Low Rank Approximation
Lecture 4

Daniel Kressner
Chair for Numerical Algorithms and HPC
Institute of Mathematics, EPFL
daniel.kressner@epfl.ch
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
  \[
  \min_{B, C} \| A - BC^T \|_\Omega, \quad \| M \|_\Omega^2 = \sum_{(i,j) \in \Omega} m_{ij}^2.
  \]

  Matrix completion problem solved by general optimization techniques (ALS, Riemannian optimization, convex relaxation). 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
  
  $I = \{i_1, \ldots, i_k\}$, \hspace{2mm} $1 \leq i_1 < i_2 < \cdots i_k \leq m$,  
  
  $J = \{j_1, \ldots, j_\ell\}$, \hspace{2mm} $1 \leq j_1 < j_2 < \cdots j_\ell \leq n$,  

  we let

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

  The full index set is denoted by $:\$, e.g., $A(I, :)$.

  $|\det A|$ denotes the volume of a square matrix $A$.

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

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


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

Because of $\det(\tilde{U}(J,:)) = \det(U(J,:)) / \det(U(I,:))$ for any $J$, submatrix $\#J = r$, $\tilde{U}(I,:)$ has maximal volume among all $r \times r$ submatrices of $\tilde{U}$. 
Maximality of $\tilde{U}(I, :)$ implies $\max |b_{ij}| \leq 1$. Argument: If there was $b_{ij}$ with $|b_{ij}| > 1$ then interchanging rows $r + i$ and $j$ of $\tilde{U}$ would increase volume of $\tilde{U}(I, :)$. We have

$$\|B\|_2 \leq \|B\|_F \leq \sqrt{(n - r)r \max |b_{ij}|} \leq \sqrt{1 + (n - r)r}.$$

This yields the result:

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

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 \(k + 1\).

There is a one-to-one connection between greedy row selection and Gaussian elimination with column pivoting!

---


\(^4\) Reinvented multiple times in the literature.
Greedy row selection from orthonormal basis

Gaussian elimination without pivoting applied to $U \in \mathbb{R}^{n\times r}$:

for $k = 1, \ldots, r$ do

$L(:, k) \leftarrow \frac{1}{u_{kk}} U(:, k), \quad R(k, :) \leftarrow U(k, :)$

$U \leftarrow U - L(:, k)R(k, :)$

end for

Let $\tilde{U}$ denote the updated matrix $U$ obtained after $k$ steps. Then:

$\tilde{U} = U - LR$ with

$L = \begin{bmatrix} L_{11} \\ L_{21} \end{bmatrix} \in \mathbb{R}^{n\times k}, \quad R = \begin{bmatrix} R_{11} & R_{12} \end{bmatrix} \in \mathbb{R}^{k\times r}$

$L_{11}$ unit lower triangular, $R_{11}$ upper triangular.

$\tilde{U}$ is zero in first $k$ rows and columns:

$\tilde{U} = \begin{bmatrix} 0 & 0 \\ 0 & \tilde{U}_{22} \end{bmatrix}, \quad \tilde{U}_{22} \in \mathbb{R}^{(n-k)\times(r-k)}$
Combining both relations gives

\[ U = LR + \tilde{U} = \begin{bmatrix} L_{11} & 0 \\ L_{12} & I_{n-r} \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} \\ 0 & \tilde{U}_{22} \end{bmatrix} \]

Back to the greedy algorithm: By a suitable permutation, suppose that the first \( k \) indices are given by \( I_k = \{1, \ldots, k\} \). Then

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

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

This is Gaussian elimination with column pivoting!

\( r \) steps of Gaussian elimination with column pivoting yields factorization of the form

\[ PU = LR, \]

where

- \( P \) is permutation matrix
- \( L = \begin{bmatrix} L_{11} \\ L_{12} \end{bmatrix} \) with \( L_{11} \in \mathbb{R}^{r \times r} \) unit lower triangular and \( \max |L_{ij}| \leq 1 \)
- \( R \in \mathbb{R}^{r \times r} \) is upper triangular
Greedy row selection from orthonormal basis

Simplified form of Gaussian elimination with column pivoting:

Input: $n \times r$ matrix $U$
Output: “Good” index set $I \subset \{1, \ldots, n\}$, $\#I = r$.

Set $I = \emptyset$.

for $k = 1, \ldots, r$ do

Choose $i^* = \arg\max_{i=1,\ldots,n} |u_{ik}|$.

Set $I \leftarrow I \cup i^*$.

$U \leftarrow U - \frac{1}{u_{i^*,k}} U(:,k) U(i^*,:)$

end for

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

Lemma (Theorem 8.15 in [Higham’2002])

Let \( T \in \mathbb{R}^{n \times n} \) be an upper triangular matrix satisfying

\[
|t_{ii}| \geq |t_{ij}| \quad \text{for} \quad j > i.
\]

Then

\[
1 \leq \min_i |t_{ii}| \cdot \|T^{-1}\|_2 \leq \frac{1}{3} \sqrt{4^n + 6n - 1} \leq 2^{n-1}.
\]

Proof. By diagonal scaling, we may assume without loss of generality that \( t_{ii} = 1 \). Let

\[
Z_n = \begin{bmatrix}
1 & -1 & \cdots & -1 \\
0 & 1 & \ddots & \\
\vdots & \ddots & \ddots & -1 \\
0 & \cdots & 0 & 1
\end{bmatrix} \in \mathbb{R}^{n \times n}.
\]

By induction, one shows that \( |T^{-1}| \leq Z_n^{-1} \) (where the absolute value and the inequality are understood elementwise).
By the monotonicity of the spectral norm

\[ \| T^{-1} \|_2 \leq \| Z_n^{-1} \|_2 \leq \| Z_n^{-1} \|_F. \]

Because of \((Z_n^{-1})_{ij} = 2^{j-i-1}\) for \(j > i\) (see exercises), we obtain

\[ \| Z_n^{-1} \|_F^2 = \sum_{j=1}^{n} \left( 1 + \sum_{i=1}^{j-1} 4^{j-i-1} \right) = \frac{1}{3} \sum_{j=1}^{n} (4^{j-1} + 2) = \frac{1}{9} (4^n + 6n - 1), \]

completing the proof.

**Theorem**

*For the index set returned by the greedy algorithm applied to orthnormal \( U \in \mathbb{R}^{n \times r} \), it holds that*

\[ \| U(I,:)^{-1} \|_2 \leq \sqrt{nr2^{r-1}}. \]
Proof. We start from
\[ PU = LR. \quad (1) \]
Partitioning \( L = \begin{bmatrix} L_1 \\ L_2 \end{bmatrix} \) with \( L_1 \in \mathbb{R}^{r \times r} \), factorization (1) implies
\[ U(I, :) = L_1 R. \]
Because \( PU \) is orthonormal, (1) also implies \( \| R^{-1} \|_2 = \| L \|_2 \Rightarrow \]
\[ \| U(I, :)^{-1} \|_2 \leq \| L_1^{-1} \|_2 \| R^{-1} \|_2 = \| L_1^{-1} \|_2 \| L \|_2. \]
Because the magnitudes of the entries of \( L \) are bounded by 1, we have
\[ \| L \|_2 \leq \| L \|_F \leq \sqrt{nr} \cdot \max |\ell_{ij}| = \sqrt{nr}. \]
Applying the lemma to \( L_1^T \) in order to bound \( \| L_1^{-1} \|_2 \) completes proof.
Vector approximation

**Goal:** Want to approximate vector $f$ in subspace $\text{range}(U)$. For $I = \{i_1, \ldots, i_k\}$ define selection operator:

$$S_I = \begin{bmatrix} e_{i_1} & e_{i_2} & \cdots & e_{i_k} \end{bmatrix}.$$ 

Minimal error attained by orthogonal projection $UU^T$. When replaced by *oblique* projection

$$U(S_I^T U)^{-1} S_I^T f$$

increase of error bounded by result of lemma.

**Lemma**

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

**Proof.** Let $\Pi = U(S_I^T U)^{-1} S_I^T$. Then

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

The proof is completed by noting (and using the exercises),

$$\|I - \Pi\|_2 = \|\Pi\|_2 \leq \|(S_I^T U)^{-1} S_I^T\|_2 = \|(S_I^T U)^{-1}\|_2.$$
Connection to interpolation

We have

\[ S_I^T (I - U(S_I^T U)^{-1}S_I^T) = 0 \]

and hence

\[ \|S_I^T (f - U(S_I^T U)^{-1}S_I^T f)\|_2 = 0. \]

**Interpretation:** \( f \) is “interpolated” exactly at selected indices.

**Example:** 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

Iteration 1, Err ≈ 14.8

Iteration 2, Err ≈ 5.7

Iteration 3, Err ≈ 0.7

Iteration 4, Err ≈ 0.14
Connection to interpolation

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

Terminology:

- **Continuous setting: EIM (Empirical Interpolation method),**

- **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\(^5\):

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

\[ X = (x(t_1) \ldots x(t_m)). \]

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 \((U)\):

\[ \dot{y}(t) = U^T A U y(t) + U^T F(Uy(t)). \]

\(^5\text{See [S. Volkwein. Proper Orthogonal Decomposition: Theory and Reduced-Order Modelling. Lecture Notes, 2013] for a comprehensive introduction.}\)
POD+DEIM

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

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

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

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

$$F(x) = \begin{pmatrix} f_1(x_1) \\ \vdots \\ f_n(x_n) \end{pmatrix} \Rightarrow S_I^T F(Uy(t)) = \begin{pmatrix} f_i_1(x_i_1) \\ \vdots \\ f_i_r(x_i_r) \end{pmatrix}$$

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*

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


**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

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

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

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

Search for largest element

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

If

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

(2) terminate algorithm. Otherwise, set $I \leftarrow I \setminus \{j^*\} \cup \{i^*\}$ and repeat.

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

**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 $\mu$ in absolute value. In particular this holds for

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

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

$$\left| \frac{\det U(I, :) \det U(I_K, :)}{\det U(I_K, :) \det U(I, :)^{-1}} \right| \leq \det(X) \leq \prod_{j=1}^{r} \|X(:, j)\|_2 \leq \sqrt{r} \prod_{j=1}^{r} \|X(:, j)\|_\infty \leq (\mu \sqrt{r})^r.$$
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 \( I \subset \{1, \ldots, m\} \) and column indices \( J \subset \{1, \ldots, n\} \) and a matrix \( S \in \mathbb{R}^{k \times k} \) such that

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

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

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

Remains to choose \( S \).
The CUR decomposition: Existence results

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

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

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

1. $U_kU_k^T(...)V_kV_k^T$:

$$\|\Sigma_k - U_k^TA(:, J)SA(I, :)V_k\|_2 = \|\Sigma_k - \Sigma_k \hat{V}S\hat{U}\Sigma_k\|_2 = \|\Sigma_k - \hat{U}^{-1}\Phi T_{\tilde{k}}(\Phi)^+\Phi \hat{V}^{-1}\|_2 = \|\hat{U}^{-1}(\Phi - T_{\tilde{k}}(\Phi)) \hat{V}^{-1}\|_2 \leq \varepsilon \sqrt{\|\hat{U}^{-1}\|_2\|\hat{V}^{-1}\|_2}.$$ 

2. $(I_m - U_kU_k^T)(...)V_kV_k^T$:

$$\|(I - U_kU_k)^TA(:, J)SA(I, :)V_k\|_2 \leq \varepsilon \|SA(I, :)V_k\|_2 = \varepsilon \|T_{\tilde{k}}(\Phi)^+\Phi \hat{V}^{-1}\| \leq \varepsilon \sqrt{\|\hat{V}^{-1}\|_2}.$$ 

3. $U_kU_k^T(...) (I - V_kV_k^T)$: As in 2, bounded by $\varepsilon \sqrt{\|\hat{U}^{-1}\|_2}$.
The CUR decomposition: Existence results

4. \((I - U_kU_k^T)(\ldots)(I - V_kV_k^T)\):

\[
\| (I - U_kU_k)^TA(: , J)SA(I, :) (I - V_kV_k^T)\|_2 \leq \varepsilon^2 \| S \|_2
\]

\[
\leq \varepsilon \sqrt{\| \hat{U}^{-1} \|_2 \| \hat{V}^{-1} \|_2}
\]

In summary, we obtain

\[
\| A - A(:, J)SA(I, :) \|_2 \leq \varepsilon \left( 1 + \left( \sqrt{\| \hat{U}^{-1} \|_2} + \sqrt{\| \hat{V}^{-1} \|_2} \right)^2 \right),
\]

which implies the result.
The CUR decomposition: Existence results

Choice of $S = (A(I, J))^{-1}$ in CUR $\sim$ 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:

\[
\text{adj}(A) = C^T, \quad c_{ij} = (-1)^{i+j} m_{ij},
\]

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,

\[
A^{-1} = \frac{1}{\det A} \text{adj}(A).
\]

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

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

\[
(A^{-1})_{r+1,r+1} = \frac{1}{a_{22} - a_{21}^TA^{-1}_{11}a_{12}}.
\]
Adaptive Cross Approximation (ACA)

ACA with full pivoting [Bebendorf/Tyrtyshnikov’2000]

1: Set \( R_0 := A \), \( I := \{\} \), \( J := \{\} \), \( k := 0 \)
2: repeat
3: \( k := k + 1 \)
4: \((i_k, j_k) := \text{arg max}_{i, j} \|R_{k-1}(i, j)\|\)
5: \( I \leftarrow I \cup \{i_k\}, J \leftarrow J \cup \{j_k\} \)
6: \( \delta_k := R_{k-1}(i_k, j_k) \)
7: \( u_k := R_{k-1}(\cdot, j_k), v_k := R_{k-1}(i_k, \cdot)^T/\delta_k \)
8: \( R_k := R_{k-1} - u_k v_k^T \)
9: until \( \|R_k\|_F \leq \varepsilon \|A\|_F \)

- This is greedy for maxvol. (Proof on next slide.)
- Still too expensive for general matrices.
Lemma (Bebendorf’2000). Let $I_k = \{i_1, \ldots, i_k\}$ and $J_k = \{j_1, \ldots, j_k\}$ 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 $j_1, \ldots, j_{k-1}$ of $A$. Hence, there is a vector $y$ such that
\[
A(I_k, J_k) = \begin{bmatrix} A(I_k, J_{k-1}) & R_{k-1}(I_k, j_k) \end{bmatrix} \begin{bmatrix} I_{k-1} \\ 0 \\ 1 \end{bmatrix}.
\]

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

1: Set $R_0 := A$, $I := \{\}$, $J := \{\}$, $k := 1$, $i^* := 1$
2: repeat
3: $j^* := \text{arg max}_j |R_{k-1}(i^*, j)|$
4: $\delta_k := R_{k-1}(i^*, j^*)$
5: if $\delta_k = 0$ then
6: if $\#I = \min\{m, n\} - 1$ then
7: Stop
8: end if
9: else
10: $u_k := R_{k-1}(\cdot, j^*)$, $v_k := R_{k-1}(i^*, \cdot)^T / \delta_k$
11: $R_k := R_{k-1} - u_k v_k^T$
12: $k := k + 1$
13: end if
14: $I \leftarrow I \cup \{i^*\}$, $J \leftarrow J \cup \{j^*\}$
15: $i^* := \text{arg max}_{i \notin I} |u_k(i)|$
16: 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 $100 \times 100$ 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

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

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 details.