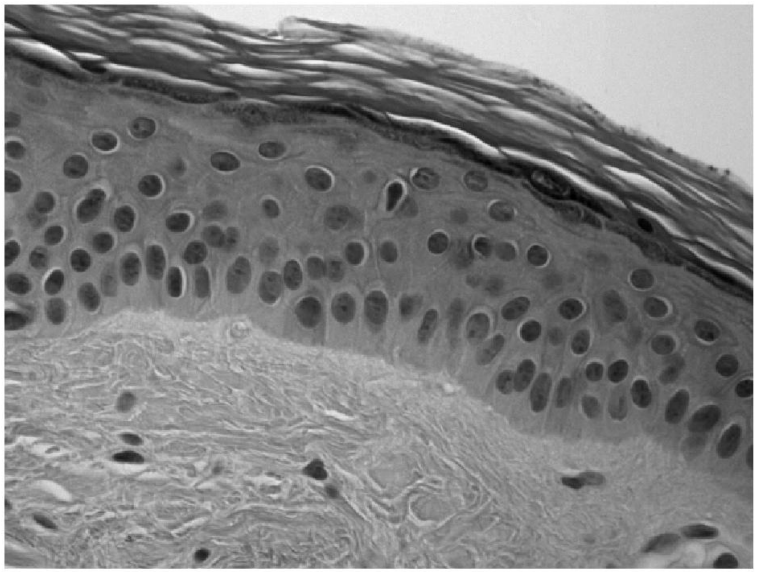
The Goal: Lossy compression, data reconstruction, and classification using a small number of samples (images and/or pixels).

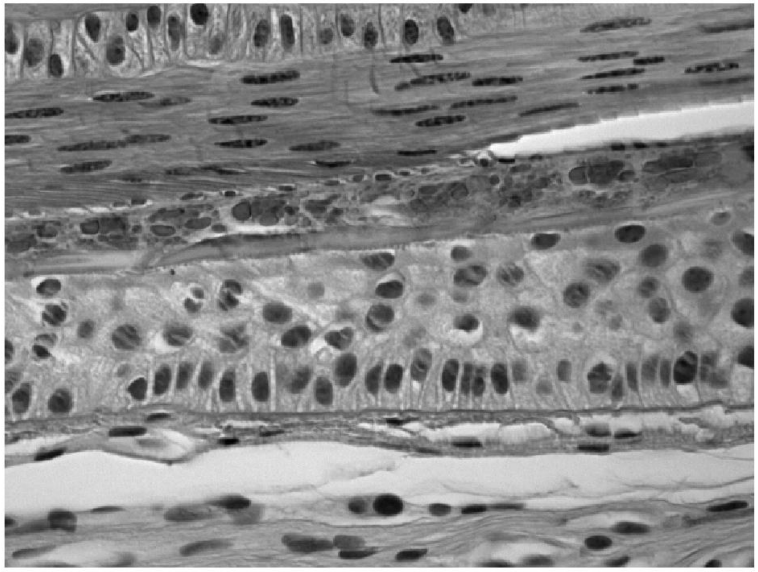


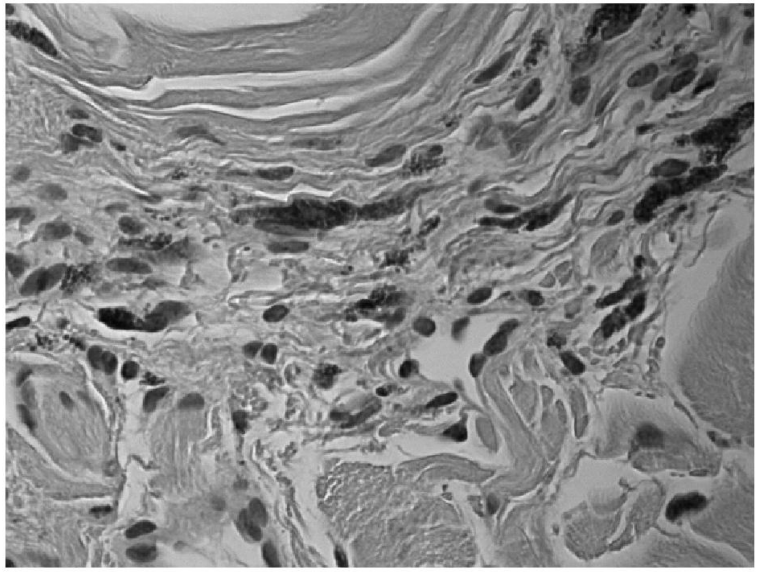
m x n x p tensor A or mn x p matrix A



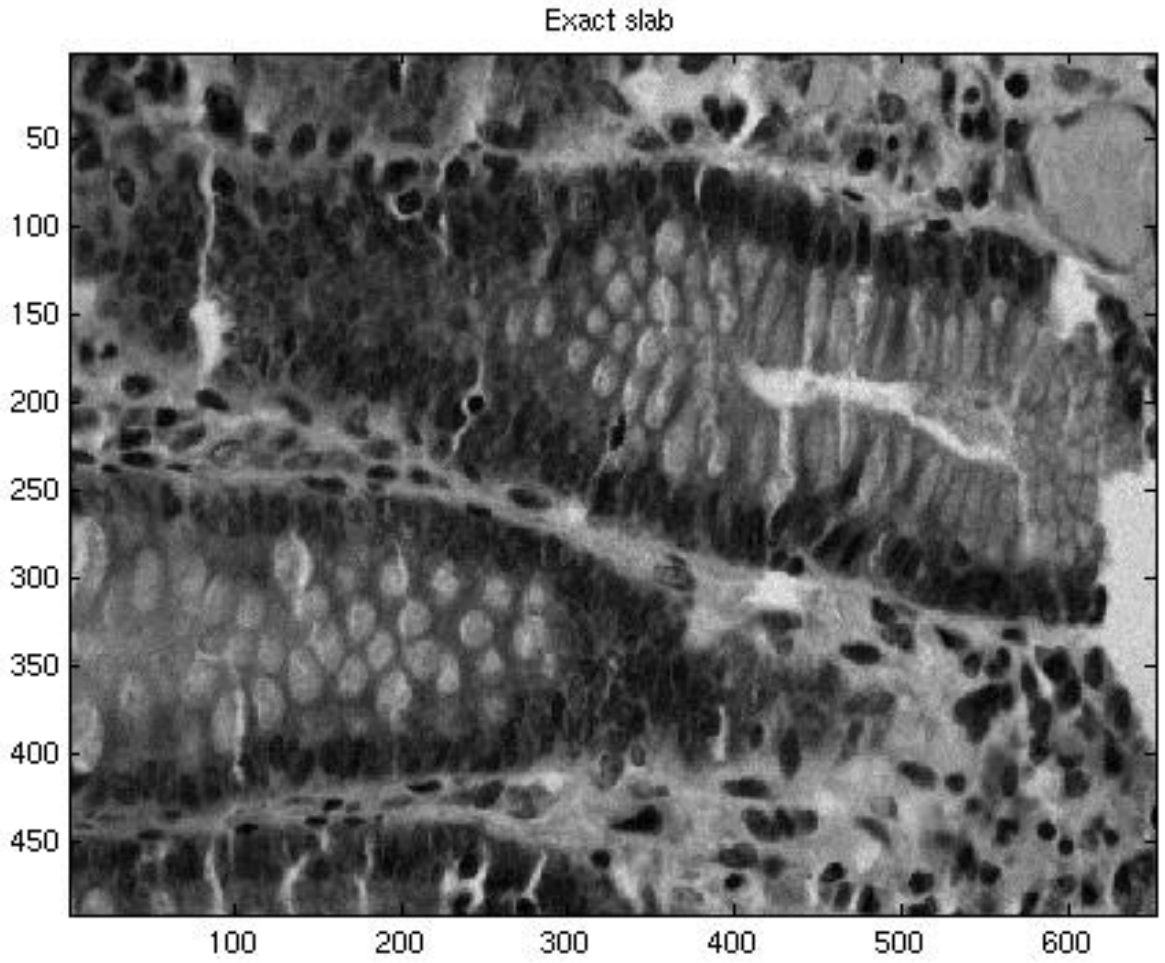

Epidermis
Dermis
Hypodermis



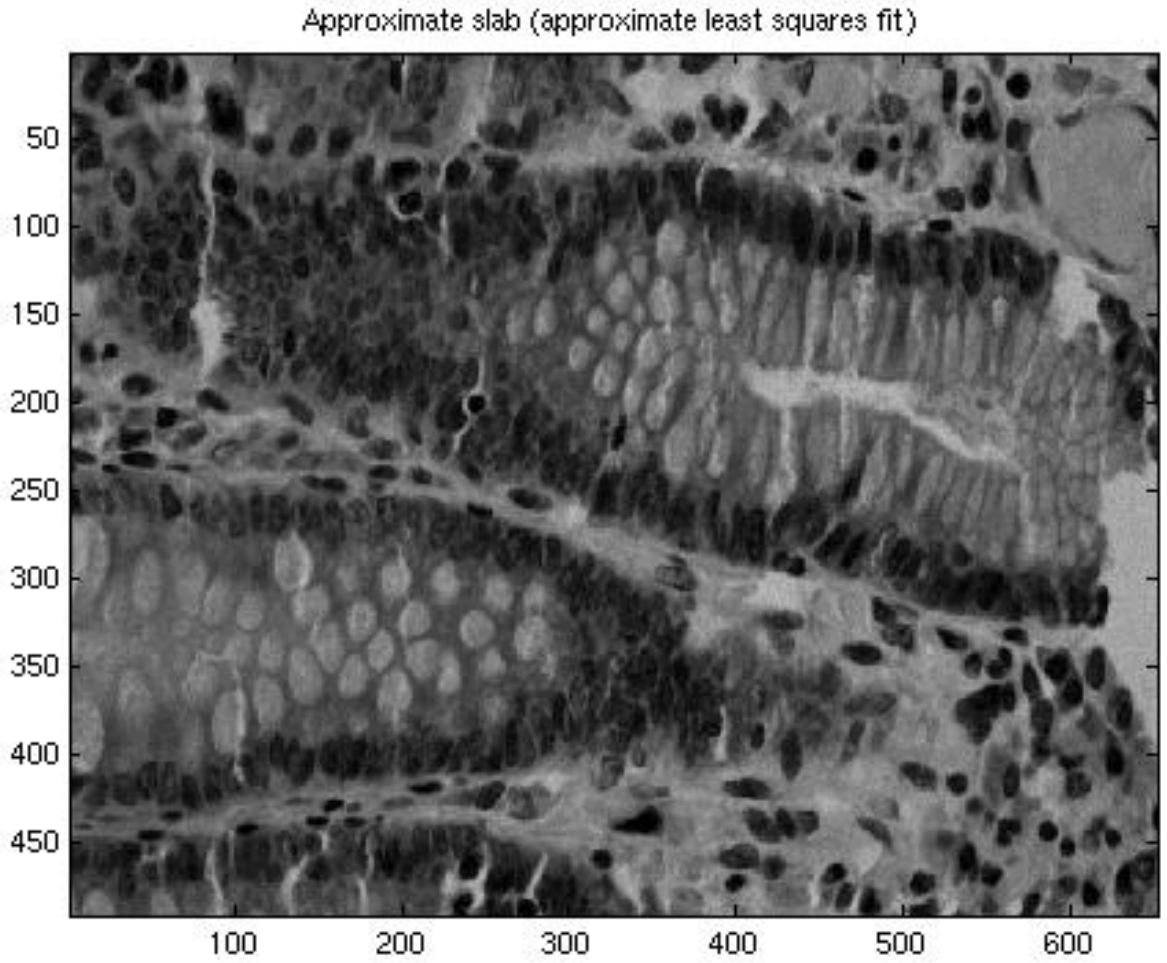




Look at the exact (65-th) slab.

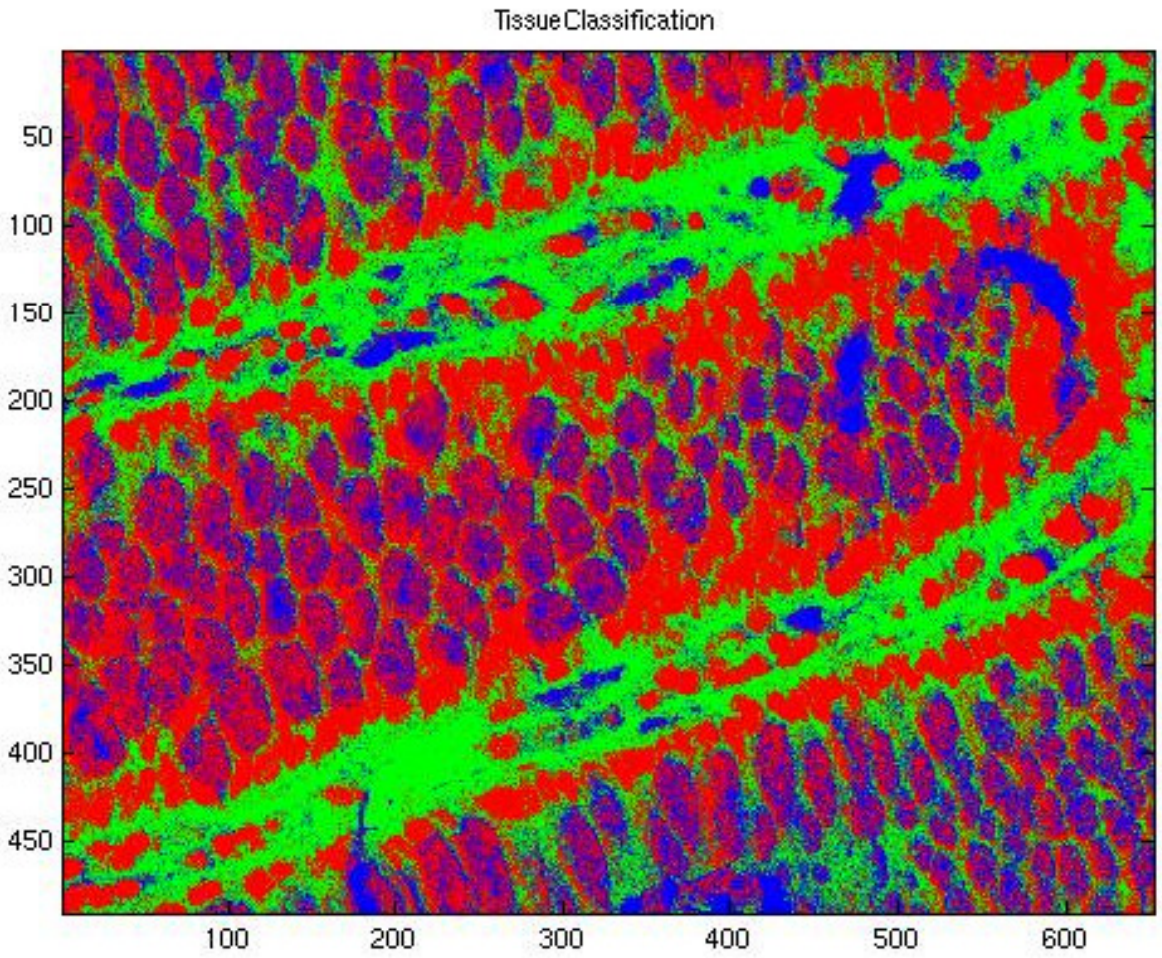


The (65-th) slab approximately reconstructed

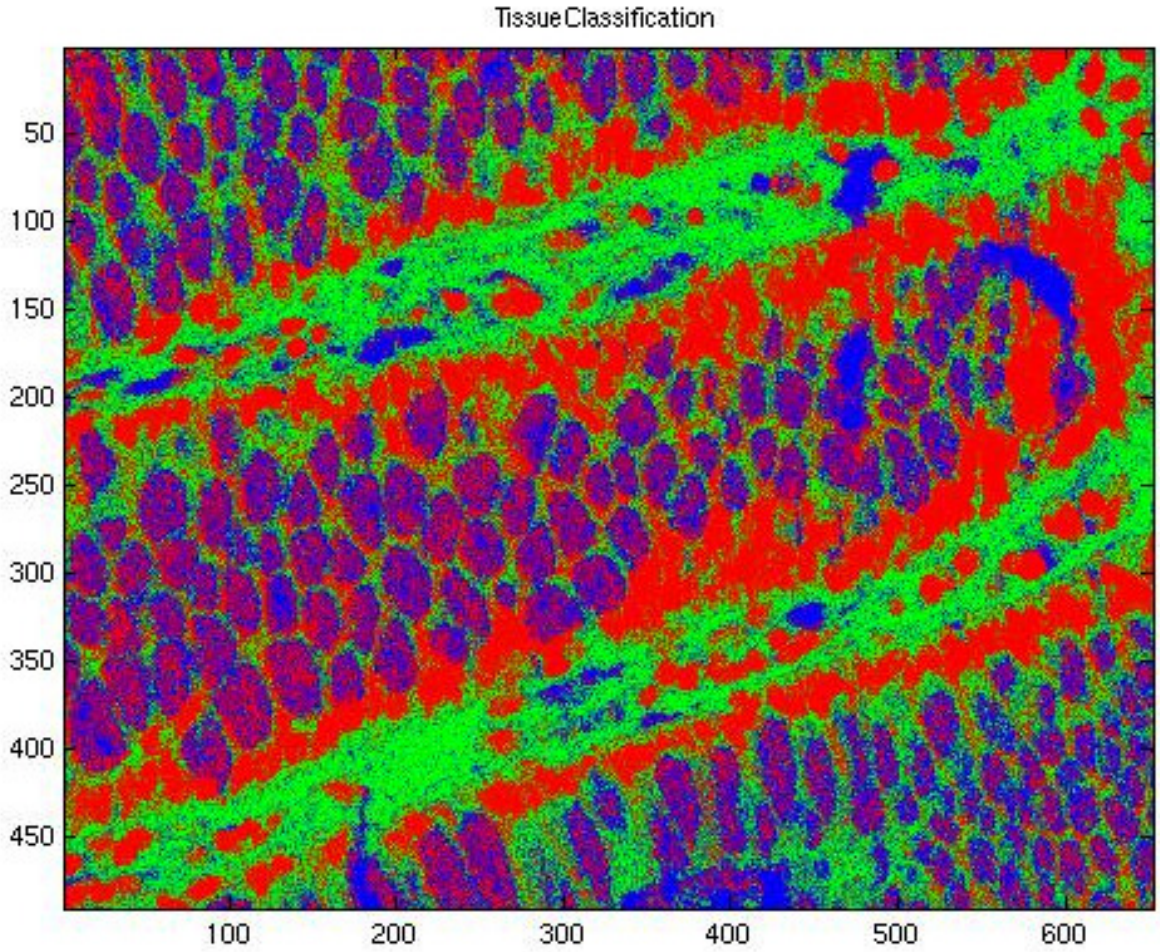


This slab was reconstructed by approximate least-squares fit to the basis from slabs 41 and 50, using 1000 (of 250K) pixels/fibers.

Tissue Classification - Exact Data



Tissue Classification - N_s=12 & N_f=1000



CUR Data Application: Recommendation Systems

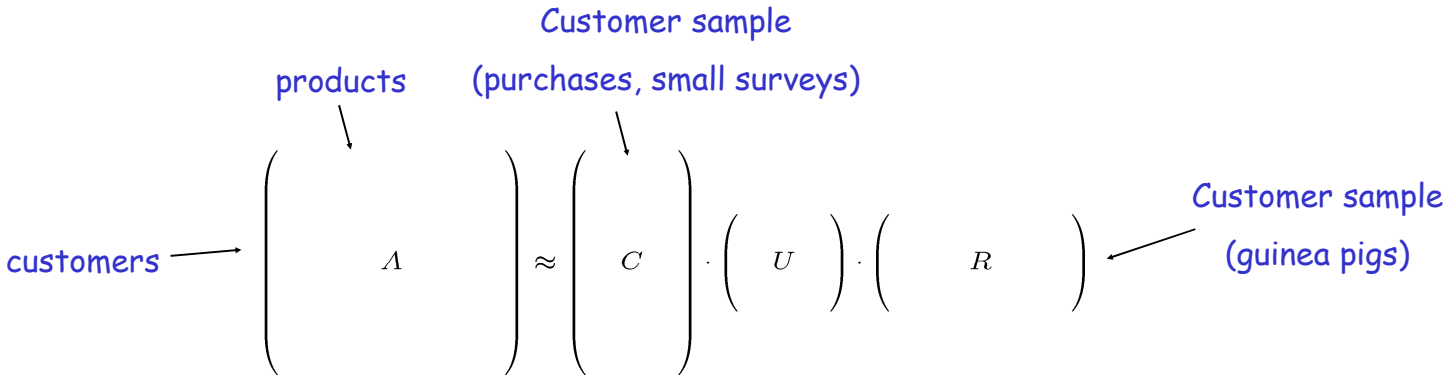
Problem: m customers and n products; A_{ij} is the (unknown) rating/utility of product j for customer i.

Goal: recreate A from a few samples to recommend high utility products.

- (KRRT98): Assuming strong clustering of the products, competitive algorithms even with only 2 samples/customer.
- (AFKMS01): Assuming sampling of $\Omega(mn)$ entries of A and a gap requirement, accurately recreate A.
- *Lots* of applied work, especially at large internet companies!

Q: Can we get competitive performance by sampling o(mn) elements?

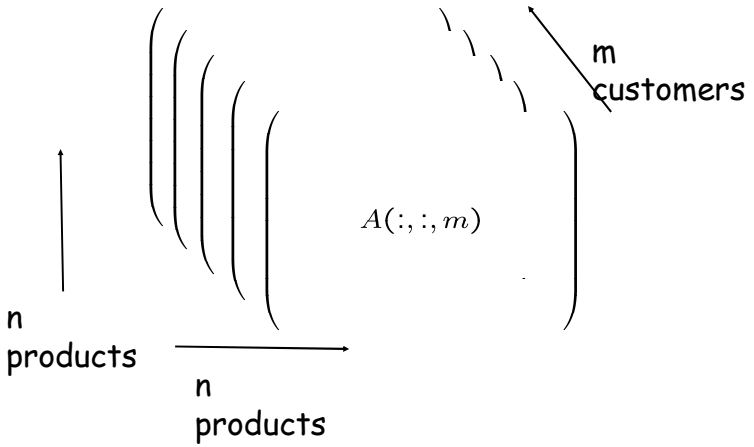
A: Apply the CUR decomposition:



Recommendation systems, cont'd

Recommendation Model Revisited:

- Given n products and m customers, *each* customer has an n x n {-1,+1}- "preference" matrix.
- Motivation: Utility is ordinal and not cardinal, so compare products; don't assign utility values.
- *Application: Did a user click on link A or link B?*



View each preference matrix as a vector, get an m x n^2 matrix, ...

... and express this matrix in terms of its columns and rows!

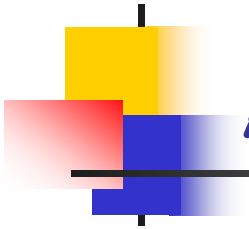
customers (m)

$$\begin{pmatrix} & A & \end{pmatrix} \approx \begin{pmatrix} & C & \end{pmatrix} \cdot \begin{pmatrix} & U & \end{pmatrix} \cdot \begin{pmatrix} & R & \end{pmatrix}$$

"preferences" (n^2)

a few "preferences" are known for all customers

all "preferences" are known for a few customers



Application to Jester Joke Recommendations

Use just the 14,140 "full" users who rated all 100 Jester jokes.

For each user, convert the utility vector to 100 x 100 pair-wise preference matrix.

Choose, e.g., 300 users (slabs), and a small number of comparisons (fibers).

Conclusion

CUR Low-Rank Matrix Decompositions:

- Uses actual columns and/or rows.
- Useful if data have low-rank structure *and* other structure.
- Provable performance guarantees within ε of "best."
- Performs well in practice on genetic, medical imaging, and internet data.