Low Rank Approximation
Lecture 3

Daniel Kressner
Chair for Numerical Algorithms and HPC
Institute of Mathematics, EPFL
daniel.kressner@epfl.ch

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

Sampling based approximation

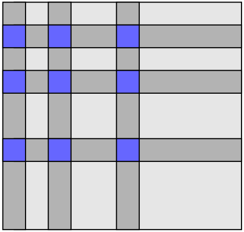
Aim: Obtain rank-r approximation of $m \times n$ matrix A from selected entries of A.
Two different situations:

- Unstructured sampling: Let $\Omega \subset \{1, \ldots, m\} \times \{1, \ldots, n\}$. Solve

$$\min \|A - BC^T\|_\Omega, \qquad \|M\|_\Omega^2 = \sum_{(i,j) \in \Omega} m_{ij}^2.$$

  Matrix completion problem solved by general optimization techniques (ALS, Riemannian optimization). Will discuss later.

- Column/row sampling:



Focus of this lecture.

Row selection from orthonormal basis

Task. Given orthonormal basis $U \in \mathbb{R}^{n\times r}$ find a "good" $r \times r$ submatrix of U.

Classical problem already considered by Knuth.[1]

Quantification of "good": Smallest singular value not too small.

Some notation:

- Given an $m \times n$ matrix A and index sets

$$\begin{aligned} I &= \{i_1, \dots, i_k\}, \quad 1 \le i_1 < i_2 < \cdots i_k \le m, \\ J &= \{j_1, \dots, j_\ell\}, \quad 1 \le j_1 < j_2 < \cdots j_\ell \le n, \end{aligned}$$

  we let

$$A(I,J) = \begin{pmatrix} a_{i_1,j_1} & \cdots & a_{i_1,j_n} \\ \vdots & & \vdots \\ a_{i_m,j_1} & \cdots & a_{i_m,j_n} \end{pmatrix} \in \mathbb{R}^{k\times\ell}.$$

  The full index set is denoted by :, e.g., $A(I,:)$.
- $|\det A|$ denotes the volume of a *square* matrix A.

[1] Knuth, Donald E. Semioptimal bases for linear dependencies. Linear and Multilinear Algebra 17 (1985), no. 1, 1–4.

Row selection from orthonormal basis

Lemma (Maximal volume yields good submatrix)

Let index set I, $\#I = r$, be chosen such that $|det(U(I,:))|$ is maximized among all $r \times r$ submatrices. Then

$$\frac{1}{\sigma_{\min}(U(I,:))} \leq \sqrt{r(n-r)+1}$$

Proof.[2] W.l.o.g. $I = \{1, \dots, r\}$. Consider

$$\tilde{U} = UU(I,:)^{-1} = \begin{pmatrix} I_r \\ B \end{pmatrix}.$$

Leading submatrix is still of maximal volume. This implies that every entry of B satisfies $|b_{ij}| \leq 1$. (EFY: Why? Hint: By contradiction + clever choice of submatrix.) Hence,

$$\|U(I,:)^{-1}\|_2 = \|UU(I,:)^{-1}\|_2 \leq \sqrt{1 + \|B\|_2^2} \leq \sqrt{1 + (n-r)r}.$$

[2]Following Lemma 2.1 in [Goreinov, S. A.; Tyrtyshnikov, E. E.; Zamarashkin, N. L. A theory of pseudoskeleton approximations. Linear Algebra Appl. 261 (1997), 1â21].

Greedy row selection from orthonormal basis

EFY. Develop an extension of the lemma: Prove that for an *arbitrary* $n \times r$ matrix U of rank r, there is an index set I with $\#I = r$ such that $\frac{1}{\sigma_{\min}(U(I,:))} \leq \sqrt{r(n-r)+1}\,\frac{1}{\sigma_{\min}(U)}$.

Finding submatrix of maximal volume is NP hard.[3]

Greedy algorithm (column-by-column):[4]

- First step is easy: Choose i such that $|u_{i1}|$ is maximal.
- Now, assume that $k < r$ steps have been performed and the first k columns have been processed. Task: Choose optimal index in column $k+1$.

[3] Civril, A., Magdon-Ismail, M.: On selecting a maximum volume sub-matrix of a matrix and related problems. Theoret. Comput. Sci. 410(47-49), 4801–4811 (2009)

[4] Reinvented multiple times in the literature.

Greedy row selection from orthonormal basis

By a suitable permutation, suppose that the first k indices are given by $I_k = \{1, \ldots, k\}$ and partition

$$U = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}, \quad U_{11} \in \mathbb{R}^{k \times k}.$$

We have

$$U = \begin{pmatrix} I_k & 0 \\ U_{21} U_{11}^{-1} & I_{n-k} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ 0 & \tilde{U}_{22} \end{pmatrix}, \qquad \tilde{U}_{22} = U_{22} - U_{21} U_{11}^{-1} U_{12}.$$

This implies

$$\det(U(I_k \cup \{k+i\}, I_k \cup \{k+1\})) = \det(U_{11}) \cdot \tilde{U}_{22}(i, 1).$$

$\rightsquigarrow$ Greedily maximizing determinant: Choose i such that $|\tilde{U}_{22}(i, 1))|$ is maximal.

Greedy row selection from orthonormal basis

Choose $i^* = \text{argmax}_{i=1,\dots,n} |u_{i1}|$. Set $I = \{i^*\}$.
for $k = 2, \dots, r$ **do**
 res $= U(:,k) - U(:,1:k)U(I,1:k)^{-1}U(I,k)$
 Choose $i^* = \text{argmax}_{i=k,\dots,n} |\text{res}(i)|$
 Set $I \leftarrow I \cup i^*$.
end for

- For $I = \{i_1, \dots, i_k\}$ define selection operator:

$$\mathbb{S}_I = \begin{pmatrix} e_{i_1} & e_{i_2} & \cdots & e_{i_k} \end{pmatrix}.$$

 Then residual can be expressed as

$$\text{res} = U(:,k) - U(:,1:k)(\mathbb{S}_I^T U(:,1:k))^{-1} \mathbb{S}_I^T U(:,k)$$

- Literally implemented, requires $\mathcal{O}(nr^2 + r^4)$ ops.

EFY. k steps of Gausian elimination (with or without pivoting) yield the Schur complement needed to form r. Use this observation to reduce the complexity to $\mathcal{O}(nr^2)$ ops

Greedy row selection from orthonormal basis

Performance of greedy algorithm in practice often quite good, but there are counter examples (see later).

Theorem

For the index set returned by the greedy algorithm, it holds that

$$\|(\mathbb{S}_I^T U)^{-1}\|_2 = \|U(I,:)^{-1}\|_2 \leq (1+\sqrt{2n})^{r-1}\|U(:,1)\|_\infty^{-1}.$$

Proof.[5] W.l.o.g., may assume $I = \{1, \ldots, r\}$. Proof by induction wrt k. For $k = 1$, u_{11} is maximal element in first column $U(:,1)$, which yields result. Now, assume it is satisfied for $k-1$ and partition

$$U = \begin{pmatrix} U_{11} & u_{12} & \star \\ u_{21}^T & u_{22} & \star \\ \star & \star & \star \end{pmatrix}, \qquad U_{11} \in \mathbb{R}^{(k-1)\times(k-1)}.$$

Aim is to estimate $\|\tilde{U}^{-1}\|_2$ for $\tilde{U} := \begin{pmatrix} U_{11} & u_{12} \\ u_{21}^T & u_{22} \end{pmatrix}$.

[5] See Lemma 3.2 in [Chaturantabut, S. and Sorensen, D. C. Nonlinear model reduction via discrete empirical interpolation. SIAM Journal on Scientific Computing, 32(5), 2737–2764, 2010].

Greedy row selection from orthonormal basis

From the construction, we have the block LU decomposition

$$\tilde{U} = \begin{pmatrix} I & 0 \\ u_{21}^T U_{11}^{-1} & 1 \end{pmatrix} \begin{pmatrix} U_{11} & u_{12} \\ 0 & \rho \end{pmatrix} = \begin{pmatrix} U_{11} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} I & 0 \\ u_{21}^T & 1 \end{pmatrix} \begin{pmatrix} I & U_{11}^{-1} u_{12} \\ 0 & \rho \end{pmatrix}$$

with $\rho = u_{22} - u_{21}^T U_{11}^{-1} u_{11}$. We have

$$\text{res} = u(:, r) - U(:, 1 : r-1) U_{11}^{-1} u_{12} = U(:, 1 : r) \begin{pmatrix} -U_{11}^{-1} u_{12} \\ 1 \end{pmatrix}.$$

By construction, ρ is the element of maximal absolute value of res. Hence,

$$\left\| \begin{pmatrix} -U_{11}^{-1} u_{12} \\ 1 \end{pmatrix} \right\|_2 = \|\text{res}\|_2 \leq \sqrt{n} \|\text{res}\|_\infty = \sqrt{n} \rho.$$

Greedy row selection from orthonormal basis

$$\tilde{U}^{-1} = \begin{pmatrix} I & -\rho^{-1} U_{11}^{-1} u_{12} \\ 0 & \rho^{-1} \end{pmatrix} \begin{pmatrix} I & 0 \\ -u_{21}^T & 1 \end{pmatrix} \begin{pmatrix} U_{11}^{-1} & 0 \\ 0 & 1 \end{pmatrix}$$

Therefore,

$$\begin{aligned} \|\tilde{U}^{-1}\|_2 &\leq \|U_{11}^{-1}\|_2 \left(1 + \rho^{-1} \left\| \begin{pmatrix} -U_{11}^{-1} u_{12} \\ 1 \end{pmatrix} \begin{pmatrix} -u_{21}^T & 1 \end{pmatrix} \right\|_2 \right) \\ &\leq \|U_{11}^{-1}\|_2 (1 + \sqrt{2n}) \end{aligned}$$

Together with induction assumption, completes proof.

Vector approximation

Goal: Want to approximate vector f in subspace range(U). Minimal error attained by orthogonal projection UU^T. When replaced by *oblique* projection

$$U(\mathbb{S}_I^T U)^{-1}\mathbb{S}_I^T f$$

increase of error bounded by result of lemma.

Lemma

$$\|f - U(\mathbb{S}_I^T U)^{-1}\mathbb{S}_I^T f\|_2 \leq \|(\mathbb{S}_I^T U)^{-1}\|_2 \cdot \|f - UU^T f\|_2.$$

Proof. Let $\Pi = U(\mathbb{S}_I^T U)^{-1}\mathbb{S}_I^T$. Then

$$\|(I - \Pi)f\|_2 = \|(I - \Pi)(f - UU^T f)\|_2 \leq \|I - \Pi\|_2 \|f - UU^T f\|_2.$$

EFY. Prove that any projector $\Pi \not\in \{0, I_n\}$ satisfies $\|I - \Pi\|_2 = \|\Pi\|_2$. Hint: Choose orthonormal bases U, $U_\perp$ of range(Π) and its complement, respectively, and express Π and $I - \Pi$ in $[U, U_\perp]$.

The proof is completed by noting

$$\|I - \Pi\|_2 = \|\Pi\|_2 \leq \|(\mathbb{S}_I^T U)^{-1}\mathbb{S}_I^T\|_2 = \|(\mathbb{S}_I^T U)^{-1}\|_2.$$

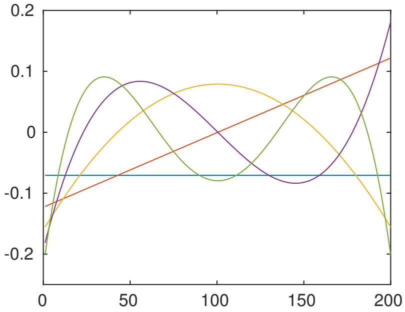
Connection to interpolation

We have

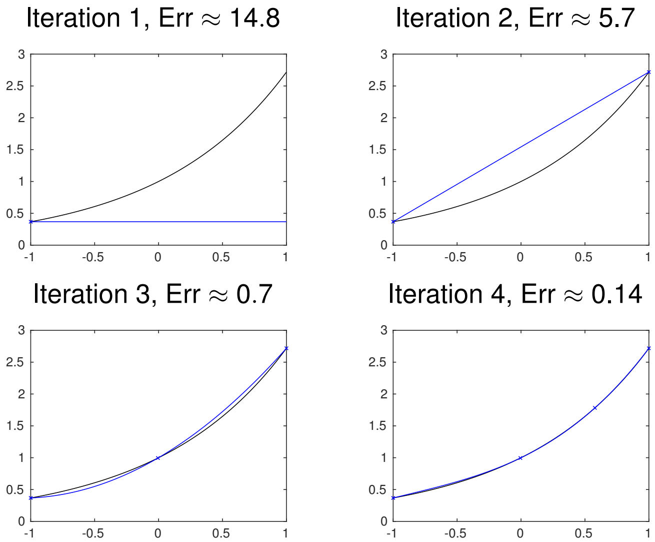
$$\|\mathbb{S}_I^T(f - U(\mathbb{S}_I^T U)^{-1}\mathbb{S}_I^T f)\|_2 = 0$$

$\rightsquigarrow$ f is "interpolated" exactly at selected indices.

Let f contain discretization of $\exp(x)$ on $[-1, 1]$ let U contain orthonormal basis of discretized monomials $\{1, x, x^2, \ldots\}$.

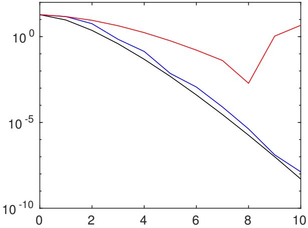


Connection to interpolation



Connection to interpolation

Comparison between best approximation, greedy approximation, approximation obtained by selecting first r indices.



Names:

- Continuous setting: EIM (Empirical Interpolation method), [M. Barrault, Y. Maday, N. C. Nguyen, and A. T. Patera, An “empirical interpolation” method: Application to efficient reduced-basis discretization of partial differential equations, C. R. Math. Acad. Sci. Paris, 339 (2004), pp. 667–672].
- Discrete setting: DEIM (Discrete EIM).

POD+DEIM

Consider LARGE ODE of the form

$$\dot{x}(t) = Ax(t) + F(x(t)).$$

A is $n \times n$ matrix. Idea of POD[6]:

1. Simulate ODE for one or more initial conditions and collect trajectories at discrete time points into snapshot matrix:

$$X = \begin{pmatrix} x(t_1) & \cdots & x(t_m) \end{pmatrix}.$$

2. Compute ONB $V \in \mathbb{R}^{n \times r}$, $r \ll n$, of dominant left subspace of X (e.g., by SVD).
3. Assume approximation $x \approx UU^T x = Uy$ and project dynamical system onto range(U):

$$\dot{y}(t) = U^T AUy(t) + U^T F(Uy(t)).$$

[6] See [S. Volkwein. Proper Orthogonal Decomposition: Theory and Reduced-Order Modelling. Lecture Notes, 2013] for a comprehensive introduction.

POD+DEIM

Problem: $U^T F(Uy(t))$ still involves (large) dimension of original system.

Using DEIM:

$$U^T F(Uy(t)) \approx (\mathbb{S}_I^T U)^{-1} \mathbb{S}_I^T F(Uy(t)).$$

$$\dot{y}(t) = U^T A U y(t) + (\mathbb{S}_I^T U)^{-1} \mathbb{S}_I^T F(Uy(t)).$$

$\rightsquigarrow$ Only need to evaluate $\#I = r$ instead of n entries of function F. Particularly efficient for

$$F(x) = \begin{pmatrix} f_1(x_1) \\ \vdots \\ f_n(x_n) \end{pmatrix} \quad \Rightarrow \quad \mathbb{S}_I^T F(Uy(t)) = \begin{pmatrix} f_{i_1}(x_{i_1}) \\ \vdots \\ f_{i_r}(x_{i_r}) \end{pmatrix}$$

Example from [Chaturantabut/Sorensen'2010]: Discretized FitzHugh-Nagumo equations involve $F(x) = x \odot (x - 0.1) \odot (1 - x)$.

Greedy row selection from orthonormal basis

QR-based variant of index selection: Inspired from Orthogonal Matching Pursuit..

In step $k+1$:

1. Select row i_{k+1} of maximal 2-norm from U.
2. Set $x = U(i_{k+1}, :)^T / \|U(i_{k+1}, :)\|_2$.
3. Update $U \leftarrow U(I_r - xx^T)$.

This is QR with column pivoting applied to U^T.

Theorem

For the index set I_Q returned by QR with pivoting, it holds that

$$\|(\mathbb{S}_{I_Q}^T U)^{-1}\|_2 = \|U(I_Q, :)^{-1}\|_2 \leq \frac{\sqrt{n-r+1}}{3}\sqrt{4^r + 6r - 1}.$$

Proof. See Theorem 2.1 in [Drmač, Z. and Gugercin, S. A New Selection Operator for the Discrete Empirical Interpolation Method—Improved A Priori Error Bound and Extensions. SIAM Journal on Scientific Computing, 2016 38:2, A631–A648].

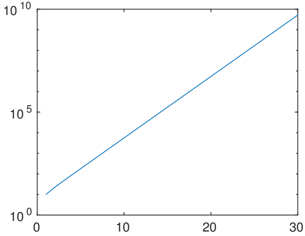
EFY. Using MATLAB's command qr, implement the method above. Apply it to the exponential function, as above, and compare with the standard greedy method.

Counter example for greedy

Let U be Q-factor of economy sized QR factorization of $n \times r$ matrix

$$A = \begin{pmatrix} 1 & & & \\ -1 & 1 & & \\ \vdots & \ddots & \ddots & \\ -1 & \cdots & -1 & 1 \\ -1 & \cdots & -1 & -1 \\ \vdots & & \vdots & \vdots \\ -1 & \cdots & -1 & -1 \end{pmatrix}$$

Variation of famous example by Wilkinson. (QR-based) greedy do no pivoting, at least in exact arithmetic.



$\|U(I,:)^{-1}\|_2$ vs. r for $n = 100$ and U returned by greedy.

Row selection beyond greedy

Improve upon maxvol-based greedy (in a deterministic framework) via Knuth's iterative exchange of rows. Given index set I, $\#I = r$, and $\mu \geq 1$, $\mu \approx 1$, form

$$\tilde{U} = UU(I,:)^{-1}.$$

Search for largest element

$$(i^*, j^*) = \operatorname{argmax} |\tilde{u}_{ij}|.$$

If

$$|\tilde{u}_{i^*j^*}| \leq \mu, \tag{1}$$

terminate algorithm. Otherwise, set $I \leftarrow I \backslash \{j^*\} \cup \{i^*\}$ and repeat.

EFY. Show that the this row exchange increases the volume of $\tilde{U}(I,:)$ and $U(I,:)$ by at least μ.

EFY. Implement this strategy and apply it to Wilkinson's example from the previous slide. How many iterates are needed for $r = 30$ to achieve $\mu = 1.01$?

QR-based greedy can be improved by existing methods for rank-revealing QR [Golub/Van Loan'2013].

Theorem

Let $U(I_K,:)$ be the submatrix obtained upon termination of Knuth's procedure. Then

$$|\det U(I_K,:)| \geq \frac{1}{(\mu\sqrt{r})^r} \max_I |\det U(I,:)|$$

Proof. By construction, all entries of

$$UU(I_K,:)^{-1}$$

are bounded by μ in absolute value. In particular this holds for

$$X = U(I,:)U(I_K,:)^{-1}$$

for any index set $I \subset \{1,\dots,n\}$ with $\#I = r$. Hence, by Hadamard's inequality,

$$\frac{|\det U(I,:)|}{|\det U(I_K,:)|} = \det(X) \leq \prod_{j=1}^{r} \|X(:,j)\|_2 \leq \sqrt{r}^r \prod_{j=1}^{r} \|X(:,j)\|_\infty \leq (\mu\sqrt{r})^r.$$

The CUR decomposition: Existence results

$$A = CUR,$$

where C contains columns of A, R contains rows of A, U is chosen "wisely".

Theorem (Goreinov/Tyrtyshnikov/Zamarshkin'1997). Let $\varepsilon := \sigma_{k+1}(A)$. Then there exist row indices $I \subset \{1, \dots, m\}$ and column indices $J \subset \{1, \dots, n\}$ and a matrix $S \in \mathbb{R}^{k \times k}$ such that

$$\|A - A(:, J)SA(I, :)\|_2 \le \varepsilon(1 + 2\sqrt{k}(\sqrt{m} + \sqrt{n})).$$

Proof. Let U_k, V_k contain k dominant left/right singular vectors of A. Choose I, J by selecting rows from U_k, V_k. According to max volume lemma, the square matrices $\hat{U} = U_k(I, :)$, $\hat{V} = V_k(J, :)$ satisfy

$$\|\hat{U}^{-1}\|_2 \le \sqrt{k(m-k)+1}, \quad \|\hat{V}^{-1}\|_2 \le \sqrt{k(n-k)+1}.$$

Remains to choose S.

The CUR decomposition: Existence results

Form $\Phi = \hat{U}\Sigma_k \hat{V}^T$ and choose $\tilde{k}$ such that

$$\|\Phi - \mathcal{T}_{\tilde{k}}(\Phi)\|_2 \leq \frac{\varepsilon}{\sqrt{\|\hat{U}^{-1}\|_2 \|\hat{V}^{-1}\|_2}}.$$

We set $S = \mathcal{T}_{\tilde{k}}(\Phi)^+$. We now estimate the four different components of $U_k \Sigma_k V_k^T - A(:, J)SA(I, :)$ wrt U_k, V_k and their complements:

1. $U_k U_k^T (...) V_k V_k^T$:

$$\begin{aligned} & \|\Sigma_k - U_k^T A(:, J) SA(I, :) V_k\|_2 = \|\Sigma_k - \Sigma_k \hat{V} S \hat{U} \Sigma_k\|_2 \\ = \;& \|\Sigma_k - \hat{U}^{-1} \Phi \mathcal{T}_{\tilde{k}}(\Phi)^+ \Phi \hat{V}^{-1}\|_2 = \|\hat{U}^{-1}(\Phi - \mathcal{T}_{\tilde{k}}(\Phi))\hat{V}^{-1}\|_2 \\ \leq \;& \varepsilon \sqrt{\|\hat{U}^{-1}\|_2 \|\hat{V}^{-1}\|_2}. \end{aligned}$$

2. $(I_m - U_k U_k^T)(...) V_k V_k^T$

$$\begin{aligned} & \|(I - U_k U_k)^T A(:, J) SA(I, :) V_k\|_2 \leq \varepsilon \|SA(I, :) V_k\|_2 \\ = \;& \varepsilon \|\mathcal{T}_{\tilde{k}}(\Phi)^+ \Phi \hat{V}^{-1}\| \leq \varepsilon \sqrt{\|\hat{V}^{-1}\|_2} \end{aligned}$$

3. $U_k U_k^T (...)(I - V_k V_k^T)$: As in 2, bounded by $\varepsilon \sqrt{\|\hat{U}^{-1}\|_2}$.

The CUR decomposition: Existence results

4. $(I - U_k U_k^T)(...)(I - V_k V_k^T)$:

$$\begin{aligned} & \|(I - U_k U_k)^T A(:,J) S A(I,:)(I - V_k V_k^T)\|_2 \le \varepsilon^2 \|S\|_2 \\ \le \quad & \varepsilon \sqrt{\|\hat{U}^{-1}\|_2 \|\hat{V}^{-1}\|_2} \end{aligned}$$

In summary, we obtain

$$\|A - A(:,J) S A(I,:)\|_2 \le \varepsilon \left(1 + \left(\sqrt{\|\hat{U}^{-1}\|_2} + \sqrt{\|\hat{V}^{-1}\|_2} \right)^2 \right),$$

which implies the result.

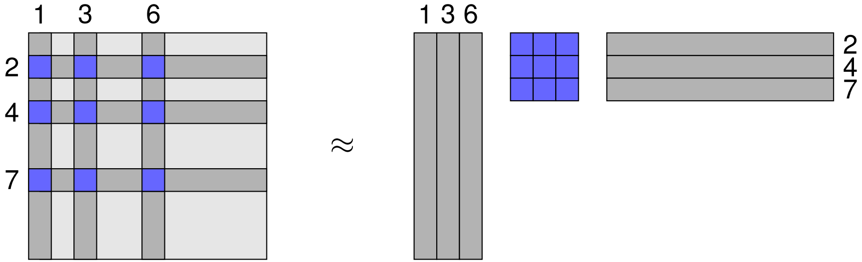
The CUR decomposition: Existence results

Choice of $S = (A(I,J))^{-1}$ in CUR $\rightsquigarrow$ Remainder term

$$R := A - A(:,J)(A(I,J))^{-1}A(I,:)$$

has zero rows at I and zero columns at J.

Cross approximation:



Adaptive Cross Approximation (ACA)

A more direct attempt to find a good cross..

Theorem (Goreinov/Tyrtyshnikov'2001). Suppose that

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

where $A_{11} \in \mathbb{R}^{r \times r}$ has maximal volume among all $r \times r$ submatrices of A. Then

$$\|A_{22} - A_{21} A_{11}^{-1} A_{12}\|_C \leq (r+1)\sigma_{r+1}(A),$$

where $\|M\|_C := \max_{ij} |m_{ij}|$

As we already know, finding A_{11} is NP hard [Çivril/Magdon-Ismail'2013].

Adaptive Cross Approximation (ACA)

Proof of theorem for $(r+1)\times(r+1)$ *matrices.* Consider

$$A = \begin{pmatrix} A_{11} & a_{12} \\ a_{21}^T & a_{22} \end{pmatrix}, \quad A_{11} \in \mathbb{R}^{r\times r},\ a_{12}, a_{21} \in \mathbb{R}^{r\times 1},\ a_{22} \in \mathbb{R},$$

with invertible A_{11}. We recall the definition of the adjunct of a matrix:

$$\mathrm{adj}(A) = C^T, \qquad c_{ij} = (-1)^{i+j} m_{ij},$$

where m_{ij} is the determinant of the matrix obtained by deleting row i and j of A. By the max-volume assumption, $|m_{r+1,r+1}|$ is maximal among all $|m_{ij}|$. On the other hand,

$$A^{-1} = \frac{1}{\det A}\mathrm{adj}(A).$$

This implies that the element of A^{-1} of maximum absolute value is at position $(r+1, r+1)$:

$$|(A^{-1})_{r+1,r+1}| = \|A^{-1}\|_C := \max_{i,j} \left|(A^{-1})_{ij}\right|.$$

Adaptive Cross Approximation (ACA)

Proof of theorem for continued. On the other hand, we have for any $k \times \ell$ matrix B that

$$\|B\|_2 \leq \|B\|_F \leq \sqrt{k\ell}\|B\|_C.$$

Thus,

$$\sigma_{r+1}(A)^{-1} = \|A^{-1}\|_2 \leq (r+1)\|A^{-1}\|_C = (r+1)|(A^{-1})_{r+1,r+1}|.$$

This completes the proof, using (e.g., via Schur complement)

$$(A^{-1})_{r+1,r+1} = \frac{1}{a_{22} - a_{21}^T A_{11}^{-1} a_{12}}.$$

Adaptive Cross Approximation (ACA)

ACA with full pivoting [Bebendorf/Tyrtyshnikov'2000]

Set $R_0 := A$, $I := \{\}$, $J := \{\}$, $k := 0$
repeat
  $k := k + 1$
  $(i_k, j_k) := \arg\max_{i,j} |R_{k-1}(i,j)|$
  $I \leftarrow I \cup \{i_k\}$, $J \leftarrow J \cup \{j_k\}$
  $\delta_k := R_{k-1}(i_k, j_k)$
  $u_k := R_{k-1}(:, j_k)$, $v_k := R_{k-1}(i_k, :)^T / \delta_k$
  $R_k := R_{k-1} - u_k v_k^T$
until $\|R_k\|_F \leq \varepsilon \|A\|_F$

- This is greedy for maxvol. (Proof on next slide.)
- Still too expensive for general matrices.

Adaptive Cross Approximation (ACA)

Lemma (Bebendorf'2000). Let $I_k = \{i_1, \dots, i_k\}$ and $J_k = \{j_1, \dots, j_k\}$ be the row/column index sets constructed in step k of the algorithm. Then

$$\det(A(I_k, J_k)) = R_0(i_1, j_1) \cdots R_{k-1}(i_k, j_k).$$

Proof. From lines 7 and 8 of the algorithm, $R_{k-1}(I_k, j_k)$ is obtained from $A(I_k, j_k)$ by subtracting scalar multiples of columns $j_1, \dots, j_{k-1}$ of A. Hence, there is a vector y such that

$$A(I_k, J_k) = \begin{bmatrix} A(I_k, J_{k-1}) & R_{k-1}(I_k, j_k) \end{bmatrix} \begin{bmatrix} I_{k-1} & y \\ 0 & 1 \end{bmatrix}.$$

This implies $\det(\tilde{A}_k) = \det(A(I_k, J_k))$. However, $R_{k-1}(i, j_k) = 0$ for all $i = i_1, \dots, i_{k-1}$ and hence

$$\det A(I_k, J_k) = R_{k-1}(i_k, j_k) \det(A(I_{k-1}, J_{k-1})).$$

Since $\det A(I_1, J_1) = A(i_1, j_1) = R_0(i_1, j_1)$, the result follows by induction.

Adaptive Cross Approximation (ACA)

ACA with partial pivoting

Set $R_0 := A$, $I := \{\}$, $J := \{\}$, $k := 1$, $i^* := 1$
repeat
  $j^* := \arg\max_j |R_{k-1}(i^*, j)|$
  $\delta_k := R_{k-1}(i^*, j^*)$
  if $\delta_k = 0$ **then**
    if $\#I = \min\{m, n\} - 1$ **then**
      Stop
    end if
  else
    $u_k := R_{k-1}(:, j^*)$, $v_k := R_{k-1}(i^*, :)^T / \delta_k$
    $R_k := R_{k-1} - u_k v_k^T$
    $k := k + 1$
  end if
  $I \leftarrow I \cup \{i^*\}$, $J \leftarrow J \cup \{j^*\}$
  $i^* := \arg\max_{i \notin I} |u_k(i)|$
until stopping criterion is satisfied

Adaptive Cross Approximation (ACA)

ACA with partial pivoting. Remarks:

- R_k is never formed explicitly. Entries of R_k are computed from

$$R_k(i,j) = A(i,j) - \sum_{\ell=1}^{k} u_\ell(i) v_\ell(j).$$

- Ideal stopping criterion $\|u_k\|_2 \|v_k\|_2 \leq \varepsilon \|A\|_F$ elusive. Replace $\|A\|_F$ by $\|A_k\|_F$, recursively computed via

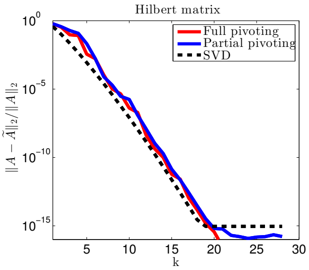
$$\|A_k\|_F^2 = \|A_{k-1}\|_F^2 + 2 \sum_{j=1}^{k-1} u_k^T u_j v_j^T v_k + \|u_k\|_2^2 \|v_k\|_2^2.$$

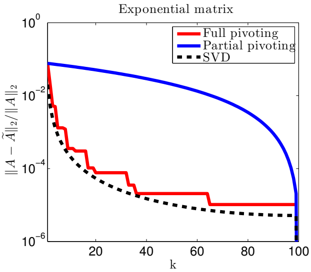
Adaptive Cross Approximation (ACA)

Two 100×100 matrices:

(a) The Hilbert matrix A defined by $A(i,j) = 1/(i+j-1)$.

(b) The matrix A defined by $A(i,j) = \exp(-\gamma|i-j|/n)$ with $\gamma = 0.1$.





1. Excellent convergence for Hilbert matrix.
2. Slow singular value decay impedes partial pivoting.

ACA is Gaussian elimination

We have

$$R_k = R_{k-1} - \delta_k R_{k-1} e_k e_k^T R_{k-1} = (I - \delta_k R_{k-1} e_k e_k^T) R_{k-1} = L_k R_{k-1},$$

where $L_k \in \mathbb{R}^{m\times m}$ is given by

$$L_k = \begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ & & & 0 & & & \\ & & & \ell_{k+1,k} & 1 & & \\ & & & \vdots & & \ddots & \\ & & & \ell_{m,k} & & & 1 \end{bmatrix}, \qquad \ell_{i,k} = -\frac{e_i^T R_{k-1} e_k}{e_k^T R_{k-1} e_k}.$$

for $i = k+1, \ldots, m$.

Matrix L_k differs only in position (k,k) from usual lower triangular factor in Gaussian elimination.

ACA for SPSD matrices

For symmetric positive semi-definite matrix $A \in \mathbb{R}^{n \times n}$:

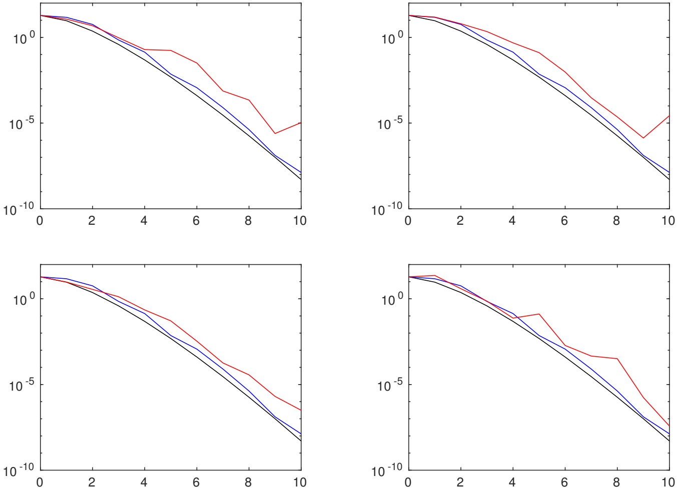
- SVD becomes spectral decomposition.
- Can use trace instead of Frobenius norm to control error.
- R_k stays SPSD.
- Choice of rows/columns, e.g., by largest diagonal element of R_k.
- ACA becomes
  - $=$ Cholesky (with diagonal pivoting). Analysis in [Higham'1990].
  - $=$ Nyström method [Williams/Seeger'2001].

See [Harbrecht/Peters/Schneider'2012] for more detais.

Outlook on randomized algorithms

Coming back to DEIM for exponential function.

Comparison between best approximation, greedy approximation, approximation obtained by randomly selecting r indices.



Outlook on randomized algorithms

A simple way to fool uniformly random selection:

$$U = \begin{pmatrix} 0_{(n-r)\times r} \\ I_r \end{pmatrix}$$

for n very large and $r \ll n$.