Randomized Numerical Linear Algebra

http://bicmr.pku.edu.cn/~wenzw/bigdata2023.html

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Outline

1. Randomized Numerical Linear Algebra (RandNLA)
2. Approximating Matrix Multiplication
3. Approximate SVD
4. Random Sampling for SVD
5. Single View Algorithm For Matrix Approximation

Why RandNLA?

Randomization and sampling allow us to design provably accurate algorithms for problems that are:

- **Massive**
  (matrices so large that can not be stored at all, or can only be stored in slow memory devices)

- **Computationally expensive or NP-hard**
  (combinatorial optimization problems such as the Column Subset Selection Problem)

RandNLA: sampling rows/columns

Randomized algorithms

- By (carefully) sampling rows/columns of a matrix, we can construct new, smaller matrices that are close to the original matrix (w.r.t. matrix norms) with high probability.

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

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

RandNLA: sampling rows/columns

Matrix perturbation theory

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

Structural results that "decouple" the "randomized" part from the "matrix perturbation" part are important in the analyses of such algorithms.

Interplay

- Applications in BIG DATA: (Data Mining, Information Retrieval, Machine Learning, Bioinformatics, etc.)
- Numerical Linear Algebra: Matrix computations and linear algebra (ie., perturbation theory)
- Theoretical Computer Science: Randomized and approximation algorithms

Issues

- 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 takes about 12 minutes.
  - 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.
- Obviously, running time is a concern.
- Machine-precision accuracy is NOT necessary!
  - Data are noisy.
  - Approximate singular vectors work well in our settings.

Issues

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

The two issues:

- Fast approximation to the top k singular vectors of a matrix, and
- Selecting columns that capture the structure of the top k singular vectors

are connected and can be tackled using the same framework

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Approximating Matrix Multiplication

Problem Statement

Given an m-by-n matrix A and an n-by-p matrix B, approximate the product AB, Or equvialently, Approximate the sum of n rank-one matrices

$$AB = \sum_{i=1}^{n} \underbrace{\left(A^{(i)} \right) \left(\quad B_{(i)} \quad \right)}_{\in \mathbb{R}^{m \times p}}$$

- $A^{(i)}$ the i-th column of A
- $B_{(i)}$ the i-th row of B
- Each term in the summation is a rank-one matrix

A sampling approach

$$AB = \sum_{i=1}^{n} \underbrace{\left(A^{(i)} \right) \left(\quad B_{(i)} \quad \right)}_{\in \mathbb{R}^{m\times p}}$$

Algorithm

- Fix a set of probabilities p_i, $i = 1, \ldots, n$, summing up to 1.
- For $t = 1, \ldots, c$,
  set $j_t = i$, where $P(j_t = i) = p_i$.
  (Pick c terms of the sum, with replacement, with respect to the p_i.)
- Approximate the product AB by summing the c terms, after scaling.

Generate Discrete Distributions

Consider a discrete random variable with possible values $c_1 < \ldots < c_n$. The probability attached to c_i is p_i. Let

$$q_0 = 0, \quad q_i = \sum_{j=1}^{i} p_j.$$

They are the cumulative probabilities associated with c_i, i.e., $q_i = F(c_i)$.

To sample this distribution

- generate a uniform U
- find $K \in \{1, \ldots, n\}$ such that $q_{K-1} < U < q_K$
- set $X = c_K$

With/without replacement

- Sampling with replacement:
  Each data unit in the population is allowed to appear in the sample more than once.
  It is easy to analyze mathematically.
- Sampling without replacement:
  Each data unit in the population is allowed to appear in the sample no more than once.

A sampling approach

$$\begin{aligned} AB &= \sum_{i=1}^{n} \underbrace{\begin{pmatrix} A^{(i)} \end{pmatrix} \begin{pmatrix} \quad B_{(i)} \quad \end{pmatrix}}_{\in \mathbb{R}^{m \times p}} \\ &\approx \frac{1}{c} \sum_{t=1}^{c} \frac{1}{p_{j_t}} \underbrace{\begin{pmatrix} A^{(j_t)} \end{pmatrix} \begin{pmatrix} \quad B_{(j_t)} \quad \end{pmatrix}}_{\in \mathbb{R}^{m \times p}} \end{aligned}$$

Keeping the terms $j_1, j_2, \ldots, j_c$

The algorithm (matrix notation)

$$\overset{m \times n}{\begin{pmatrix} \\ \quad\quad A \quad\quad \\ \\ \end{pmatrix}} \overset{n \times p}{\begin{pmatrix} \\ \quad\quad B \quad\quad \\ \\ \end{pmatrix}} \approx \overset{m \times c}{\begin{pmatrix} \\ \quad\quad C \quad\quad \\ \\ \end{pmatrix}} \overset{c \times p}{\begin{pmatrix} \quad\quad R \quad\quad \end{pmatrix}}$$

Algorithm:

- Pick c columns of A to form an m-by-c matrix C and the corresponding c rows of B to form a c-by-p matrix R.
- Approximate AB by CR.

Note

- We pick the columns and rows with non-uniform probabilities.
- We scale the columns (rows) prior to including them in $C(R)$.

The algorithm (matrix notation)

$$\begin{array}{ccccc} m \times n & n \times p & & m \times c & c \times p \\ \begin{pmatrix} & & \\ & A & \\ & & \end{pmatrix} & \begin{pmatrix} & & \\ & B & \\ & & \end{pmatrix} & \approx & \begin{pmatrix} & & \\ & C & \\ & & \end{pmatrix} & \begin{pmatrix} & R & \end{pmatrix} \end{array}$$

Algorithm:

- Create C and R by performing c i.i.d. trials, with replacement.
- For $t = 1, \ldots, c$, pick a column $A^{(j_t)}$ and a row $B_{(j_t)}$ with probability

$$\mathbf{P}(j_t = i) = \frac{\|A^{(i)}\|_2 \|B_{(i)}\|_2}{\sum_{j=1}^{n} \|A^{(j)}\|_2 \|B_{(j)}\|_2}$$

- Include $A^{(j_t)}/(cp_{j_t})^{1/2}$ as a column of C, and $B_{(j_t)}/(cp_{j_t})^{1/2}$ as a row of R

The algorithm (matrix notation)

- Let S be an n-by-c matrix whose t-th column (for $t = 1, \ldots, c$) has a single non-zero entry, namely

  $$S_{j_t t} = \frac{1}{\sqrt{c p_{j_t}}}$$

  Clearly:

  $$AB \approx CR = (AS)(S^T B)$$

  Note: S is sparse (has exactly c non-zero elements, one per column).
- It is easy to implement this particular sampling in two passes.

A bound for the Frobenius norm

For the above algorithm,

$$\mathbf{E}[\|AB - CR\|_F] = \mathbf{E}[\|AB - ASS^T B\|_F] \leq \frac{1}{c}\|A\|_F\|B\|_F$$

- The expectation of CR (element-wise) is AB (unbiased estimator), regardless of the sampling probabilities.
- Our particular choice of sampling probabilities minimizes the variance of the estimator (w.r.t. the Frobenius norm of the error AB-CR).
- prove using elementary manipulations of expectation
- Measure concentration follows from a martingale argument.
- The above bound also implies an upper bound for the spectral norm of the error $AB - CR$.

Proofs

Let $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{p\times p}$, $1 \le c \le n$, and $p_i \ge 0$, $\sum_i p_i = 1$. Then

$$\mathbf{E}[(CR)_{ij}] = (AB)_{ij}, \quad \mathrm{Var}[(CR)_{ij}] = \frac{1}{c}\sum_{i=1}^{n}\frac{A_{ik}^2 B_{kj}^2}{p_k} - \frac{1}{c}(AB)_{ij}^2$$

- Define $X_t = \left(\frac{A^{(i_t)}B_{(i_t)}}{cp_{i_t}}\right)_{ij} = \frac{A_{ii_t}B_{i_tj}}{cp_{i_t}}$. Then

$$\mathbf{E}[X_t] = \sum_{k=1}^{n} p_k \frac{A_{ik}B_{kj}}{cp_k} = \frac{1}{c}(AB)_{ij} \text{ and } \mathbf{E}[X_t^2] = \sum_{k=1}^{n}\frac{A_{ik}^2 B_{kj}^2}{c^2 p_k}$$

- $\mathbf{E}[(CR)_{ij}] = \sum_{t=1}^{c} \mathbf{E}[X_t] = (AB)_{ij}$

$$\mathrm{Var}[X_t] = E[X_t^2] - E[X_t]^2 = \sum_{k=1}^{n}\frac{A_{ik}^2 B_{kj}^2}{c^2 p_k} - \frac{1}{c^2}(AB)_{ij}^2$$

Proofs

Lemma:

$$\mathbf{E}[\|AB - CR\|_F^2] = \sum_{k=1}^{n} \frac{|A^{(k)}|^2 |B_{(k)}|^2}{cp_k} - \frac{1}{c}\|AB\|_F^2$$

Proof:

$$\begin{aligned}
\mathbf{E}[\|AB - CR\|_F^2] &= \sum_{i=1}^{n}\sum_{j=1}^{p} \mathbf{E}[(AB - CR)_{ij}^2] = \sum_{i=1}^{n}\sum_{j=1}^{p} \mathrm{Var}[(CR)_{ij}] \\
&= \frac{1}{c}\sum_{k=1}^{n} \frac{1}{p_k}\left(\sum_i A_{ik}^2\right)\left(\sum_i B_{kj}^2\right) - \frac{1}{c}\|AB\|_F^2 \\
&= \frac{1}{c}\sum_{k=1}^{n} \frac{1}{p_k}|A^{(k)}|^2 |B_{(k)}|^2 - \frac{1}{c}\|AB\|_F^2
\end{aligned}$$

Proofs

- Find p_k to minimize $\mathbf{E}[\|AB - CR\|_F^2]$:

$$\min_{\sum_{k=1}^n p_k = 1} f(p_1, \ldots, p_n) = \sum_{k=1}^n \frac{1}{p_k} |A^{(k)}|^2 |B_{(k)}|^2$$

- Introduce $L = f(p_1, \ldots, p_n) + \lambda(\sum_{k=1}^n p_k - 1)$ and solve $\frac{\partial L}{\partial p_i} = 0$

- It gives $p_k = \frac{|A^{(k)}||B_{(k)}|}{\sum_{k'=1}^n |A^{(k')}||B_{(k')}|}$. Then

$$\begin{aligned}
\mathbf{E}[\|AB - CR\|_F^2] &= \frac{1}{c}\left(\sum_{k=1}^n |A^{(k)}||B_{(k)}|\right)^2 - \frac{1}{c}\|AB\|_F^2 \\
&\leq \frac{1}{c}\|A\|_F^2 \|B\|_F^2
\end{aligned}$$

Special case: $B = A^T$

If $B = A^T$, then the sampling probabilities are

$$\mathbf{P}(j_t = i) = \frac{\|A^{(i)}\|_2^2}{\|A\|_F^2}$$

Also, $R = C^T$, and the error bounds are:

$$\mathbf{E}[\|AA^T - CC^T\|_F] = \mathbf{E}[\|AA^T - ASS^TA^T\|_F] \leq \frac{1}{c}\|A\|_F^2$$

Special case: $B = A^T$

A better spectral norm bound via matrix Chernoff/Bernstein inequalities:

Assumptions:

- Spectral norm of A is one (not important, just normalization)
- Frobenius norm of A is at least 0.2 (not important, simplifies bounds).
- Important: Set

$$c = \Omega\left(\frac{\|A\|_F^2}{\epsilon^2}\ln\left(\frac{\|A\|_F^2}{\epsilon^2\sqrt{\delta}}\right)\right)$$

Then: for any $0 < \epsilon < 1$ with probability at least $1 - \delta$

$$\mathbf{E}[\|AA^T - CC^T\|_F] = \mathbf{E}[\|AA^T - ASS^TA^T\|_F] \leq \epsilon$$

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Low-Rank Matrix Approximation

Problem Statement:
Given: mxn matrix A, and $0 < k < \min(m,n) = n$.
Goal: Compute a rank-k approximation to A.

- Fast low-rank matrix approximation is key to efficiency of superfast direct solvers for integral equations and many large sparse linear systems.
- Indispensable tool in mining large data sets.
- Randomized algorithms compute accurate truncated SVD.
- Minimum work and communication/Exceptionally high success rate.

Low-rank Approximation

seek to compute a rank-k approximation with $k \ll n$

$$\overset{m \times n}{\begin{pmatrix} & & \\ & & \\ & A & \\ & & \\ & & \end{pmatrix}} \approx \overset{m \times k}{\begin{pmatrix} & & \\ & & \\ & U_k & \\ & & \\ & & \end{pmatrix}} \overset{k \times n}{\begin{pmatrix} & & \\ & X & \\ & & \end{pmatrix}}$$

- Eigenvectors corresponding to leading eigenvalues.
- Singular Value Decomposition (SVD) / Principal Component Analysis (PCA).
- Spanning columns or rows.

The problem being addressed is ubiquitous in applications.

Review of existing methods: dense matrix

For a dense $n \times n$ matrix that fits in RAM, excellent algorithms are already part of LAPACK (and incorporated into Matlab, Mathematica, etc).

- Double precision accuracy.
- Very stable.
- $O(n^3)$ asymptotic complexity. Reasonably small constants.
- Require extensive random access to the matrix.
- When the target rank k is much smaller than n, there also exist $O(n^2k)$ methods with similar characteristics (the well-known Golub-Businger method, RRQR by Gu and Eisentstat, etc).
- For small matrices, the state-of-the-art is quite satisfactory. (By "small" we mean something like $n \leq 10000$ on today's computers.)

Review of existing methods: structured matrix

If the matrix is large, but can rapidly be applied to a vector (if it is sparse, or sparse in Fourier space, or amenable to the FMM, etc.), so called Krylov subspace methods often yield excellent accuracy and speed.

Lanczos-based methods:

1. From $v \in \mathbb{R}^n$, computes orthonormal basis V for

$$\mathcal{K}(A, v) = span\left\{v, Av, A^2v, \cdots, A^{k-1}v\right\}$$

2. Rayleigh-Ritz: $eig(V^TAV) \Rightarrow$ Ritz pairs $\approx$ eigenpairs
3. If “not converged”, update v and go to Step 1.

Strength and weakness:

- Most efficient in terms of the number of Av (or SpMv)
- Fast and reliable for computing “not too many” eigenpairs
- Lower concurrency and unable to be warm-started

“New” challenges in algorithmic design

The existing state-of-the-art methods of numerical linear algebra that we have very briefly outlined were designed for an environment where the matrix fits in RAM and the key to performance was to minimize the number of floating point operations required. Currently, communication is becoming the real bottleneck:

- While clock speed is hardly improving at all anymore, the cost of a flop keeps going down rapidly. (Multi-core processors, GPUs, cloud computing, etc.)
- The cost of slow storage (hard drives, flash memory, etc.) is also going down rapidly.
- Communication costs are decreasing, but not rapidly. Moving data from a hard-drive. Moving data between nodes of a parallel machine. (Or cloud computer ...) The amount of fast cache memory close to a processor is not improving much. (In fact, it could be said to be shrinking — GPUs, multi-core, etc.)
- “Deluge of data”. Driven by ever cheaper storage and acquisition techniques. Web search, data mining in archives of documents

Review of existing randomized methods

- Random column/row selection
  Draw at random some columns and suppose that they span the entire column space. If rows are drawn as well, then spectral properties can be estimated. Crude sampling leads to less than O(mn) complexity, but is very dangerous.

- Sparsification
  Zero out the vast majority of the entries of the matrix. Keep a random subset of entries, and boost their magnitude to preserve "something".

- Quantization and sparsification
  Restrict the entries of the matrix to a small set of values (-1/0/1 for instance).

- Randomized Subspace iteration
  Random sampling + Rayleigh Rtiz procedure

Linear Time SVD Algorithm

- Input: m-by-n matrix A, $1 \leq k \leq c \leq n$, $\{p_i\}_{i=1}^n$ such that $p_i \geq 0$ and $\sum_i p_i = 1$
- Sampling:
  - For $t = 1$ to c

    pick $i_t \in \{1, \ldots, n\}$ with $\mathcal{P}(i_t = \alpha) = p_\alpha$.

    Set $C^{(t)} = \frac{A^{(i_t)}}{\sqrt{cp_{i_t}}}$
- Compute $C^T C$ and its eigenvalue decomposition, say $C^T C = \sum_{t=1}^c \sigma_t(C)^2 y_t y_t^T$
- Compute $h_t = \frac{Cy_t}{\sigma_t(C)}$ for $t = 1, \ldots, k$.

  (Note: $A = U\Sigma V^T$ and $C = H\Sigma_C Y^T \Longrightarrow H = CY\Sigma_C^{-1}$)
- Return H_k where $H_k^{(t)} = h_t$ and $\sigma_t(C)$ for $t = 1, \ldots, k$

The left singular vectors of C are with high probability approximations to the left singular vectors of A

Extract approximate SVD

- Given A. Let X be an approximation of the left singular vectors of A corresponding to k largest singular values

```
method = 2;    % = 1 or 2
Y = (X'*A)';     % Y = A'*X;
switch method
    case 1;
        [V,S,W] = svd(Y,0);
        U = X*W;
    case 2;
        [V,R] = qr(Y,0);
        [W,S,Z] = svd(R');
        U = X*W; V = V*Z;
 end
```

- The pair (U, S, V) is an approximation of the k-dominant SVD

Main theoretical results

Let H_k be constructed the linear Time SVD

$$\mathbf{E}[\|A - H_k H_k^T A\|_F^2] \leq \|A - A_k\|_F^2 + \epsilon \|A\|_F^2$$

- Exact SVD of $A = U\Sigma V^T$, $A_k = U_k \Sigma_k V_k^T = U_k U_k^T A = AV_k V_k^T$.
  $\min_{\text{rank}(B)\leq k} \|A - B\|_2 = \|A - A_k\|_2 = \sigma_{k+1}(A)$
  $\min_{\text{rank}(B)\leq k} \|A - B\|_F^2 = \|A - A_k\|_F^2 = \sum_{t=k+1}^{r} \sigma_t^2(A)$
- perturbation theory of matrices

  $$\max_{1\leq t\leq n} |\sigma_t(A+E) - \sigma_t(A)| \leq \|E\|_2, \quad \sum_{k=1}^{n} (\sigma_k(A+E) - \sigma_k(A))^2 \leq \|E\|_F^2$$

  the latter is known as Hoffman-Wielandt inequality
- Exact SVD of $C = H\Sigma_C Y^T$

Proofs

Lemma:

$$\begin{aligned} \|A - H_k H_k^T A\|_F^2 &\leq \|A - A_k\|_F^2 + 2\sqrt{k}\|AA^T - CC^T\|_F \\ \|A - H_k H_k^T A\|_2^2 &\leq \|A - A_k\|_2^2 + 2\|AA^T - CC^T\|_2 \end{aligned}$$

Proof of the first inequality

- $\|X\|_F^2 = \mathrm{Tr}(X^T X)$ and $\mathrm{Tr}(X+Y) = \mathrm{Tr}(X) + \mathrm{Tr}(Y)$

$$\begin{aligned} \|A - H_k H_k^T A\|_F^2 &= \mathrm{Tr}((A - H_k H_k^T A)^T (A - H_k H_k^T A)) \\ &= \mathrm{Tr}(A^T A) - \mathrm{Tr}(A^T H_k H_k^T A) = \|A\|_F^2 - \|A^T H_k\|_F^2 \end{aligned}$$

- Using Cauchy-Schwartz inequality:

$$\left| \|A^T H_k\|_F^2 - \sum_{t=1}^{k} \sigma_t^2(C) \right| \leq \sqrt{k} \left(\sum_{t=1}^{k} (|A^T h_t|^2 - \sigma_t^2(C))^2 \right)^{1/2}$$

$$\begin{aligned} &= \sqrt{k} \left(\sum_{t=1}^{k} (|A^T h_t|^2 - |C^T h_t|^2)^2 \right)^{1/2} = \sqrt{k} \left(\sum_{t=1}^{k} ((h_t)^T (AA^T - CC^T) h_t)^2 \right)^{1/2} \\ &\leq \sqrt{k} \|AA^T - CC^T\|_F \end{aligned}$$

Proofs

- by Hoffman-Wielandt inequality

$$
\begin{aligned}
& \left|\sum_{t=1}^{k}\sigma_t^2(C)-\sum_{t=1}^{k}\sigma_t^2(A)\right| \le \sqrt{k}\left(\sum_{t=1}^{k}(\sigma_t^2(C)-\sigma_t^2(A))^2\right)^{1/2} \\
= \quad & \sqrt{k}\left(\sum_{t=1}^{k}(\sigma_t(CC^T)-\sigma_t(AA^T))^2\right)^{1/2} \\
\le \quad & \sqrt{k}\left(\sum_{t=1}^{m}(\sigma_t(CC^T)-\sigma_t(AA^T))^2\right)^{1/2} \le \sqrt{k}\|CC^T-AA^T\|_F
\end{aligned}
$$

- Therefore

$$
\left|\|A^TH_k\|_F^2-\sum_{t=1}^{k}\sigma_t^2(A)\right| \le 2\sqrt{k}\|AA^T-CC^T\|_F
$$

Proofs

- matrix approximation gives

$$\mathbf{E}[\|AB - CR\|_F^2] \quad \leq \quad \frac{1}{c}\|A\|_F^2\|B\|_F^2$$

  which yields

$$2\sqrt{k}\mathbf{E}[\|AA^T - CC^T\|_F] \quad \leq \quad \left(\frac{4k}{c}\right)^{1/2}\|A\|_F^2$$

-

$$\|A^T H_k\|_F^2 \geq \sum_{t=1}^{k}\sigma_t^2(A) - 2\sqrt{k}\|AA^T - CC^T\|_F$$

- If $c \geq 4k/\epsilon^2$, then

$$\begin{aligned}\mathbf{E}[\|A - H_k H_k^T A\|_F^2] \quad &\leq \quad \|A\|_F^2 - \sum_{t=1}^{k}\sigma_t^2(A) + 2\sqrt{k}\mathbf{E}[\|AA^T - CC^T\|_F] \\ &\leq \quad \|A - A_k\|_F^2 + \epsilon\|A\|_F^2\end{aligned}$$

The CX decomposition

Mahoney & Drineas (2009) PNAS

$$\overset{m \times n}{\begin{pmatrix} & & \\ & & \\ & A & \\ & & \\ & & \end{pmatrix}} \approx \overset{m \times c}{\begin{pmatrix} & & \\ & & \\ & C & \\ & & \\ & & \end{pmatrix}} \overset{c \times n}{\begin{pmatrix} & & \\ & X & \\ & & \end{pmatrix}}$$

- Goal: make (some norm) of $A - CX$ small.
- C: c columns of A, with c being as close to k as possible
- Moore-Penrose pseudoinverse of A:

$$AA^{\dagger}A = A, A^{\dagger}AA^{\dagger} = A^{\dagger}, (AA^{\dagger})^{*} = AA^{\dagger}, (A^{\dagger}A)^{*} = A^{\dagger}A$$

The CX decomposition

$$\overset{m \times n}{\begin{pmatrix} \\ \quad A \quad \\ \\ \end{pmatrix}} \approx \overset{m \times c}{\begin{pmatrix} \\ \quad C \quad \\ \\ \end{pmatrix}} \overset{c \times n}{\begin{pmatrix} \quad X \quad \end{pmatrix}}$$

- Easy to prove that optimal $X = C^{\dagger}A$. (with respect to unitarily invariant norms; $C^{\dagger}$ is the Moore-Penrose pseudoinverse of C). Thus, the challenging part is to find good columns of A to include in C.

- From a mathematical perspective, this is a combinatorial optimization problem, closely related to the so-called Column Subset Selection Problem (CSSP); the CSSP has been heavily studied in Numerical Linear Algebra.

objective for the CX decomposition

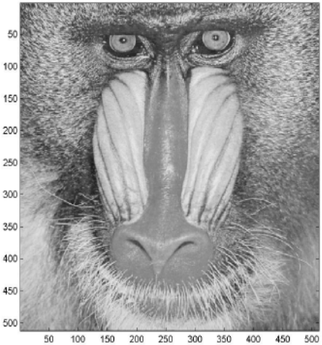
We would like to get theorems of the following form

Given an m-by-n matrix A, there exists an efficient algorithm that picks a small number of columns of A such that with reasonable probability:

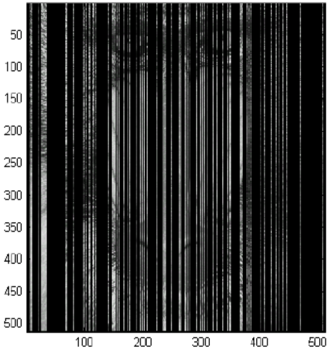
$$\|A - CX\|_F = \|A - CC^\dagger A\|_F \leq (1+\epsilon)\|A - A_k\|_F$$

- Best rank-k approximation to A: $A_k = U_k U_k^\top A$
- Let's start with a simpler, weaker result, connecting the spectral norm of A-CX to matrix multiplication.

Approximating singular vectors



Original matrix

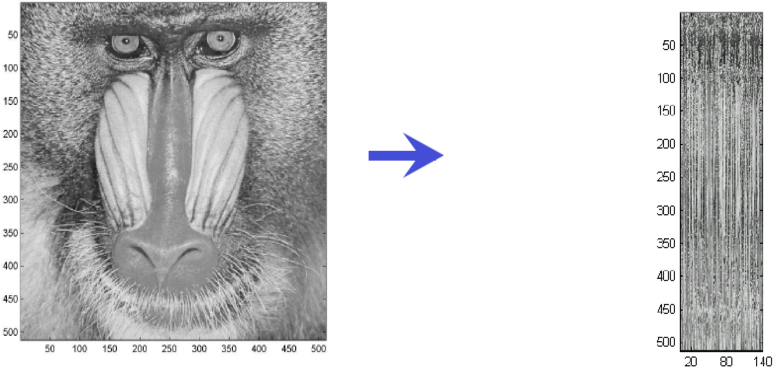


Sampling (c = 140 columns)

- Sample c (=140) columns of the original matrix A and rescale them appropriately to form a 512-by-c matrix C.
- Show that $A - CX$ is “small”.

($C^\dagger$ is the pseudoinverse of C and $X = C^\dagger A$)

Approximating singular vectors



Original matrix

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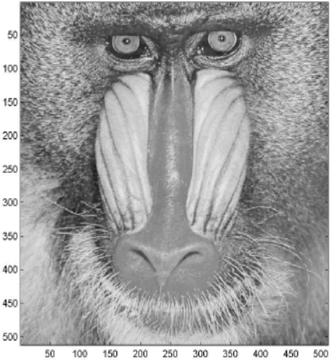
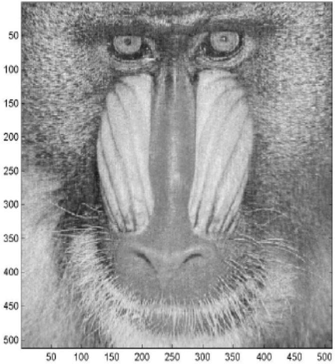
Approximating singular vectors



A



CX

The fact that $AA^T - CC^T$ is small will imply that $A - CX$ is small as well.

Proof (spectral norm)

Using the triangle inequality and properties of norms,

$$\begin{aligned}
\|A - CC^{\dagger}A\|_2^2 &= \|(I - CC^{\dagger})A\|_2^2 \\
&= \|(I - CC^{\dagger})AA^T(I - CC^{\dagger})^T\|_2 \\
&= \|(I - CC^{\dagger})(AA^T - CC^{\dagger})(I - CC^{\dagger})^T\|_2 \\
&\leq \|AA^T - CC^{\dagger}\|_2
\end{aligned}$$

- $I - CC^{\dagger}$ is a projection matrices
- $(I - CC^{\dagger})CC^{\dagger} = 0$

Proof (spectral norm)

Assume that our sampling is done in c i.i.d. trials and the sampling probabilities are:

$$\mathbf{P}(j_t = i) = \frac{\|A^{(i)}\|_2^2}{\|A\|_F^2}$$

We can use our matrix multiplication result: (We will upper bound the spectral norm by the Frobenius norm to avoid concerns about c, namely whether c exceeds the threshold necessitated by the theory.)

$$\begin{aligned} \mathbf{E}[\|A - CC^{\dagger}A\|_2] &\leq \mathbf{E}[\|AA^T - CC^T\|_2] \\ &\leq \frac{1}{c^{1/4}}\|A\|_F \end{aligned}$$

Is this a good bound?

$$\mathbf{E}[\|A - CC^{\dagger}A\|_2] \leq \mathbf{E}[\|AA^T - CC^T\|_2] \leq \frac{1}{c^{1/4}}\|A\|_F$$

- Problem 1: If c = n we 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 non-uniform sampling without replacement.)
- Problem 2: If A had rank exactly k, we would like a column selection procedure that drives the error down to zero when c = k. This can be done deterministically simply by selecting k linearly independent columns.
- Problem 3: 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.

Such deterministic bounds exist when c = k and depend on $(k(n-k))^{1/2}\|A - A_k\|_2$

Relative-error Frobenius norm bounds

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

$$O((k/\epsilon^2)\ln(k/\epsilon^2)) \text{ columns of } A$$

such that with probability at least 0.9

$$\|A - CX\|_F = \|A - CC^\dagger A\|_F \leq (1+\epsilon)\|A - A_k\|_F$$

Outline

1. Randomized Numerical Linear Algebra (RandNLA)
2. Approximating Matrix Multiplication
3. Approximate SVD
4. Random Sampling for SVD
5. Single View Algorithm For Matrix Approximation

Range finding problem

Given an $m \times n$ matrix A and an integer $k < \min(m, n)$, find an orthonormal $m \times k$ matrix Q such that

$$A \approx QQ^T A$$

Solving the primitive problem via randomized sampling — intuition

- Draw random vectors $r_1, r_2, \ldots, r_k \in \mathbb{R}^n$.
- Form "sample" vectors $y_1 = Ar_1, y_2 = Ar_2, \ldots, y_k = Ar_k \in \mathbb{R}_m$.
- Form orthonormal vectors $q_1, q_2, \ldots, q_k \in \mathbb{R}^m$ such that

$$\mathrm{span}\{q_1, q_2, \ldots, q_k\} = \mathrm{span}\{y_1, y_2, \ldots, y_k\}$$

Almost always correct if A has exact rank k

Low-Rank Approximation: Randomized Sampling

Algorithm RandSam0

Input: mxn matrix A, int k, p.

- Draw a random $n \times (k+p)$ matrix Ω
- Compute $QR = A\Omega$
- and SVD: $Q^T A = \hat{U}\hat{\Sigma}\hat{V}^T$
- Truncate SVD: $\hat{U}_k\hat{\Sigma}_k\hat{V}_k^T$

Output: $B = (Q\hat{U}_k)\hat{\Sigma}_k\hat{V}_k^T$

- Easy to implement.
- Very efficient computation.
- Minimum communication.

error for Gaussian test matrices

Ref: Halko, Martinsson, Tropp, 2009 & 2011; Martinsson, Rokhlin, Tygert (2006)

- Let A denote an $m \times n$ matrix with singular values $\{\sigma_j\}_{j=1}^{\min(m,n)}$
- Let k denote a target rank and let p denote an over-sampling parameter.
- Let Ω denote an $n \times (k+p)$ Gaussian matrix.
- Let Q denote the $m \times (k+p)$ matrix $Q = \texttt{orth}(A\Omega)$.

If $p \geq 4$, then

$$\|A - QQ^*A\|_2 \leq \left(1 + 6\sqrt{(k+p)p\log p}\right)\sigma_{k+1} + 3\sqrt{k+p}\left(\sum_{j>k}\sigma_j^2\right)^{1/2}$$

except with probability at most $3p^{-p}$.

Improved Randomized Sampling

Algorithm RandSam1

```
Input: mxn matrix A, int k, p, c.
    ▶ Draw a random $n \times (k+p+c)$ matrix $\Omega$
    ▶ Compute $QR = A\Omega$
    ▶ and SVD: $Q^T A = \hat{U}\hat{\Sigma}\hat{V}^T$
    ▶ Truncate SVD: $\hat{U}_k\hat{\Sigma}_k\hat{V}_k^T$
Output: $B = (Q\hat{U}_k)\hat{\Sigma}_k\hat{V}_k^T$
```

- Only change from RandSam0: p becomes p + c
- Smallest modification of any algorithm.
- c allows a drastically different error bound, controls accuracy.
- p remains in control of failure chance.

Randomized Power Method

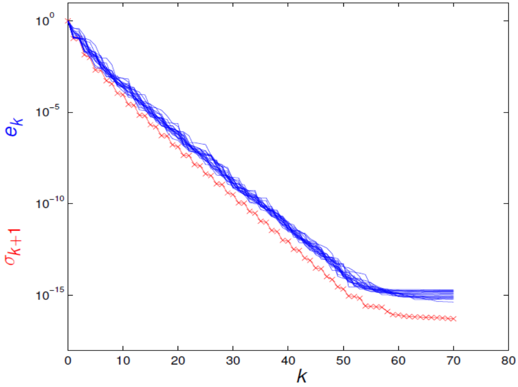
Algorithm RandSam2

```
Input: mxn matrix A, int k, p, c, q
    Draw a random $n \times (k+p+c)$ matrix $\Omega$
    Compute $QR = (AA^T)^q A\Omega$
    and SVD: $Q^T A = \hat{U}\hat{\Sigma}\hat{V}^T$
    Truncate SVD: $\hat{U}_k\hat{\Sigma}_k\hat{V}_k^T$
Output: $B = (Q\hat{U}_k)\hat{\Sigma}_k\hat{V}_k^T$
```

- QR needs done carefully for numerical accuracy.
- Algorithm is old one when q = 0; but q = 1 far more accurate.
- Should converge faster when singular values do not decay very fast.

Example 1

We consider a 1000×1000 matrix A whose singular values are shown below:



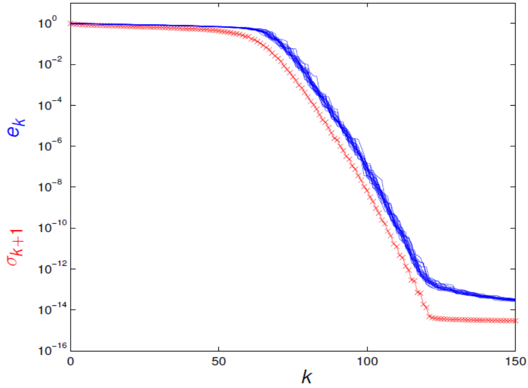
The red line indicates the singular values σ_{k+1} of **A**. These indicate the theoretically minimal approximation error.

The blue lines indicate the actual errors e_k incurred by 20 instantiations of the proposed method.

A is a discrete approximation of a certain compact integral operator normalized so that $\|A\| = 1$. Curiously, the nature of A is in a strong sense irrelevant: the error distribution depends only on $\{\sigma_j\}_{j=1}^{\min(m,n)}$.

Example 2

We consider a 1000×1000 matrix A whose singular values are shown below:



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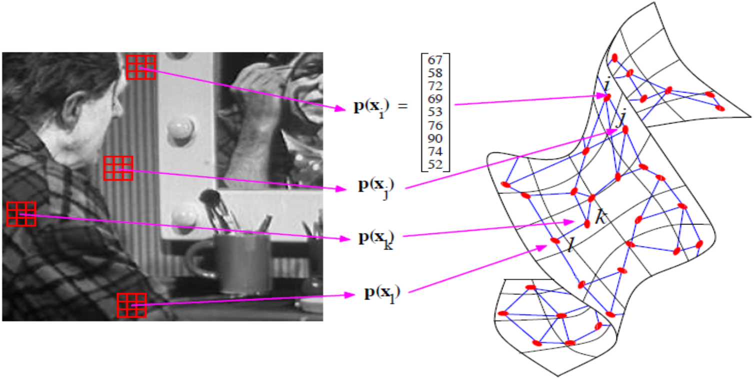
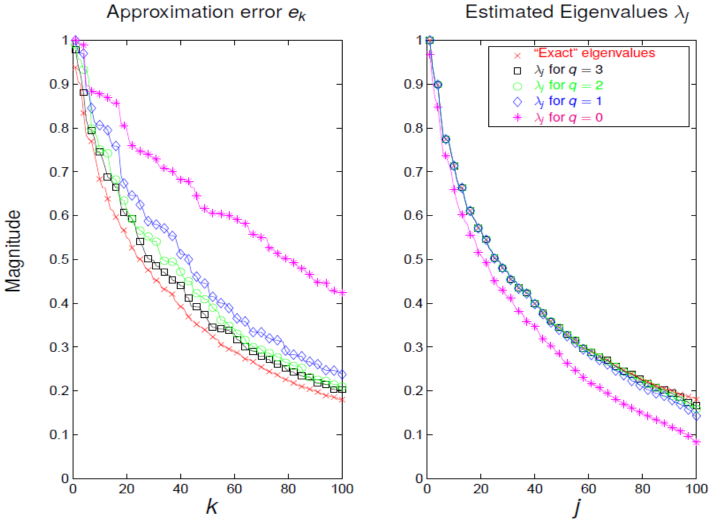
A is a discrete approximation of a certain compact integral operator normalized so that $\|A\| = 1$. Curiously, the nature of A is in a strong sense irrelevant: the error distribution depends only on $\{\sigma_j\}_{j=1}^{\min(m,n)}$.

Example 3

The matrix A being analyzed is a 9025×9025 matrix arising in a diffusion geometry approach to image processing.

To be precise, A is a graph Laplacian on the manifold of 3×3 patches.





The pink lines illustrates the performance of the basic random sampling scheme. The errors for q = 0 are huge, and the estimated eigenvalues are much too small.

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Low-rank reconstruction

Given $A \in \mathbb{R}^{m\times n}$ and a target rank r. Select k and ℓ. Given random matrices $\Omega \in \mathbb{R}^{n\times k}$ and $\Psi \in \mathbb{R}^{\ell\times m}$. Compute

$$Y = A\Omega, \qquad W = \Psi A,$$

Then an approximation $\hat{A}$ is computed:

- Form an orthogonal-triangular factorization $Y = QR$ where $Q \in \mathbb{R}^{m\times k}$.
- Solve a least-squares problem to obtain $X = (\Psi Q)^{\dagger} W \in \mathbb{R}^{k\times n}$
- Construct the rank-k approximation $\hat{A} = QX$

Suppose $k = 2r + 1$ and $\ell = 4r + 2$, then

$$\mathbf{E}\|A - \hat{A}\|_F \leq 2 \min_{\mathrm{rank}(Z)\leq r} \|A - Z\|_F$$

Linear update of A

- Suppose that A is sent as a sequence of additive updates:

  $$A = H_1 + H_2 + H_3 + \cdots$$

  Then one compute

  $$Y \leftarrow Y + H\Omega, \quad W = W + \Psi H$$

- Suppose that A is sent as a sequence of additive updates:

  $$A = \theta A + \eta H$$

  Then one compute

  $$Y \leftarrow \theta Y + \eta H\Omega, \quad W = \theta W + \eta \Psi H$$

Intuition

- Suppose

$$A \approx QQ^*A.$$

  We want to form the rank-k approximation $Q(Q^*A)$, but we cannot compute the factor Q^*A without revisiting the target matrix A.

- Note

$$W = \Psi(QQ^*A) + \Psi(A - QQ^*A) \approx (\Psi Q)(Q^*A)$$

- The construction of X:

$$X = (\Psi Q)^\dagger W \approx Q^*A$$

- Hence

$$\hat{A} = QX \approx QQ^*A \approx A$$

Projection onto a Convex Set.

Let C be a closed and convex set. Define the projection:

$$\Pi_C(M) = \arg\min_X \quad \|X - M\|_F^2, \text{ s.t. } X \in C$$

- Suppose $A \in C$. Let $\hat{A}_{in}$ be an initial approximation of A,

$$\|A - \Pi_C(\hat{A}_{in})\|_F \leq \|A - \hat{A}_{in}\|_F$$

- Conjugate Symmetric Approximation

$$H^n = \{X \in \mathcal{C}^{n\times n} | X = X^*\}$$

The projection

$$\Pi_{H^n}(M) = \frac{1}{2}(M + M^*)$$

Conjugate Symmetric Approximation.

Let $A \in H^n$. Let $\hat{A} = QX$.

- $$\Pi_{H^n}(\hat{A}) = \frac{1}{2}(QX + X^* Q^*) = \frac{1}{2}[Q, X^*] \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} [Q, X^*]^*$$
- Let $[Q, X^*] = U[T_1, T_2]$. Then $$S = \frac{1}{2}(T_1 T_2^* + T_2 T_1^*)$$
- Construct $$\hat{A}_{sym} = USU^*$$

PSD Approximation

Let A be positive semidefinite (PSD). Let $\hat{A} = QX$.

- Form eigenvalue decomposition
$$S = VDV^*$$
- Compute
$$\hat{A}_{sym} = (UV)D(UV)^*$$
- Construct
$$\hat{A}_+ = \Pi_{H_+^n}(\hat{A}) = (UV)D_+(UV)^*$$