ALORA: Affine low-rank approximation

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Introduction and motivation

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- The SVD approximation can be constructed iteratively as (affine) subspace fitting of a set of columns.
- Matrix (hierarchical) structure must be exploited to increase precision with small cost.
- Black-box fast solvers can efficiently replace classical solvers for PDE's and integral equations.

Truncated SVD

Given $A \in \mathbb{R}^{m\times n}$, $m \geq n$, there exits orthogonal matrices $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ such that

$$A = U\Sigma V^T = \begin{bmatrix} u_1 & \cdots & u_m \end{bmatrix} \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \\ & 0 & \end{bmatrix} \begin{bmatrix} v_1 & \cdots & v_n \end{bmatrix}^T.$$

where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$ are the singular values and u_j and v_j are the left and right singular vectors associated to σ_j.

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The truncated SVD decomposition is defined as

$$\mathcal{T}_k(A) := U_k \Sigma_k V_k^T, \tag{1}$$

where $U_k := [u_1 \ \cdots \ u_k]$, $\Sigma_k := \text{diag}(\sigma_1, \ldots, \sigma_k)$ and $V_k := [v_1 \ \cdots \ v_k]$.

Error of TSVD approximation

For the spectral and Frobenius norms it holds

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

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Theorem (Eckart and Young)

Let $A \in \mathbb{R}^{m \times n}$, then

$$\|\mathcal{T}_k(A) - A\| = \min\{\|A - B\| : \ B \in \mathbb{R}^{m \times n} \text{ has at most rank } k\} \tag{2}$$

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Remark

- *Problem (2) has a unique solution when the Frobenius norm is used, provided all σ_j are different.*
- *If the spectral norm is used, the solutions are not unique since, e.g. for any $0 \le \theta \le 1$, $B = \mathcal{T}_k(A) - \theta\sigma_{k+1}U_kV_k^T$ is a solution, [Gu, M., 2014].*

Householder reflections

Definition (Householder reflector)

It is s a linear transformation that describes a reflection about an hyperplane containing the origin and orthogonal to $\mathbf{u}$,

$$\mathcal{H}_{\mathbf{u}} := I - \frac{2}{\|\mathbf{v}\|^2}\mathbf{v}\mathbf{v}^T, \tag{3}$$

where $\mathbf{v} = \mathbf{u} - \|\mathbf{u}\|\mathbf{e}$ is the Householder vector and $\mathbf{e} = (1, 0, \cdots, 0)^T$.

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Since $\mathcal{H}_{\mathbf{u}}(\mathbf{u}) = \|\mathbf{u}\|\mathbf{e}$, a complete pivoted QR factorization can be constructed via Householder reflections, this is

$$A\Pi = \underbrace{Q_1 \cdots Q_n}_{=:Q} R = QR, \tag{4}$$

where Π is a permutation, $Q_1 = \mathcal{H}_1$ and for $j = \{2 \cdots n\}$

$$Q_j = \begin{bmatrix} I_j & 0 \\ 0 & \mathcal{H}_j \end{bmatrix}$$

I_j: Identity matrix of size $(j-1) \times (j-1)$.

Error of QR approximation

For a rank-k QR approximation only consider the first k reflections as follows

$$A = QR\Pi^T = \begin{array}{c} \\ m \end{array} \begin{array}{cc} k & r-k \\ [Q_{11} & Q_{12}] \end{array} \begin{array}{c} \\ k \\ r-k \end{array} \begin{array}{c} \begin{array}{cc} k & n-k \end{array} \\ \begin{bmatrix} R_{11} & R_{12} \\ 0 & {\color{red}R_{22}} \end{bmatrix} \end{array} \Pi^T$$

$$= \underbrace{Q_{11}\begin{bmatrix} R_{11} & R_{12} \end{bmatrix}\Pi^T}_{{\color{blue}=:A_k}} + \underbrace{Q_{12}\begin{bmatrix} 0 & R_{22} \end{bmatrix}\Pi^T}_{{\color{red}\text{"residual"}}}.$$

where $Q = Q_1 \cdots Q_k$, and

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- The choice of Π is of great importance to control the error.
- Note that $\sigma_k(A) = \sigma_k(R)$.

Choosing the pivot using the maximal volume criteria

Theorem (Goreinov and Tyrtyshnikov, 2001)

Let us consider

$$R = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix}$$

where $R_{11} \in \mathbb{R}^{k\times k}$ *has maximal volume (i.e., maximum determinant in absolute value) among all* $k \times k$ *submatrices of* R*. Then*

$$\|R_{22} - R_{21}R_{11}^{-1}R_{12}\|_{\max} \leq (k+1)\sigma_{k+1}(R).$$

where $\|M\|_{\max} := \max_{i,j}|M(i,j)|$.

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Good news: Since for a low-rank QR factorization we have $R_{21} = 0$, then

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Bad news: Finding a submatrix of maximum volume has been proven to be NP-hard, Civril and Magdon-Ismail (2011).

Choosing the pivot using the classical column pivoting QRCP

QRCP takes as pivot the column of largest norm at each step, the error is bounded as

$$\|R_{22}\|_2 \leq 2^k \sqrt{n-k}\, \sigma_{k+1}(A). \tag{6}$$

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Method	**Reference**	**g(k,n)**	**Time**
Pivoted QR	[Golub, 1965]	$\sqrt{(n-k)}2^k$	$O(mnk)$
High RRQR	[Foster, 1986]	$\sqrt{n(n-k)}2^{n-k}$	$O(mn^2)$
High RRQR	[Chan, 1987]	$\sqrt{n(n-k)}2^{n-k}$	$O(mn^2)$
RRQR	[Hong and Pan, 1992]	$\sqrt{k(n-k)+k}$	-
Low RRQR	[Chan and Hansen, 1994]	$\sqrt{(k+1)n}2^{k+1}$	$O(mn^2)$
Hybrid-I RRQR	[Chandr. and Ipsen, 1994]	$\sqrt{(k+1)(n-k)}$	-
Hybrid-II RRQR		$\sqrt{(k+1)(n-k)}$	-
Hybrid-III RRQR		$\sqrt{(k+1)(n-k)}$	-
Algorithm 3	[Gu and Eisenstat, 1996]	$\sqrt{k(n-k)+1}$	-
Algorithm 4		$\sqrt{f^2k(n-k)+1}$	$O(kmn\log_f(n))$
DGEQPY	[Bischof and Orti, 1998]	$O(\sqrt{(k+1)^2(n-k)})$	-
DGEQPX		$O(\sqrt{(k+1)(n-k)})$	-
SPQR	[Stewart, 1999]	-	-
PT Algorithm 1	[Pan and Tang, 1999]	$O(\sqrt{(k+1)(n-k)})$	-
PT Algorithm 2		$O(\sqrt{(k+1)^2(n-k)})$	-
PT Algorithm 3		$O(\sqrt{(k+1)^2(n-k)})$	-
Pan Algorithm 2	[Pan, 2000]	$O(\sqrt{k(n-k)+1})$	-

Figure: Different algorithms for low-rank QR approximation, Mahoney et al. (2010).

Low rank approximation using subspace iteration

The following algorithm is the basic subspace iteration method,

Algorithm 1 $[A_k] = \text{SubspaceIter}(A,\Omega,k,q)$

Requires: $\Omega \in \mathbb{R}^{n\times l}$, with $l \geq k$.
Returns: rank-k approximation of A.

1: Perform $Y = (AA^T)^q A\Omega$.
2: Compute (economic) QR decomposition $Y = QR$.
3: Form $B = Q^T A$.
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- Note that setting $k = l = 1$ then Algorithm 1 is the classical *power method.*
- If Ω is a random Gaussian matrix, then setting $l = 2k$ and $q = 0$, we get the expected error [Halko, N. et al, 2014]

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

Error of subspace iteration approximation

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$$\widehat{\Omega} := V^T\Omega = \begin{matrix} l-p \\ n-l+p \end{matrix} \begin{bmatrix} \widehat{\Omega}_1 \\ \widehat{\Omega}_2 \end{bmatrix}, \quad 0 \leq p \leq l-k.$$

If $\widehat{\Omega}_1$ is full row rank, then the error is bounded as ([Gu, M., 2014])

$$\|A - A_k\|_2 \leq \sqrt{\sigma_{k+1}^2 + \omega^2 \|\widehat{\Omega}_2\|_2^2 \ \|\widehat{\Omega}_1^\dagger\|_2^2}, \tag{7}$$

where $\omega = \sqrt{k}\sigma_{l-p+1}\left(\frac{\sigma_{l-p+1}}{\sigma_k}\right)^{2q}$ and $\widehat{\Omega}_1\widehat{\Omega}_1^\dagger = I$.

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Remark

If G is a $(l-p) \times l$ is a Gaussian matrix, then rank$(G) = l - p$ with probability 1.

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2. How do we measure the distance between subspaces?
   - Consider $W_1, W_2 \in \mathbb{R}^{m \times k}$ with orthogonal columns.
   - Let let $S_1 := \text{ran}(W_1)$ and $S_2 := \text{ran}(W_2)$, then

$$\text{dist}(S_1, S_2) := \|W_1 W_1^T - W_2 W_2^T\|_2.$$

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Theorem (Ayala et al., 2017)

Using the notation from Algorithm 1, Let $S_u = \text{ran}([u_1 \cdots u_l])$ *and* $S_q = \text{ran}(Q)$, *considering* $\widehat{\Omega}_1$ *nonsingular and* $p = 0$, *then*

$$\text{dist}(S_u, S_q) \leq \left(\frac{\sigma_{l+1}}{\sigma_l}\right)^{2q+1} \|\widehat{\Omega}_2\|_2 \; \|\widehat{\Omega}_1^{-1}\|_2,$$

provided $\sigma_{l+1} > \sigma_l$.

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Given $A = [a_1 \;\; a_2 \;\; \cdots \;\; a_n]$, let $u \in \mathbb{R}^m$ be any unitary vector, then

$$\mathcal{H}_u A = [h_{a_1} \;\; h_{a_2} \;\; \cdots \;\; h_{a_n}].$$

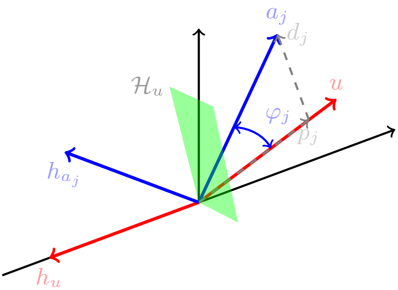

Figure: Householder reflection: p_j and d_j denote the projections of a_j along and orthogonal to u respectively.

Error for a rank-one approximation with arbitrary Householder vector.

$$\mathcal{H}_u A = \begin{bmatrix} \|a_1\|_2 \cos(\varphi_1) & \|a_2\|_2 \cos(\varphi_2) & \cdots & \|a_n\|_2 \cos(\varphi_n) \\ r_1 & r_2 & \cdots & r_n \end{bmatrix}, \tag{8}$$

where $r_j \in \mathbb{R}^{m-1}$.

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where $r_j \in \mathbb{R}^{m-1}$. The rank-one matrix

$$A_1 = \frac{u}{\|u\|_2}(\|a_1\|_2 \cos(\varphi_1), \cdots, \|a_n\|_2 \cos(\varphi_n)) \tag{9}$$

approximates A with an error given by the norm of the residual matrix $E := [r_1 \cdots r_n]$. By the Pythagorean theorem $\|r_j\|_2 = \|a_j\|_2 \sin(\varphi_j)$, then

$$\|A - A_1\|_F^2 = \|E\|_F^2 = \sum_{j=1}^{n} \|r_j\|_2^2 = \sum_{j=1}^{n} \|a_j\|_2^2 \sin^2(\varphi_j). \tag{10}$$

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Which choice of u minimizes this error?

Solving the optimization problem

We seek the hyperline in the m dimensional space that minimizes the sum of squared orthogonal distances from the points a_j's to itself. This is the *total least-square problem*.

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Define the matrix

$$Y := [a_1 - g \cdots a_n - g]. \tag{12}$$

- The best fitting line of the points $\{a_j\text{'s}\}$ is given by

$$\mathcal{L} := \{\ g + u\tau \quad | \quad \tau \in \mathbb{R}\}. \tag{13}$$

where $g := (1/n)\sum_{j=1}^{n} a_j$ and $u = u_1(Y)$, [Schneider et al., 2003].

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Define the matrix

$$Y := [a_1 - g \cdots a_n - g]. \tag{12}$$

- The best fitting line of the points $\{a_j\text{'s}\}$ is given by

$$\mathcal{L} := \{\ g + u\tau \quad | \quad \tau \in \mathbb{R}\}. \tag{13}$$

  where $g := (1/n)\sum_{j=1}^{n} a_j$ and $u = u_1(Y)$, [Schneider et al., 2003].

- If we impose the condition that the line passes through the origin, then the solution would be

$$\tilde{\mathcal{L}} := \{\ \tilde{u}\tau \quad | \quad \tau \in \mathbb{R}\}. \tag{14}$$

  where $\tilde{u} = u_1(A)$.

Best fitting (affine) subspace.

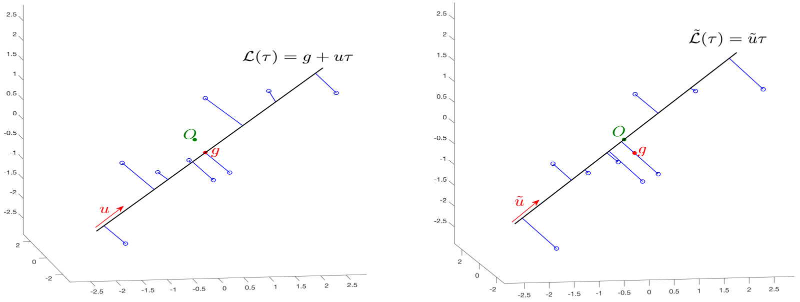

Figure: Solution of the total least-square problem (left) and its solution by imposing the condition to pass through the origin O (right).

Best fitting (affine) subspace.

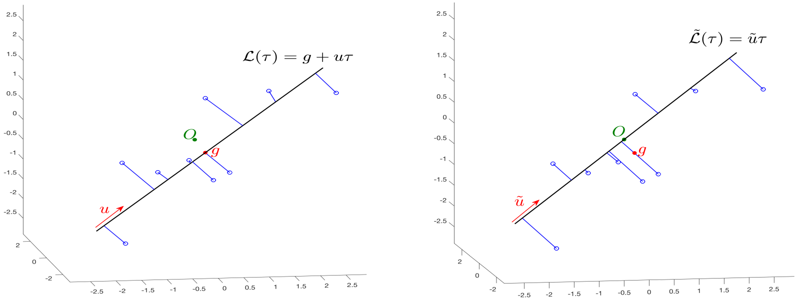

Figure: Solution of the total least-square problem (left) and its solution by imposing the condition to pass through the origin O (right).

- To approximate $u_1(Y)$ we can use the fact that it is the principal component of $C = YY^T$, the *covariance matrix*.
- There exists work on PCA on trimming around affine subspaces [Croux et al., 2014].

Error approximation for ALORA

Consider $c = [1, \cdots, 1]^T \in \mathbb{R}^m$. Let $u = u_1(Y) = u_1(A - gc)$ and define

$$B = A - T, \qquad T = (g - \alpha u)c, \tag{15}$$

where $\alpha \in \mathbb{R}$.

- Considering $g_B = (1/n) \sum_{j=1}^{n} b_j$, then clearly $g_B = u$.

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- Next, we prove that $u_1(B) = \frac{g_B}{\|g_B\|}$ and then the best fitting line of B is

$$\mathcal{L}^{(B)} := \left\{ \frac{g_B}{\|g_B\|}\tau \quad | \quad \tau \in \mathbb{R} \right\}.$$

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Lemma

Let $r = \text{rank}(Y)$ $\alpha \in R$, *then rank*$(B) = r$ *and*

$$u_j(B) = u_j(Y) \qquad \forall j \in \{1 \cdots r\}.$$

$$\sigma_1(B) = \sqrt{\sigma_1(Y)^2 + n\alpha^2} \quad \text{and} \quad v_1(B) = (\alpha c + \sigma_1(Y)v_1(Y))/\sigma_1(B).$$

$$\sigma_j(B) = \sigma_j(Y) \quad \text{and} \quad v_j(B) = v_j(Y) \quad \forall j \in \{2 \cdots r\}.$$

Lemma

Let B_k be a rank-k approximation of B such that

$$\|B - B_k\|_2 \leq g(k,n)\sigma_{k+1}(B),$$

where g is a function of k and n. Define $A_{k+1} = B_k + T$, then

$$\|A - A_{k+1}\|_2 \leq g(k,n)\sigma_{k+1}(A).$$

Lemma

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Corollary

$$\sigma_{k+1}(B) \leq \sigma_{k+1}(A) \leq \sigma_k(B). \tag{16}$$

Error approximation for ALORA

Lemma

Consider $A_l = B_{l-1} + T$*, where* B_{l-1} *is a rank* $l-1$ *approximation of* B*, then*

$$\|A - A_l\|_2 \leq g(l, n, C)\sigma_{l+1}(A),$$

where $C == (A-g)(A-g)^T$ *is the covariance matrix and*

$$g(l, n, C) = \sqrt{\frac{r + s\sqrt{\frac{n-l}{l}}}{r - s\sqrt{\frac{l}{n-l}}}}$$

with $r = \frac{\mathrm{tr}(C)}{n}$ *and* $s = \sqrt{\frac{\mathrm{tr}(C^2)}{n} - r^2}$.

Error approximation for ALORA

Lemma

Consider $A_l = B_{l-1} + T$, where B_{l-1} is a rank $l-1$ approximation of B, then

$$\|A - A_l\|_2 \leq g(l, n, C)\sigma_{l+1}(A),$$

where $C == (A - g)(A - g)^T$ is the covariance matrix and

$$g(l, n, C) = \sqrt{\frac{r + s\sqrt{\frac{n-l}{l}}}{r - s\sqrt{\frac{l}{n-l}}}}$$

with $r = \frac{\mathrm{tr}(C)}{n}$ and $s = \sqrt{\frac{\mathrm{tr}(C^2)}{n} - r^2}$.

Proof.

Use Theorem 3.1 from [Merikosky et al., 1983] on matrix C. □

Affine low rank approximation (ALORA)

Algorithm 4 $[A_{k+1}]$ = ALORA(A,k)

Require: $A = [a_1 \;\; a_2 \;\; \cdots \;\; a_n] \in \mathbb{R}^{m\times n}$.
Returns: rank $k+1$ approximation of A.

1: $g = (1/n)\sum_{j=1}^{n} a_j$, $c = [1 \cdots 1] \in \mathbb{R}^{1\times n}$.
2: $u :=$ first singular vector of Y.
3: $\alpha = g(1)/u(1)$.
4: $T = (g - \alpha u)c$.
5: Compute B_k: a rank-k approximation of $B = Y + \alpha uc$.
6: $A_{k+1} = T + B_k$

Ensure: $\|A - A_{k+1}\|_2 \le \sigma_k(A)$

Note that if the directions of the fitting lines are computed using a rank-revealing QR algorithm, then ALORA will produce a translated QR factorization.

Approximation error using ALORA with QRCP

- Using QRCP to approximate the direction of the best fitting line, then ALORA yields a QRCP factorization plus a rank-one translation matrix.

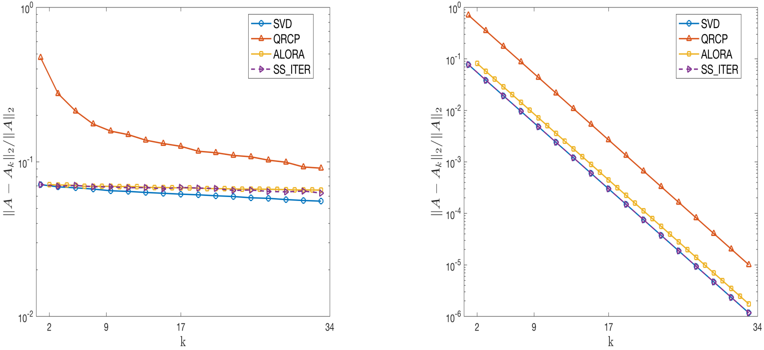


Figure: Low-rank approximation of a random matrix with slowly decreasing singular values (left), and the Kahan matrix (right), size $m = n = 256$.

ALORA with QRCP

- For matrices with slowly decreasing singular values, typically the first part of the spectrum is better approximated by ALORA.

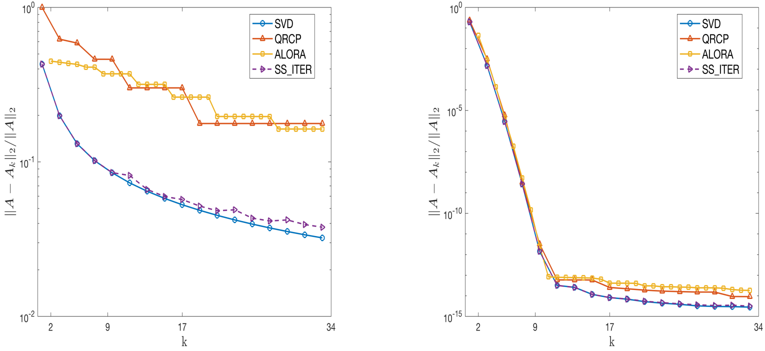


Figure: Low-rank approximation of matrices GKS (left), and Baart1 (right), size $m = n = 256$.

Approximation error using ALORA with Subspace Iteration

- Using Subspace iteration (Alg. 1 with $p = 2, q = 1$), to approximate the direction of the best fitting line, then ALORA improves the convergence error.
- The error get smaller while increasing p or q in Alg. 1.

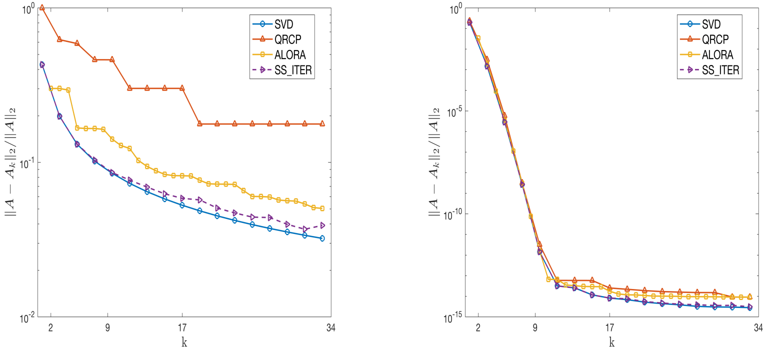
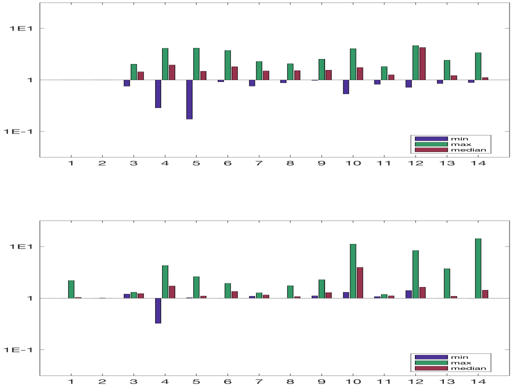


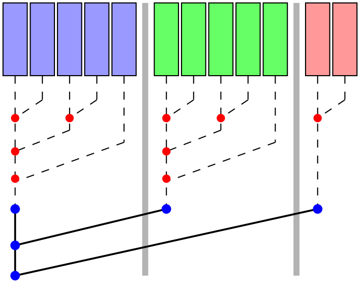
Figure: Low-rank approximation of matrices GKS (left), and Baart1 (right), size $m = n = 256$.

Approximation of singular values



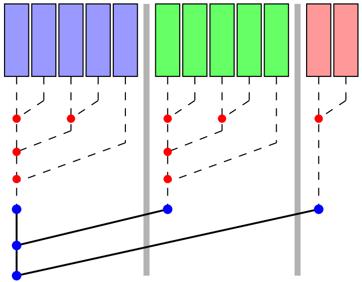
- For QRCP (top) we plot $\frac{|R(i,i)|}{\sigma_i}$.
- For ALORA (bottom) we plot $\frac{|R^{(B)}(i,i)|}{\sigma_i}$.

Reduction with tournament pivoting



- Tournament pivoting scheme (CARRQR, [Demmel et al., 2015]) on a m-by-10 matrix using 3 processors.

Reduction with tournament pivoting



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- The umber of messages (two) is independent of the number of columns and it is obviously optimal.

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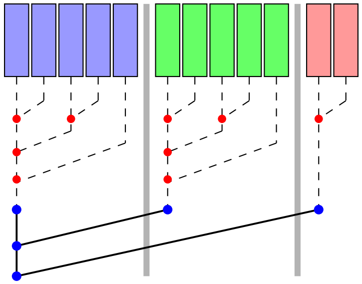


- Tournament pivoting scheme (CARRQR, [Demmel et al., 2015]) on a m-by-10 matrix using 3 processors.
- The umber of messages (two) is independent of the number of columns and it is obviously optimal.
- We use this reduction to in general select approximative *directions* instead of *pivot columns*.

- PALORA: Parallel ALORA using QRCP.
- CALRQR: Low-rank version of CARRQR.
- PDGEKQP: A low-rank version of the ScaLapack routine PDGEQP.

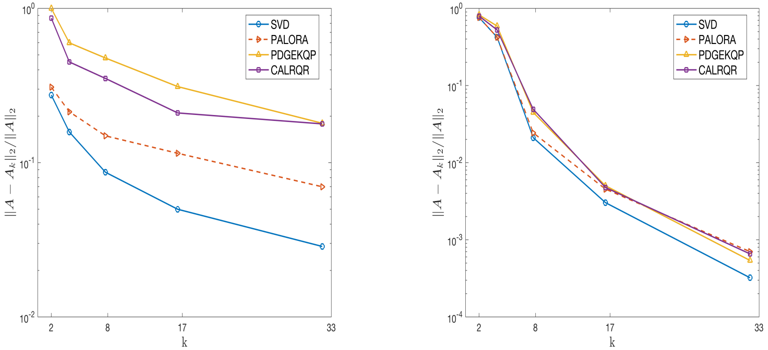


Figure: Low-rank approximation of matrices GKS (left), and Phillips (right), size $m = n = 512$.

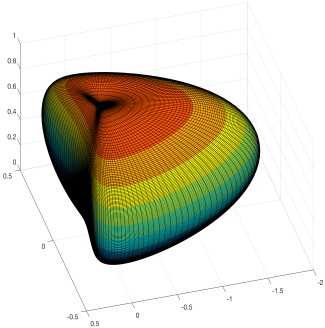
ALORA_IE: modified ALORA for integral equations

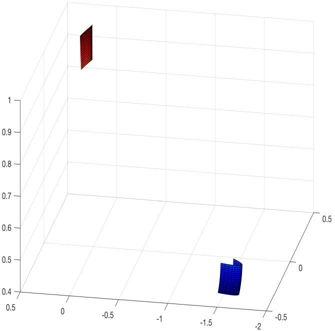
- We create a (hierarchical) partition of the domain.
- In such a way that the matrix corresponding to each subdomain has a best fitting line which direction can be approximated with its gravity center.
- Take advantage of the rapidly decreasing singular values.
- Construct a linear cost Householder reflection.
- Example: Consider the inner Dirichlet problem $\mathcal{A}u = f$

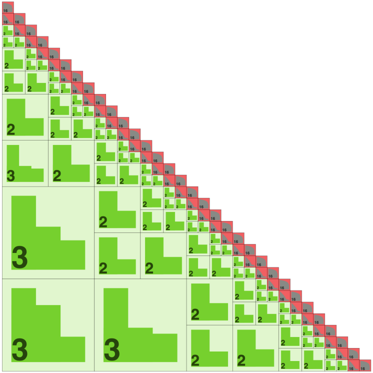
$$\mathcal{A}u(x) = \frac{1}{4\pi} \int_{\Gamma} \frac{u(y)}{|x-y|} ds_y.$$

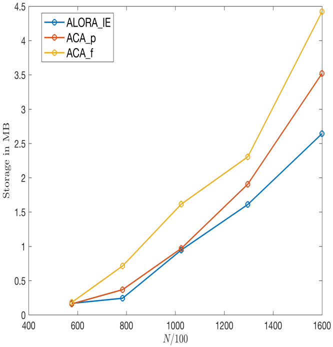
Defined over a 3D domain Γ.

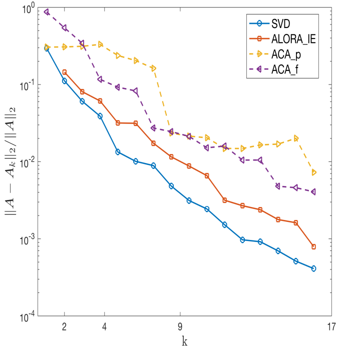
1. Discretize the equation by the classical Boundary element method and get the linear system $Ax = b$.
2. Factorize A using QRCP, ALORA_IE, and the Adaptive Cross Approximation (ACA) algorithm.

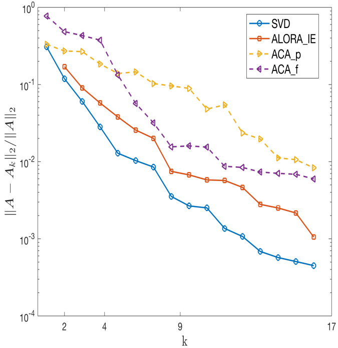

1
0.8
0.6
0.4
0.2
0
0.5
0
-0.5
0.5
0
-0.5
-1
-1.5
-2


1
0.9
0.8
0.7
0.6
0.5
0.4
0.5
0
-0.5
-1
-1.5
-2
0.5
0
-0.5




ALORA_IE
ACA_p
ACA_f
Storage in MB
N/100
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
400
600
800
1000
1200
1400
1600


SVD
ALORA_IE
ACA_p
ACA_f
$\|A - A_k\|_2/\|A\|_2$
k
10^0
10^-1
10^-2
10^-3
10^-4
2
4
9
17


SVD
ALORA_IE
ACA_p
ACA_f
$\|A - A_k\|_2/\|A\|_2$
k
10^0
10^-1
10^-2
10^-3
10^-4
2
4
9
17

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