Matrices with Hierarchical Low-Rank Structures

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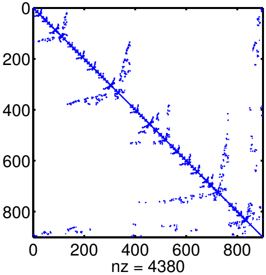
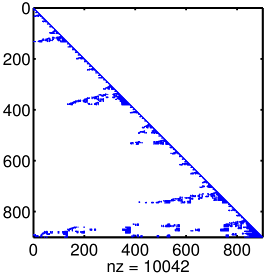
Introduction

- Limitations of (approximate) sparsity
- HODLR for $(\text{tridiagonal})^{-1}$
- HSS for $(\text{tridiagonal})^{-1}$

Sparse matrices



Discretized 2D Laplace
(reord. by `symamd`)



Cholesky factor

- Cholesky factor (nearly) inherits sparsity.
- Look for nothing else when solving $Ax = b$ for matrices A from 2D FE or FD discretizations.

Limitations of sparsity

Sparse factorizations are of limited use when:

- The matrix A itself is full. Examples:
  - nonlocal operators: BEM, fractional PDEs;
  - nonlocal basis functions (Trefftz-like methods).
- A^{-1} is explicitly needed. Examples:
  - Inverse covariance matrix estimation;
  - Matrix iterations for computing $f(A)$, for example sign function iteration;
  - $\operatorname{diag}(A^{-1})$ in electronic structure analysis.
- Cholesky/LU factors of (reordered) A have too much fill-in:
  - FE discretizations of 3D PDEs;
  - "random" sparsity.

Does approximate sparsity help?

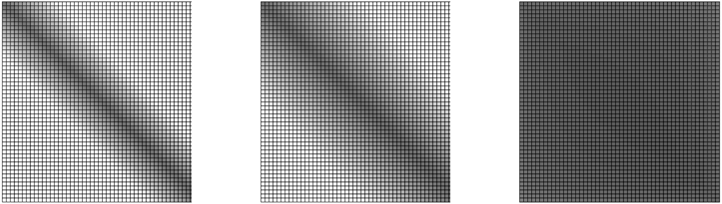
A tridiagonal matrix

$$A = (n+1)^2 \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix} + \sigma(n+1)^2 I_n,$$

- $\sigma \geq 0$ is chosen to control $\kappa(A) = \|A\|_2 \|A^{-1}\|_2$.

Inverse of a tridiagonal matrix

Approximate sparsity of A^{-1} for $n = 50$ and different values of σ:



(a) $\sigma = 4, \kappa(A) \approx 2$ (b) $\sigma = 1, \kappa(A) \approx 5$ (c) $\sigma = 0, \kappa(A) \approx 10^3$

In accordance with result by [Demko et al.'1984]:

$$\left|[A^{-1}]_{ij}\right| \le C \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^{2|i-j|}, \quad C = \max \left\{ \lambda_{\min}^{-1}, (2\lambda_{\max})^{-1}(1+\sqrt{\kappa(A)})^2 \right\}.$$

See also [Benzi/Razouk'2007].

Inverse of a tridiagonal matrix

- Idea: Exploit data-sparsity instead of sparsity.
- Low rank: $n \times n$ matrix M with rank $r \ll n$ can be represented with $2nr$ parameters: $M = BC^T$.
- But: $(\text{tridiagonal})^{-1}$ does not have low rank $\rightsquigarrow$ need for partitioning.

Assume A is tridiagonal spd and partition with $A_{11} \in \mathbb{R}^{n_1 \times n_1}$, $A_{22} \in \mathbb{R}^{n_2 \times n_2}$:

$$A = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix} - a_{n_1,n_1+1} \begin{pmatrix} e_{n_1} \\ -e_1 \end{pmatrix} \begin{pmatrix} e_{n_1} \\ -e_1 \end{pmatrix}^T .$$

Inverse of a tridiagonal matrix

SMW implies

$$A^{-1} = \begin{pmatrix} A_{11}^{-1} & 0 \\ 0 & A_{22}^{-1} \end{pmatrix} + \frac{a_{n_1,n_1+1}}{1 + e_{n_1}^T A_{11}^{-1} e_{n_1} + e_1^T A_{22}^{-1} e_1} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}^T,$$

with $w_1 = A_{11}^{-1} e_{n_1}$ and $w_2 = -A_{22}^{-1} e_1$.

- Off-diagonal blocks of A^{-1} have rank at most 1.
- But: A_{11} and A_{22} are still large!
- $\rightsquigarrow$ hierarchical partitioning.

Inverse of a tridiagonal matrix: Hierarchical partitioning

Suppose n is integer multiple of 4, partition

$$A = \left(\begin{array}{cc|c} A_{11}^{(2)} & A_{12}^{(2)} & \\ \hline A_{21}^{(2)} & A_{22}^{(2)} & A_{12} \\ \hline & & \begin{array}{c|c} A_{33}^{(2)} & A_{34}^{(2)} \\ \hline A_{43}^{(2)} & A_{44}^{(2)} \end{array} \\ \multicolumn{2}{c|}{A_{21}} & \end{array}\right),$$

$$A^{-1} = \left(\begin{array}{cc|c} B_{11}^{(2)} & B_{12}^{(2)} & \\ \hline B_{21}^{(2)} & B_{22}^{(2)} & B_{12} \\ \hline & & \begin{array}{c|c} B_{33}^{(2)} & B_{34}^{(2)} \\ \hline B_{43}^{(2)} & B_{44}^{(2)} \end{array} \\ \multicolumn{2}{c|}{B_{34}} & \end{array}\right),$$

such that $A_{ij}^{(2)}, B_{ij}^{(2)} \in \mathbb{R}^{n/4 \times n/4} \rightsquigarrow$ all off-diagonal blocks have rank 1.
Continuing recursively for $n = 2^k$:

$$2n/2 + 4n/4 + \cdots + 2^k n/2^k + n = n \log_2 n + O(n)$$

storage for A^{-1}.

Inverse of a tridiagonal matrix: Nested bases

Goal: Remove log-factor in $n \log_2 n$.

Let $U_j^{(2)} \in \mathbb{R}^{n/4 \times 2}$, $j = 1, \ldots, 4$, be orthonormal bases such that

$$\operatorname{span}\left\{(A_{jj}^{(2)})^{-1} e_1, (A_{jj}^{(2)})^{-1} e_{n/4}\right\} \subseteq \operatorname{range}(U_j^{(2)}).$$

Applying SMW to $A_{11} = \begin{pmatrix} A_{11}^{(2)} & A_{12}^{(2)} \\ A_{21}^{(2)} & A_{22}^{(2)} \end{pmatrix}$ shows

$$A_{11}^{-1} e_1 \in \operatorname{range} \begin{pmatrix} U_1^{(2)} & 0 \\ 0 & U_2^{(2)} \end{pmatrix}, \quad A_{11}^{-1} e_{n/2} \in \operatorname{range} \begin{pmatrix} U_1^{(2)} & 0 \\ 0 & U_2^{(2)} \end{pmatrix}.$$

Similarly,

$$A_{22}^{-1} e_1 \in \operatorname{range} \begin{pmatrix} U_3^{(2)} & 0 \\ 0 & U_4^{(2)} \end{pmatrix}, \quad A_{22}^{-1} e_{n/2} \in \operatorname{range} \begin{pmatrix} U_3^{(2)} & 0 \\ 0 & U_4^{(2)} \end{pmatrix}.$$

Inverse of a tridiagonal matrix: Nested bases

If we let $U_j \in \mathbb{R}^{n/2\times 2}$, $j = 1, 2$, be orthonormal basis such that

$$\operatorname{span}\left\{A_{jj}^{-1}e_1, A_{jj}^{-1}e_{n/2}\right\} \subseteq \operatorname{range}(U_j),$$

then there exist $X_j \in \mathbb{R}^{4\times 2}$ s.t. $U_j = \begin{pmatrix} U_{2j-1}^{(2)} & 0 \\ 0 & U_{2j}^{(2)} \end{pmatrix} X_j$.

- no need to store the bases $U_1, U_2 \in \mathbb{R}^{n/2\times 2}$ explicitly
- availability of $U_j^{(2)}$ and the small matrices X_1, X_2 suffices

Summary: Can represent A^{-1} as

$$\left(\begin{array}{c|c} \begin{array}{c|c} B_{11}^{(2)} & U_1^{(2)}S_{12}^{(2)}(U_2^{(2)})^T \\ \hline U_2^{(2)}(S_{12}^{(2)})^T(U_1^{(2)})^T & B_{22}^{(2)} \end{array} & U_1 S_{12} U_2^T \\ \hline U_2 S_{12}^T U_1^T & \begin{array}{c|c} B_{33}^{(2)} & U_3^{(2)}S_{34}^{(2)}(U_4^{(2)})^T \\ \hline U_4^{(2)}(S_{34}^{(2)})^T(U_3^{(2)})^T & B_{44}^{(2)} \end{array} \end{array}\right)$$

for some matrices $S_{12}, S_{ij}^{(2)} \in \mathbb{R}^{2\times 2}$. Storage requirements:

$$\underbrace{4 \times 2n/4}_{\text{for } U_j^{(2)}} + \underbrace{2 \times 8}_{\text{for } X_j} + \underbrace{(2+1) \times 4}_{\text{for } S_{12}, S_{12}^{(2)}, S_{34}^{(2)}}.$$

$n = 2^k \rightsquigarrow O(n)$ total storage for A^{-1}.

Literature landscape of hierarchical low-rank structures

Without nested bases:

- HODLR: Aminfar, Ambikasaran, Darve, Greengard, Hogg, O'Neil, ...
- $\mathcal{H}$-matrices: Bebendorf, Grasedyck, Hackbusch, Khoromskij, ...
- Mosaic-Skeleton approximations: Tyrtyshnikov and collaborators

With nested bases:

- Semi-separable / quasi-separable matrices: *Lots* of classical and modern literature, including Bini, Chandrasekaran, Dewilde, Eidelman, Fasino, Gantmacher, Gemignani, Gohberg, Krein, Olshevsky, Pan, Rozsa, Tyrtyshnikov, Zhlobich. See survey papers and books by Vandebril/Van Barel/Mastronardi.
- HSS matrices: Chandrasekaran, Greengard, Martinsson, Rokhlin, Xia, Zorin, ...
- $\mathcal{H}^2$-matrices: Börm, Hackbusch, Mach, ...

Note: Red items not covered in this lecture.

Low-rank approximation

- SVD and best low-rank approximation
- Stability of SVD and low-rank approximation
- Algorithms: SVD, Lanczos, ACA, Randomized
- A priori approximation results

SVD

Theorem (SVD). Let $A \in \mathbb{R}^{m\times n}$ with $m \geq n$. Then there are orthogonal matrices $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ such that

$$A = U\Sigma V^T, \quad \text{with} \quad \Sigma = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ & 0 & \end{pmatrix} \in \mathbb{R}^{m\times n}$$

and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$.

- $m \geq n$ for notational convenience only.
- MATLAB: `[U,S,V] = svd(A,'econ')` computes economic SVD with $O(mn^2)$ ops.
- Pay attention to roundoff error: `semilogy(svd(hilb(100)))` vs. exponential decay established by [Beckermann'2000].
- *Sometimes* more accuracy possible: [DGESVD'1999], [Drmač/Veselić'2007].

SVD: low-rank approximation

Consider $k < n$ and let

$$U_k := \begin{pmatrix} u_1 & \cdots & u_k \end{pmatrix}, \quad \Sigma_k := \mathrm{diag}(\sigma_1, \dots, \sigma_k), \quad V_k := \begin{pmatrix} u_1 & \cdots & u_k \end{pmatrix}.$$

Then

$$\mathcal{T}_k(A) := U_k \Sigma_k V_k$$

has rank at most k. For any unitarily invariant norm $\|\cdot\|$:

$$\|\mathcal{T}_k(A) - A\| = \big\|\mathrm{diag}(\sigma_{k+1}, \dots, \sigma_n)\big\|$$

In particular, for spectral norm and the Frobenius norm:

$$\|A - \mathcal{T}_k(A)\|_2 = \sigma_{k+1}, \qquad \|A - \mathcal{T}_k(A)\|_F = \sqrt{\sigma_{k+1}^2 + \cdots + \sigma_n^2}.$$

SVD: best low-rank approximation

Theorem (Schmidt-Mirsky). Let $A \in \mathbb{R}^{m \times n}$. Then

$$\|A - \mathcal{T}_k(A)\| = \min \left\{ \|A - B\| : \ B \in \mathbb{R}^{m \times n} \text{ has rank at most } k \right\}$$

holds for any unitarily invariant norm $\|\cdot\|$.

Proof for $\|\cdot\|_2$: For any $B \in \mathbb{R}^{m \times n}$ of rank $\leq k$, null space $\mathrm{kernel}(B)$ has dimension $\geq n - k$. Hence, $\exists w \in \mathrm{kernel}(B) \cap \mathrm{range}(V_{k+1})$ with $\|w\|_2 = 1$. Then

$$\begin{aligned}
\|A - B\|_2^2 &\geq \|(A - B)w\|_2^2 = \|Aw\|_2^2 = \|AV_{k+1}V_{k+1}^T w\|_2^2 \\
&= \|U_{k+1}\Sigma_{k+1}V_{k+1}^T w\|_2^2 \\
&= \sum_{j=1}^{r+1} \sigma_j |v_j^T w|^2 \geq \sigma_{k+1} \sum_{j=1}^{r+1} |v_j^T w|^2 = \sigma_{k+1}.
\end{aligned}$$

Stability of SVD

Weyl's inequality (see, e.g., [Horn/Johnson'2013]):

$$\sigma_{i+j-1}(A+E) \le \sigma_i(A) + \sigma_j(E), \qquad 1 \le i,j \le n, \quad i+j \le q+1.$$

Setting $j = 1 \rightsquigarrow$

$$\sigma_i(A+E) \le \sigma_i(A) + \|E\|_2, \qquad i = 1,\dots,n.$$

Singular vectors tend to be less stable! Example:

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 1+\varepsilon \end{pmatrix}, \qquad E = \begin{pmatrix} 0 & \varepsilon \\ \varepsilon & -\varepsilon \end{pmatrix}.$$

- A has right singular vectors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.
- $A+E$ has right singular vectors $\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

Stability of SVD

Theorem (Wedin). Let $k < n$ and assume

$$\delta := \sigma_k(A + E) - \sigma_{k+1}(A) > 0.$$

Let $\mathcal{U}_k/\tilde{\mathcal{U}}_k/\mathcal{V}_k/\tilde{\mathcal{V}}_k$ denote subspaces spanned by first k left/right singular vectors of A / $A + E$. Then

$$\sqrt{\|\sin\Theta(\mathcal{U}_k, \tilde{\mathcal{U}}_k)\|_F^2 + \|\sin\Theta(\mathcal{V}_k, \tilde{\mathcal{V}}_k)\|_F^2} \leq \sqrt{2}\frac{\|E\|_F}{\delta}. \tag{1}$$

Θ: diagonal matrix containing canonical angles between two subspaces.

- Perturbation on input multiplied by $\delta^{-1} \approx [\sigma_k(A) - \sigma_{k+1}(A)]^{-1}$.
- Bad news?

Stability of low-rank approximation

Lemma (folklore / Hackbusch). Let $A \in \mathbb{R}^{m\times n}$ have rank $\le k$. Then

$$\|\mathcal{T}_k(A+E) - A\| \le C\|E\|$$

holds with $C = 2$ for any unitarily invariant norm $\|\cdot\|$. For the Frobenius norm, the constant can be improved to $C = (1+\sqrt{5})/2$.

Proof. Schmidt-Mirsky gives $\|\mathcal{T}_k(A+E) - (A+E)\| \le E$. Triangle inequality implies

$$\|\mathcal{T}_k(A+E) - (A+E) + (A+E) - A\| \le 2\|E\|.$$

See [Hackbusch'2014] for second part. $\square$

Implication for general matrix A:

$$\begin{aligned}\|\mathcal{T}_k(A+E) - \mathcal{T}_k(A)\| &= \big\|\mathcal{T}_k\big(\mathcal{T}_k(A) + (A - \mathcal{T}_k(A)) + E\big) - \mathcal{T}_k(A)\big\| \\ &\le C\|(A - \mathcal{T}_k(A)) + E\| \le C(\|A - \mathcal{T}_k(A)\| + \|E\|).\end{aligned}$$

Perturbations on the level of truncation error pose no danger.

Stability of low-rank approximation: Application

Consider partitioned matrix

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \qquad A_{ij} \in \mathbb{R}^{m_i \times n_j},$$

and desired rank $k \le m_i, n_j$. Let $\varepsilon := \|\mathcal{T}_k(A) - A\|$.

$$E_{ij} := \mathcal{T}_k(A_{ij}) - A_{ij} \qquad \Rightarrow \qquad \|E_{ij}\| \le \varepsilon.$$

By stability of low-rank approximation,

$$\left\| \mathcal{T}_k \begin{pmatrix} \mathcal{T}_k(A_{11}) & \mathcal{T}_k(A_{12}) \\ \mathcal{T}_k(A_{21}) & \mathcal{T}_k(A_{22}) \end{pmatrix} - A \right\|_F = \left\| \mathcal{T}_k \left(A + \begin{pmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{pmatrix} \right) - A \right\|_F \le C\varepsilon,$$

with $C = \frac{3}{2}(1+\sqrt{5})$.

Algorithms for low-rank approximation

Three main classes of algorithms:

1. All entries of A (cheaply) available and $\min\{m, n\}$ small $\rightsquigarrow$ `svd`.
   Related situation: A large but has small rank.
2. Large m, n and matvec possible $\rightsquigarrow$
   Lanczos-based methods and randomized algorithms.
3. Entries of A expensive to compute $\rightsquigarrow$ adaptive cross approximation and its cousins.

SVD for recompression

SVD frequently used for recompression. Suppose that

$$A = BC^T, \quad \text{with} \quad B \in \mathbb{R}^{m\times K}, C \in \mathbb{R}^{n\times K}, \tag{2}$$

where $K > k$, but still (much) smaller than m, n.

Typical example: Sum of J matrices of rank k:

$$A = \sum_{j=1}^{J} \underbrace{B_i}_{\in\mathbb{R}^{m\times k}} \underbrace{C_i}_{\in\mathbb{R}^{n\times k}}{}^T = \underbrace{\begin{pmatrix} B_1 & \cdots & B_J \end{pmatrix}}_{\mathbb{R}^{m\times Jk}} \underbrace{\begin{pmatrix} C_1 & \cdots & C_J \end{pmatrix}}_{\mathbb{R}^{m\times Jk}}{}^T. \tag{3}$$

Algorithm to recompress A:

1. Compute (economic) QR decomps $B = Q_B R_B$ and $C = Q_C R_C$.
2. Compute truncated SVD $\mathcal{T}_k(R_B R_C^T) = \tilde{U}_k \Sigma_k \tilde{V}_k$.
3. Set $U_k = Q_B \tilde{U}_k$, $V_k = Q_C \tilde{V}_k$ and return $\mathcal{T}_k(A) := U_k \Sigma_k V_k^T$.

Returns best rank-k approximation of A with $O((m+n)K^2)$ ops.

Lanczos for low-rank approximation

Normalized starting vector u_1. Consider Krylov subspaces

$$\begin{aligned}\mathcal{K}_{K+1}(AA^T, u_1) &= \operatorname{span}\left\{u_1, AA^T u_1, \ldots, (AA^T)^K u_1\right\}, \\ \mathcal{K}_{K+1}(A^T A, v_1) &= \operatorname{span}\left\{v_1, A^T A v_1, \ldots, (A^T A)^K v_1\right\},\end{aligned}$$

with $v_1 = A^T u_1 / \|A^T u_1\|_2$.

Two-sided Lanczos process

1: $\tilde{v} \leftarrow A^T u_1$, $\alpha_1 \leftarrow \|\tilde{v}\|_2$, $v_1 \leftarrow \tilde{v}/\alpha_1$.
2: **for** $j = 1, \ldots, K$ **do**
3: $\quad \tilde{u} \leftarrow Av_j - \alpha_j u_j$, $\beta_{j+1} \leftarrow \|\tilde{u}\|_2$, $u_{j+1} \leftarrow \tilde{u}/\beta_{j+1}$.
4: $\quad \tilde{v} \leftarrow A^T u_{j+1} - \beta_{j+1} v_j$, $\alpha_{j+1} \leftarrow \|\tilde{v}\|_2$, $v_{j+1} \leftarrow \tilde{v}/\beta_{j+1}$.
5: **end for**

- Returns orthonormal bases $U_{K+1} \in \mathbb{R}^{m\times(K+1)}$, $V_{K+1} \in \mathbb{R}^{n\times(K+1)}$ of $\mathcal{K}_{K+1}(AA^T, u_1)$, $\mathcal{K}_{K+1}(A^T A, v_1)$
- Reorthogonalization assumed.

Lanczos for low-rank approximation

Collect scalars from Gram-Schmidt into bidiagonal matrix:

$$B_K = \begin{pmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & \beta_K & \alpha_K \end{pmatrix}. \tag{4}$$

$\rightsquigarrow$ two-sided Lanczos decomposition

$$A^T U_K = V_K B_K^T, \qquad AV_K = U_K B_K + \beta_{K+1} u_{K+1} e_K^T,$$

Assuming $K \geq k$:
How to extract rank-k approximation to A?

Lanczos for low-rank approximation

- Do *not* use `svds`, `eigs`, PROPACK, or anything else that aims at computing singular vectors!

[Simon/Zha'2000]:

$$\mathcal{T}_k(A) \approx A_K := U_K \mathcal{T}_k(B_K) V_K^T.$$

Cheap error estimate in Frobenius norm:

Lemma.

$$\|A_K - A\|_F \leq \sqrt{\sigma_{k+1}(B_K)^2 + \cdots + \sigma_K(B_K)^2} + \omega_K.$$

where $\omega_K^2 = \|A\|_F^2 - \alpha_1^2 \sum_{j=2}^K (\alpha_j^2 + \beta_j^2)$.

Proof. By the triangular inequality

$$\begin{aligned}\|A_K - A\|_F &\leq \left\|U_K(\mathcal{T}_k(B_K) - B_K)V_K^T + U_K B_K V_K^T - A\right\|_F \\ &\leq \sqrt{\sigma_{k+1}(B_K)^2 + \cdots + \sigma_K(B_K)^2} + \left\|U_K B_K V_K^T - A\right\|_F.\end{aligned}$$

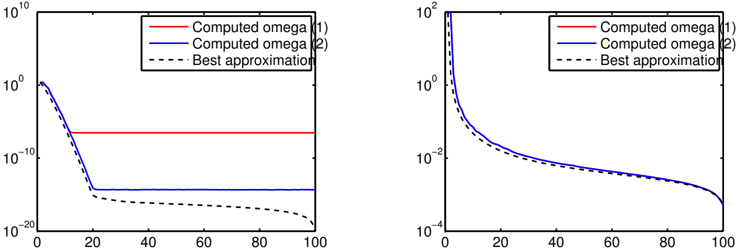
$\|A\|_F^2 = \|B_K\|_F^2 + \left\|U_K B_K V_K^T - A\right\|_F^2$ because of orthogonality.

Lanczos for low-rank approximation

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.
2. Formula for ω_K from lemma suffers from cancellation.

Lanczos for low-rank approximation

Two open problems:

1. Convergence theory that explains excellent convergence. Specifically, show that

$$\|A_{2k} - A\|_F \leq 2\|\mathcal{T}_k(A) - A\|_F$$

   under mild conditions on u_1. (Hint: Do *not* proceed via convergence of singular vectors.)
2. Derive cheap, accurate, and reliable error estimates for $\|\cdot\|_F, \|\cdot\|_2$.

Adaptive Cross Approximation (ACA)

Idea: Construct low-rank approximation from rows and columns of A.

- Which columns and rows? How?

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

$$\|A - A(:, c)SA(r, :)\|_2 \leq \varepsilon(1 + 2\sqrt{k}(\sqrt{m} + \sqrt{n})).$$

- Consider k dominant left/right singular vectors U_k, V_k. Proof proceeds by showing that $\exists$submatrices of U_k, V_k such that

$$\begin{aligned} \sigma_{\min}(U_k(c, :)) &\geq \left(\sqrt{k(m-k)+1}\right)^{-1/2} \\ \sigma_{\min}(V_k(r, :)) &\geq \left(\sqrt{k(n-k)+1}\right)^{-1/2} \end{aligned}$$

  Choice of S not difficult but technical, and involves full matrix A.
- By no means constructive.

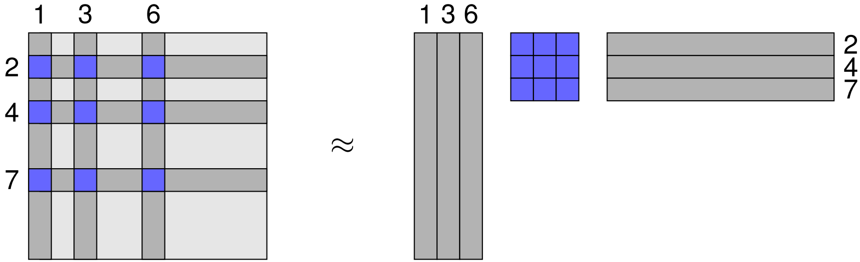
Adaptive Cross Approximation (ACA)

Choice of $S = (A(r,c))^{-1}$ in ACA $\rightsquigarrow$ Remainder term

$$R := A - A(:,c)(A(r,c))^{-1}A(r,:)$$

has zero rows at r and zero columns at c.

Cross approximation:



Adaptive Cross Approximation (ACA)

Another brave 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 $A_{11} \in \mathbb{R}^{k \times k}$ has maximal volume (i.e., max abs(det)) among all $k \times k$ submatrices of A. Then

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

where $\|M\|_C := \max_{i,j} |M(i,j)|$

Unfortunately, finding A_{11} is NP hard [Çivril/Magdon-Ismail'2013].

Adaptive Cross Approximation (ACA)

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

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

with invertible A_{11}. Using the Schur complement,

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

If $|\det A_{11}|$ is maximal among all possible selections of $k\times k$ submatrices of $A \rightsquigarrow |(A^{-1})_{k+1,k+1}| = \|A^{-1}\|_C := \max_{i,j}\left|(A^{-1})_{ij}\right|$.

$$\begin{aligned}
\sigma_{k+1}(A)^{-1} &= \|A^{-1}\|_2 = \max_x \frac{\|A^{-1}x\|_2}{\|x\|_2} \\
&\geq \frac{1}{k+1}\max_x \frac{\|A^{-1}x\|_\infty}{\|x\|_1} = \frac{1}{k+1}\|A^{-1}\|_C
\end{aligned}$$

and thus

$$|a_{22}-a_{12}A_{11}^{-1}a_{21}| = \frac{1}{\|A^{-1}\|_C} \leq (k+1)\sigma_{k+1}(A).$$

Adaptive Cross Approximation (ACA)

ACA with full pivoting [Bebendorf/Tyrtyshnikov'2000]

Set $R_0 := A$, $r := \{\}$, $c := \{\}$, $k := 0$
repeat
  $k := k + 1$
  $(i^*, j^*) := \arg\max_{i,j} |R_{k-1}(i,j)|$
  $r := r \cup \{i^*\}$, $c := c \cup \{j^*\}$
  $\delta_k := R_{k-1}(i^*, j^*)$
  $u_k := R_{k-1}(:, j^*)$, $v_k := R_{k-1}(i^*, :)^T / \delta_k$
  $R_k := R_{k-1} - u_k v_k^T$
until $\|R_k\|_F \le \varepsilon \|A\|_F$

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

Adaptive Cross Approximation (ACA)

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

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

Proof. From lines 7 and 8, it follows that the last column of $A(r_k, c_k)$ is a linear combination of the columns of the matrix

$$\tilde{A}_k := [A(r_k, c_{k-1}), R_{k-1}(r_k, j_k)] \in \mathbb{R}^{k \times k},$$

which implies $\det(\tilde{A}_k) = \det(A(r_k, c_k))$. However, $\tilde{A}_k(i, j_k) = 0$ for all $i = i_1, \ldots, i_{k-1}$ and hence

$$\det(\tilde{A}_k) = R_{k-1}(i_k, j_k) \det(A(r_{k-1}, c_{k-1})).$$

Since $\det A(r_1, c_1) = A(i_1, j_1) = R_0(i_1, j_1)$, the result follows by induction.

Adaptive Cross Approximation (ACA)

ACA with partial pivoting

Set $R_0 := A$, $r := \{\}$, $c := \{\}$, $k := 1$, $i^* := 1$
repeat
  $j^* := \arg\max_j |R_{k-1}(i^*, j)|$
  $\delta_k := R_{k-1}(i^*, j^*)$
  if $\delta_k = 0$ **then**
    if $\#r = \min\{m, n\} - 1$ **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
  $r := r \cup \{i^*\}$, $c := c \cup \{j^*\}$
  $i^* := \arg\max_{i, i \notin r} |u_k(i)|$
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 $\|u_k\|_2 \|v_k\|_2 \le \varepsilon \|A\|_F$ elusive.
  Replace $\|A\|_F$ by $\|A_k\|_F$, recursively computed via

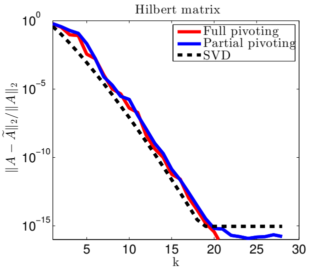
$$\|A_k\|_F^2 = \|A_{k-1}\|_F^2 + 2 \sum_{j=1}^{k-1} u_k^T u_j v_j^T v_k + \|u_k\|_2^2 \|v_k\|_2^2.$$

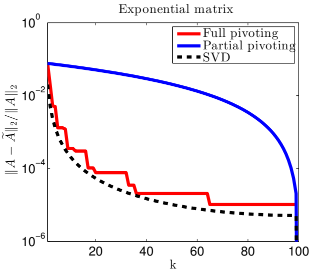
Adaptive Cross Approximation (ACA)

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.

Benefits from spd

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

- SVD becomes spectral decomposition.
- Can replace two-sided Lanczos by standard Lanczos.
- Can use trace instead of Frobenius norm to control error.
- 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].

Randomized algorithms for low-rank approximation

Must read: Halko/Martinsson/Tropp'2010: Finding Structure with Randomness...

Randomized Algorithm:

1. Choose standard Gaussian random matrix $\Omega \in \mathbb{R}^{n \times k}$.
2. Perform block mat-vec $Y = A\Omega$.
3. Compute (economic) QR decomposition $Y = QR$.
4. Form $B = Q^T A$.
5. Set $\mathcal{T}_k(A) \approx \widehat{A} := Q\mathcal{T}_k(B)$

Exact recovery: If A has rank k, we recover $\widehat{A} = A$ with probability 1.

Randomized algorithms for low-rank approximation

Must read: Halko/Martinsson/Tropp'2010: Finding Structure with Randomness...

Randomized Algorithm:

1. Choose standard Gaussian random matrix $\Omega \in \mathbb{R}^{n\times(k+p)}$.
2. Perform block mat-vec $Y = A\Omega$.
3. Compute (economic) QR decomposition $Y = QR$.
4. Form $B = Q^T A$.
5. Set $\mathcal{T}_k(A) \approx \widehat{A} := Q\mathcal{T}_k(B)$

HMT'2010: If A is a general matrix then choosing $k + p = 2k$ yields

$$\mathbb{E}\|A - \widehat{A}\|_2 \leq \left(2 + 4\sqrt{\frac{2\min\{m,n\}}{k-1}}\right)\sigma_{k+1}.$$

Bound can be improved (dramatically) by performing a few steps of subspace iteration on Y.

Randomized algorithms for low-rank approximation

Two 100×100 matrices:

(a) The Hilbert matrix A defined by $A(i,j) = 1/(i+j-1)$.
$k = 5$:

Exact	$p = 0$	$p = 1$	$p = 5$
1.88×10^{-3}	2.82×10^{-3}	1.89×10^{-3}	1.88×10^{-3}

(b) The matrix A defined by $A(i,j) = \exp(-\gamma|i-j|/n)$ with $\gamma = 0.1$.
$k = 40$:

Exact	$p = 0$	$p = 10$	$p = 40$	$p = 80$
1.45×10^{-3}	5×10^{-3}	4×10^{-3}	1.6×10^{-3}	1.45×10^{-3}

A priori approximation results

Need to know *a priori* which matrices admit good low-rank approximations.

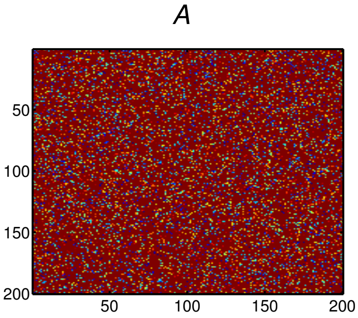
Why?

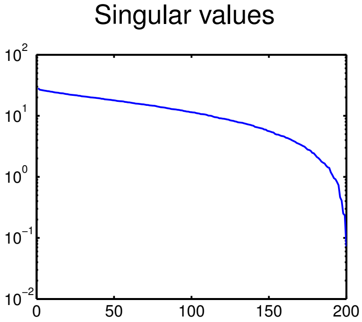
- Know which situations call for (hierarchical) low-rank approximations.
- Drive clustering/partitioning of matrix.

Schmidt-Mirsky: Equivalently, establish (quick) decay of singular values.

Singular values of random matrices

```
A = rand(200);
semilogy(svd(A))
```



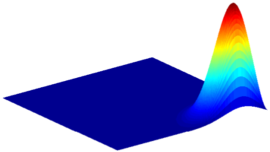


No reasonable low-rank approximation possible

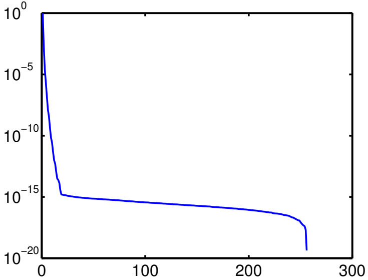
Singular values of smooth function

- Discretized smooth bivariate function.
- Arranged function values into a matrix.

Smooth function



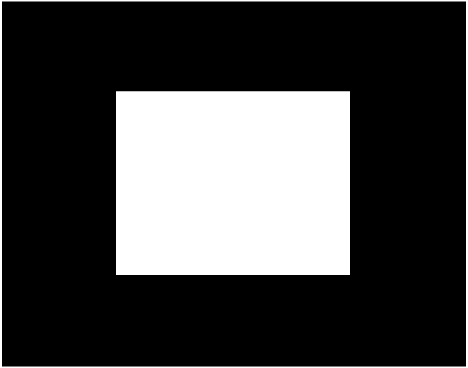
Singular values



Excellent rank-10 approximation possible

Exceptional case: Singularities along coordinate axes

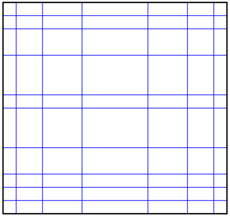
Rule of thumb: Smoothness helps, but not always needed.



Discretization of bivariate function

- Bivariate function: $f(x,y):\ [x_{\min}, x_{\max}] \times [y_{\min}, y_{\max}] \to \mathbb{R}$.
- Function values on tensor grid $[x_1, \dots, x_n] \times [y_1, \dots, y_m]$:

$$F = \begin{bmatrix} f(x_1,y_1) & f(x_1,y_2) & \cdots & f(x_1,y_n) \\ f(x_2,y_1) & f(x_2,y_2) & \cdots & f(x_2,y_n) \\ \vdots & \vdots & & \vdots \\ f(x_m,y_1) & f(x_m,y_2) & \cdots & f(x_m,y_n) \end{bmatrix}$$



Basic but crucial observation: $f(x,y) = g(x)h(y) \rightsquigarrow$

$$F = \begin{bmatrix} g(x_1)h(y_1) & \cdots & g(x_1)h(y_n) \\ \vdots & & \vdots \\ g(x_m)h(y_1) & \cdots & g(x_m)h(y_n) \end{bmatrix} = \begin{bmatrix} g(x_1) \\ \vdots \\ g(x_m) \end{bmatrix} \begin{bmatrix} h(y_1) & \cdots & h(y_n) \end{bmatrix}$$

Separability implies rank 1.

Separability and low rank

Approximation by sum of separable functions

$$f(x,y) = \underbrace{g_1(x)h_1(y) + \cdots + g_k(x)h_k(y)}_{=:f_k(x,y)} + \text{error},$$

or (*not* more generally)

$$f(x,y) = \underbrace{\sum_{j=1}^{k} s_{ij} g_i(x) h_j(y)}_{=:f_k(x,y)} + \text{error}$$

Define

$$F_k = \begin{bmatrix} f_k(x_1,y_1) & \cdots & f_k(x_1,y_n) \\ \vdots & & \vdots \\ f_k(x_m,y_1) & \cdots & f_k(x_m,y_n) \end{bmatrix}.$$

Then F_k has rank $\leq k$ and $\|F - F_k\|_F \leq \sqrt{mn} \times$ error.

$$\rightsquigarrow \sigma_{k+1}(F) \leq \|F - F_k\|_2 \leq \|F - F_k\|_F \leq \sqrt{mn} \times \text{error}.$$

Semi-separable approximation implies low-rank approximation.

Semi-separable approximation by Taylor

Example: 1D integral operator with shift-invariant kernel

$$f(x,y) := \begin{cases} g(x-y) & \text{if } x > y, \\ g(y-x) & \text{if } y > x, \\ 0 & \text{otherwise,} \end{cases}$$

with $g(z) = \log(z)$.

Taylor expansion of g around $z_0 > 0$:

$$g(z) \approx g_k(z) := \sum_{i=0}^{k-1} \frac{g^{(i)}(z_0)}{i!}(z - z_0)^i.$$

$\rightsquigarrow$ polynomial expansion of f around (x_0, y_0) with $z_0 = x_0 - y_0$:

$$f(x,y) \approx g_k(x-y) = \sum_{i=0}^{k-1} \sum_{j=0}^{k-1-i} (-1)^j f^{(i+j)}(x_0 - y_0) \frac{(x-x_0)^i}{i!} \frac{(y-y_0)^j}{j!}$$

Semi-separable approximation by Taylor

Summary:

$$\big(\text{discr. } f\big) \approx \big(\text{discr. } (x-x_0)^i\big) \times \big(f^{(i+j)}(x_0-y_0)\big) \times \big(\text{discr. } (y-y_0)^j\big)^T$$

$\rightsquigarrow$ rank-k approximation with approximation error governed by Tayor remainder

$$|g(z)-g_k(z)| \le \max_{\xi\in[a,b]} \left| \frac{f^{(k)}(\xi)}{k!}(z-z_0)^k \right| \le \frac{1}{k}\left(\frac{b-a}{2a}\right)^k$$

for all $0 < a \le z \le b$ with $z_0 = (a+b)/2$.

Semi-separable approximation by Taylor

Corollary. Consider real intervals I_x, I_y and $0 < \eta < 1$ such that

$$\mathrm{diam}(I_x) + \mathrm{diam}(I_y) \leq 2\eta \cdot \mathrm{dist}(I_x, I_y).$$

Then

$$|f(x,y) - f_k(x,y)| \leq \frac{1}{k}\eta^k$$

Proof. For $z = x - y$ with $x \in I_x, y \in I_y$, we have $z \in [a, b]$ with

$$\frac{b-a}{2a} = \frac{\mathrm{diam}(I_x) + \mathrm{diam}(I_y)}{2\mathrm{dist}(I_x, I_y)} \leq \eta.$$

Semi-separable approximation by interpolation

Solution of approximation problem

$$f(x,y) = g_1(x)h_1(y) + \cdots + g_k(x)h_k(y) + \text{error}.$$

by tensorized polynomial interpolation.

General construction:

1. Lagrange interpolation of $f(x,y)$ in y-coordinate:

$$\mathcal{I}_y[f](x,y) = \sum_{j=1}^{k} f(x,\theta_j)L_j(y)$$

   with Lagrange polynomials L_j of degree $k-1$ on $\mathcal{I}_y$.

2. Interpolation of $\mathcal{I}_y[f]$ in x-coordinate:

$$\mathcal{I}_x[\mathcal{I}_y[f]](x,y) = \sum_{i,j=1}^{k} f(\xi_i,\theta_j)L_i(x)L_j(y).$$

Semi-separable approximation by interpolation

Summary:

$$\big(\text{discr. } f\big) \approx \big(\text{discr. } L_i(x)\big) \times \big(f(\xi_i, \theta_j)\big) \times \big(\text{discr. } L_j(y)\big)^T$$

$\rightsquigarrow$ rank-k approximation with approximation error governed by

$$\begin{aligned} \text{error} &\leq \|f - \mathcal{I}_x[\mathcal{I}_y[f]]\|_\infty \\ &= \|f - \mathcal{I}_x[f] + \mathcal{I}_x[f] - \mathcal{I}_x[\mathcal{I}_y[f]]\|_\infty \\ &\leq \|f - \mathcal{I}_x[f]\|_\infty + \|\mathcal{I}_x\|_\infty \|f - \mathcal{I}_y[f]\|_\infty \end{aligned}$$

with Lebesgue constant $\|\mathcal{I}_x\|_\infty \sim \log r$ when using Chebyshev interpolation nodes.

Interpolation usually much better than Taylor [Börm'2010] $\rightsquigarrow$
η can be choosen smaller (roughly half) in adminissibility condition.

Semi-separable approximation: further results

If we do not insist on polynomials:

- For $f(x, y) = 1/(x - y)$ and similar functions, much better approximation by sum of exponentials [Hackbusch'2010].
- [Temlyakov'1992, Uschmajew/Schneider'2013]:

$$\sup_{f \in B^s} \inf \left\| f(x, y) - \sum_{k=1}^{r} g_k(x) h_k(y) \right\|_{L^2} \sim r^{-s},$$

with Sobolev space B^s of periodic functions with partial derivatives up to order s.