Numerical Matrix Analysis

Notes #22 — Eigenvalues
Computing the Singular Value Decomposition

Peter Blomgren
⟨blomgren.peter@gmail.com⟩

Department of Mathematics and Statistics
Dynamical Systems Group
Computational Sciences Research Center
San Diego State University
San Diego, CA 92182-7720

http://terminus.sdsu.edu/

Spring 2020

Outline

1. Flashback
   - The QR-Algorithm with Shifts
2. The Big Prize — Computing the SVD
   - $\sigma(A)$ and $\lambda(A^*A)$
   - Stable Approach for $\sigma(A)$
3. The Computation, Phase 1
   - Golub-Kahan Bidiagonalization
   - Lawson-Hanson-Chan Bidiagonalization, when $m \gg n$
   - Hybrid LHC/GK 3-Step Bidiagonalization
4. The Computation, Phase 2
   - OLD: QR-Like Algorithm, NEW: Divide-and-Conquer
   - Divide-and-Conquer
   - Implementations

Last Time: The QR-Algorithm with Shifts

Starting from the pure QR-Algorithm, which converges linearly, we made a number of critical connections with three other algorithms:

1. Inverse Iteration
2. Shifted Inverse Iteration
3. Rayleigh Quotient Iteration

Adding the tie-breaking Wilkinson shift, we were able to define an algorithm which diagonalizes a real symmetric matrix with **cubic convergence** in general, and **quadratic convergence** in the worst case.

We describe the algorithm to the point where we can quickly identify **one** eigenvalue/eigenvector pair. **Deflation**, *i.e.* further sub-division of the problem is necessary to identify the full diagonalization.

The Core QR-Algorithm with Wilkinson Shift

Algorithm

The QR-Algorithm with Wilkinson Shifts

$\mathbf{A}^{(0)} = \texttt{hessenberg\_form}(\mathbf{A})$

`for k = 1:...`

$\quad \texttt{Select}\ \mu_{\texttt{W}}^{(k)} = a_m - \frac{\text{sign}(\delta) b_{m-1}^2}{|\delta| + \sqrt{\delta^2 + b_{m-1}^2}}, \quad \delta = \frac{a_{m-1} - a_m}{2}$

$\quad \left[\mathbf{Q}^{(\mathbf{k})}, \mathbf{R}^{(\mathbf{k})}\right] = \texttt{qr}\left(\mathbf{A}^{(\mathbf{k-1})} - \mu_{\texttt{W}}^{(\mathbf{k})} \mathbf{I}\right)$

$\quad \mathbf{A}^{(\mathbf{k})} = \mathbf{R}^{(\mathbf{k})} \mathbf{Q}^{(\mathbf{k})} + \mu_{\texttt{W}}^{(\mathbf{k})} \mathbf{I}$

`endfor`

Where,

$$\begin{bmatrix} a_{m-1} & b_{m-1} \\ b_{m-1} & a_m \end{bmatrix} \stackrel{\text{def}}{=} A_{\texttt{(m-1):m,(m-1):m}}$$

Computing the SVD

Computing the SVD in a **stable** way is non-trivial.

Formally, computation of the SVD can be reduced to an eigenvalue decomposition of a Hermitian square matrix, but the most obvious approach is unstable. *(Which is not stopping some people from using it...)*

Better informed individuals base their SVD computations on a different form of reduction to Hermitian form. As with diagonalizations, **for maximum efficiency** SVD computations are usually done in two phases.

Singular Values of A and Eigenvalues of A^*A

We know that every matrix $A \in \mathbb{C}^{m\times n}$ has a singular value decomposition $A = U\Sigma V^*$, and hence

$$A^*A = V\Sigma^*\Sigma V^* = V\,\mathrm{diag}(\sigma_1^2, \dots, \sigma_n^2)\,V^*.$$

Since A^*A and $\mathrm{diag}(\sigma_1^2, \dots, \sigma_n^2)$ are related by a similarity transformation, we must have that $\lambda_i(A^*A) = \sigma_i^2$. Thus, in **infinite** precision the algorithm is clear:

Do-Not-Use-Algorithm (SVD in Infinite Precision)

1. Form A^*A.
2. Compute the eigenvalue decomposition $A^*A = V\Lambda V^*$.
3. Let $\Sigma = \sqrt{\Lambda}$, zero-padded to $m \times n$.
4. Solve $U\Sigma = AV$ for unitary U, via QR-factorization.

Singular Values of A and Eigenvalues of A^*A

The algorithm described is unstable since it reduces the SVD to an eigenvalue problem which may be **extremely sensitive to perturbations** — due to ill-conditioning; here $\kappa(A^*A) = (\sigma_1/\sigma_n)^2$.

However, this algorithm is used quite frequently; usually by someone who has "rediscovered" the SVD; — even though it has many names: *the Proper Orthogonal Decomposition, the Karhunen-Loève (KL-) Decomposition, Principal Component Analysis, Empirical Orthogonal Functions, etc...*, the SVD keeps getting "rediscovered."

Rewind — [Notes#4] Hits on `scholar.google.com`

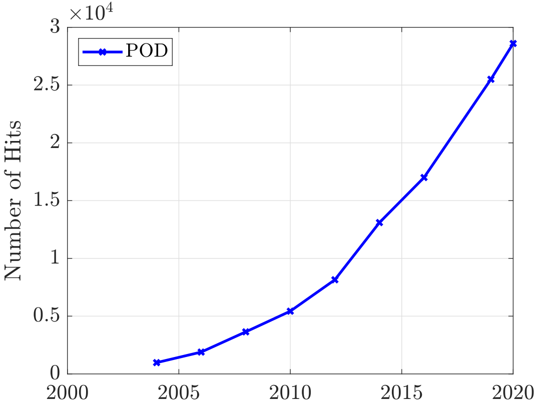


Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for "`Proper.Orthogonal.Decomposition`"

Rewind — [NOTES#4]

Hits on scholar.google.com

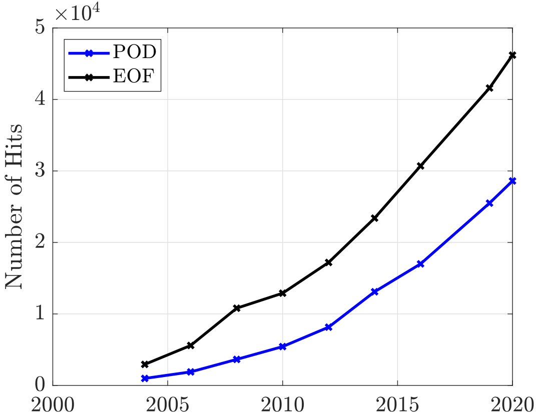


Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for "`Proper.Orthogonal.Decomposition`", "`Empirical.Orthogonal.(Function|Functions)`"

Rewind — [Notes#4] Hits on scholar.google.com

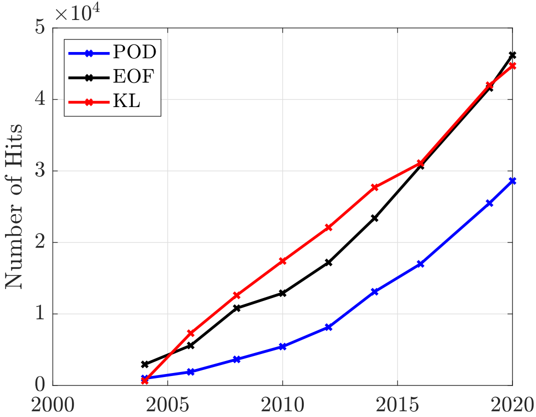


Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for "`Proper.Orthogonal.Decomposition`", "`Empirical.Orthogonal.(Function|Functions)`", "`Karhunen.Loeve`"

Rewind — [NOTES#4] Hits on scholar.google.com

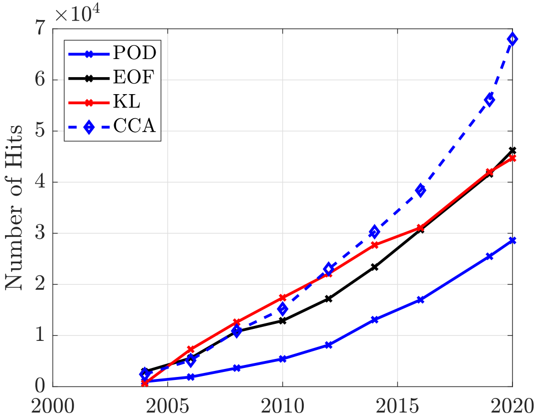


Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for "`Proper.Orthogonal.Decomposition`", "`Empirical.Orthogonal.(Function|Functions)`", "`Karhunen.Loeve`", "`Canonical.Correlation.Analysis`"

Rewind — [NOTES#4] Hits on scholar.google.com

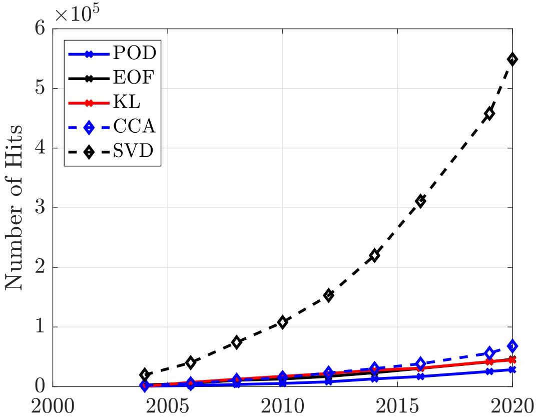


Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for "`Proper.Orthogonal.Decomposition`", "`Empirical.Orthogonal.(Function|Functions)`", "`Karhunen.Loeve`", "`Canonical.Correlation.Analysis`", "`Singular.Value.Decomposition`"

Rewind — [Notes#4] Hits on scholar.google.com

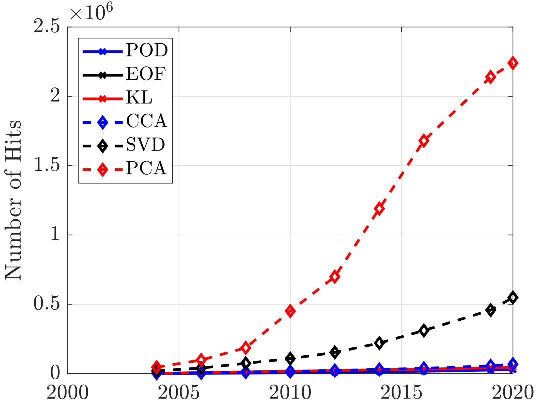


Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for "Proper.Orthogonal.Decomposition", "Empirical.Orthogonal.(Function|Functions)", "Karhunen.Loeve", "Canonical.Correlation.Analysis", "Singular.Value.Decomposition", "Principal.Component.Analysis"

Rewind — [Notes#4] Hits on scholar.google.com

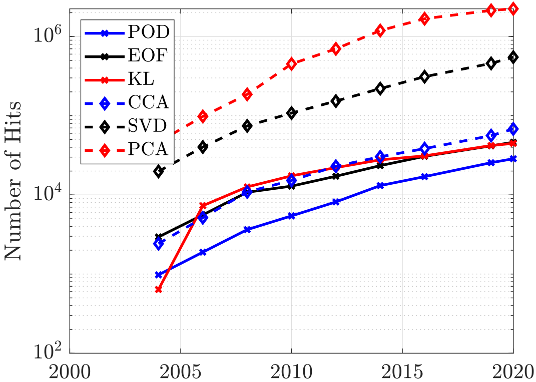


Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for `“Proper.Orthogonal.Decomposition”`, `“Empirical.Orthogonal.(Function|Functions)”`, `“Karhunen.Loeve”`, `“Canonical.Correlation.Analysis”`, `“Singular.Value.Decomposition”`, `“Principal.Component.Analysis”`

Singular Values of A and Eigenvalues of A^*A

The matrix A^*A has familiar and useful interpretations in many fields.

It shows up in linear least squares, as the *normal equations*, and also in the *general orthogonal projector*, $P = A(A^*A)^{-1}A^*$ built from a non-orthogonal matrix. Further, in statistics and other fields, it (or something very much like it) is known as the **co-variance matrix**.

Bottom Line

There are many tempting reasons to form A^*A... **Don't!!!**

SAN DIEGO STATE UNIVERSITY

Singular Values of A and Eigenvalues of A^*A

We can quantify the instability.

When the Hermitian matrix A^*A is perturbed by δB, the following holds for the perturbation of the eigenvalues

$$|\lambda_k\,(A^*A + \delta B) - \lambda_k\,(A^*A)\,| \leq \|\delta B\|_2$$

Singular Values of A and Eigenvalues of A^*A

We can quantify the instability.

When the Hermitian matrix A^*A is perturbed by δB, the following holds for the perturbation of the eigenvalues

$$|\lambda_k(A^*A + \delta B) - \lambda_k(A^*A)| \leq \|\delta B\|_2$$

A similar bound holds for the perturbation of the singular values

$$|\sigma_k(A + \delta A) - \sigma_k(A)| \leq \|\delta A\|_2.$$

Singular Values of A and Eigenvalues of A^*A

We can quantify the instability.

When the Hermitian matrix A^*A is perturbed by δB, the following holds for the perturbation of the eigenvalues

$$|\lambda_k(A^*A + \delta B) - \lambda_k(A^*A)| \leq \|\delta B\|_2$$

A similar bound holds for the perturbation of the singular values

$$|\sigma_k(A + \delta A) - \sigma_k(A)| \leq \|\delta A\|_2.$$

A backward stable SVD algorithm must give $\tilde{\sigma}_k$ satisfying

$$\tilde{\sigma}_k = \sigma_k(A + \delta A), \quad \frac{\|\delta A\|}{\|A\|} = \mathcal{O}(\epsilon_{\text{mach}}),$$

San Diego State University

Singular Values of A and Eigenvalues of A^*A

We can quantify the instability.

When the Hermitian matrix A^*A is perturbed by δB, the following holds for the perturbation of the eigenvalues

$$|\lambda_k(A^*A + \delta B) - \lambda_k(A^*A)| \leq \|\delta B\|_2$$

A similar bound holds for the perturbation of the singular values

$$|\sigma_k(A + \delta A) - \sigma_k(A)| \leq \|\delta A\|_2.$$

A backward stable SVD algorithm must give $\tilde{\sigma}_k$ satisfying

$$\tilde{\sigma}_k = \sigma_k(A + \delta A), \quad \frac{\|\delta A\|}{\|A\|} = \mathcal{O}(\epsilon_{\text{mach}}),$$

which implies

$$|\tilde{\sigma}_k - \sigma_k| = \mathcal{O}(\|A\|\epsilon_{\text{mach}}).$$

Singular Values of A and Eigenvalues of A^*A

Now, consider $\tilde{\lambda}_k(A^*A)$... If computed using a backward stable algorithm, we expect

$$|\tilde{\lambda}_k - \lambda_k| = \mathcal{O}(\|A^*A\|\epsilon_{\text{mach}}) = \mathcal{O}(\|A\|^2\epsilon_{\text{mach}}).$$

Singular Values of A and Eigenvalues of A^*A

Now, consider $\tilde{\lambda}_k(A^*A)$... If computed using a backward stable algorithm, we expect

$$|\tilde{\lambda}_k - \lambda_k| = \mathcal{O}(\|A^*A\|\epsilon_{\text{mach}}) = \mathcal{O}(\|A\|^2\epsilon_{\text{mach}}).$$

Since $\sigma_k = \sqrt{\lambda_k}$ we get

$$|\tilde{\sigma}_k - \sigma_k| = \mathcal{O}\left(\frac{|\tilde{\lambda}_k - \lambda_k|}{\sqrt{\lambda_k}}\right) = \mathcal{O}\left(\frac{\|A\|^2\epsilon_{\text{mach}}}{\sigma_k}\right).$$

Singular Values of A and Eigenvalues of A^*A

Now, consider $\tilde{\lambda}_k(A^*A)$... If computed using a backward stable algorithm, we expect

$$|\tilde{\lambda}_k - \lambda_k| = \mathcal{O}(\|A^*A\|\epsilon_{\text{mach}}) = \mathcal{O}(\|A\|^2\epsilon_{\text{mach}}).$$

Since $\sigma_k = \sqrt{\lambda_k}$ we get

$$|\tilde{\sigma}_k - \sigma_k| = \mathcal{O}\left(\frac{|\tilde{\lambda}_k - \lambda_k|}{\sqrt{\lambda_k}}\right) = \mathcal{O}\left(\frac{\|A\|^2\epsilon_{\text{mach}}}{\sigma_k}\right).$$

This result is off by a factor of $\frac{\|A\|}{\sigma_k}$, which is OK for the dominant singular values, but a disaster for small singular values $\sigma_k \ll \|A\|$, in this case we expect a loss of accuracy of order $\kappa(A)$. In a sense we are "squaring the condition number," much like in the least squares case.

Toward a Correct, Stable, Approach...

Given $A \in \mathbb{C}^{m \times m}$, consider (intellectually) the Hermitian matrix

$$H = \begin{bmatrix} 0 & A^* \\ A & 0 \end{bmatrix} = \begin{bmatrix} 0 & V\Sigma U^* \\ U\Sigma V^* & 0 \end{bmatrix}.$$

San Diego State University

Toward a Correct, Stable, Approach...

Given $A \in \mathbb{C}^{m\times m}$, consider (intellectually) the Hermitian matrix

$$H = \begin{bmatrix} 0 & A^* \\ A & 0 \end{bmatrix} = \begin{bmatrix} 0 & V\Sigma U^* \\ U\Sigma V^* & 0 \end{bmatrix}.$$

We can now write the eigenvalue decomposition of H

$$\begin{bmatrix} 0 & A^* \\ A & 0 \end{bmatrix} \begin{bmatrix} V & V \\ U & -U \end{bmatrix} = \begin{bmatrix} V & V \\ U & -U \end{bmatrix} \begin{bmatrix} \Sigma & 0 \\ 0 & -\Sigma \end{bmatrix}.$$

It is clear that from the eigenvalue decomposition of H, we can identify the singular values and singular vectors of A.

Toward a Correct, Stable, Approach...

Given $A \in \mathbb{C}^{m \times m}$, consider (intellectually) the Hermitian matrix

$$H = \begin{bmatrix} 0 & A^* \\ A & 0 \end{bmatrix} = \begin{bmatrix} 0 & V\Sigma U^* \\ U\Sigma V^* & 0 \end{bmatrix}.$$

We can now write the eigenvalue decomposition of H

$$\begin{bmatrix} 0 & A^* \\ A & 0 \end{bmatrix} \begin{bmatrix} V & V \\ U & -U \end{bmatrix} = \begin{bmatrix} V & V \\ U & -U \end{bmatrix} \begin{bmatrix} \Sigma & 0 \\ 0 & -\Sigma \end{bmatrix}.$$

It is clear that from the eigenvalue decomposition of H, we can identify the singular values and singular vectors of A.

Many SVD computations are (implicitly) based on / derived from this observation. We never explicitly form H, and are thus not constrained by the requirement that A is square.

The Two Phases of SVD Computation

$$\begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix} \xrightarrow{\text{Phase 1}} \begin{bmatrix} * & * & & \\ & * & * & \\ & & * & * \\ & & & * \\ & & & \\ & & & \end{bmatrix} \xrightarrow{\text{Phase 2}} \begin{bmatrix} * & & & \\ & * & & \\ & & * & \\ & & & * \\ & & & \\ & & & \end{bmatrix}$$

The **Bi-Diagonalization** in **Phase 1** requires a finite number of operations $\sim \mathcal{O}(mn^2)$.

The **Diagonalization** in **Phase 2** is done iteratively, and requires "infinitely many" operations. In practice $\mathcal{O}(n^2)$ operations are sufficient to identify the singular values.

Phase 1: Golub-Kahan Bidiagonalization

Phase-1-Bidiagonalization (for the SVD) is very similar to Phase-1-Hessenberg-transformation (for the QR-algorithm); the main difference here is that we are **not** constrained to a similarity transform, and hence we can apply a different sequence of unitary transforms from the left and right.

$$
\begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix}
\xrightarrow{U_1^*}
\begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \end{bmatrix}
\xrightarrow{V_1}
\begin{bmatrix} * & * & 0 & 0 \\ & * & * & * \\ & * & * & * \\ & * & * & * \\ & * & * & * \\ & * & * & * \end{bmatrix}
$$

$$
\xrightarrow{U_2^*}
\begin{bmatrix} * & * & & \\ & * & * & * \\ & 0 & * & * \\ & 0 & * & * \\ & 0 & * & * \\ & 0 & * & * \end{bmatrix}
\xrightarrow{V_2}
\begin{bmatrix} * & * & & \\ & * & * & 0 \\ & & * & * \\ & & * & * \\ & & * & * \\ & & * & * \end{bmatrix}
$$

Phase 1: Golub-Kahan Bidiagonalization

The unitary matrices U_i are built from full Householder reflectors, and V_i are built from "one-short" reflectors (like in the Hessenberg transformation algorithm)

$$U^* A V = U_n^* \cdots U_1^* \, A \, V_1 \cdots V_{n-2} = \begin{bmatrix} * & * & & \\ & * & * & \\ & & * & * \\ & & & * \\ & & & \\ & & & \end{bmatrix}$$

Essentially, this is a QR-factorization from the right and the left, so the total work ends up being

$$\texttt{Work} \sim \left(4mn^2 - \frac{4}{3} n^3 \right).$$

San Diego State University

Faster Methods for Phase 1

When $A \in \mathbb{R}^{m\times n}$, $m \gg n$, Golub-Kahan bidiagonalization is wasteful. In this case, a QR-factorization of A, followed by a the Golub-Kahan bidiagonalization of R is better

$$\begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix} \xrightarrow{\textbf{Phase 1a}} \begin{bmatrix} * & * & * & * \\ & * & * & * \\ & & * & * \\ & & & * \\ & & & \\ & & & \end{bmatrix} \xrightarrow{\textbf{Phase 1b}} \begin{bmatrix} * & * & & \\ & * & * & \\ & & * & * \\ & & & * \\ & & & \\ & & & \end{bmatrix}$$

i.e. $A \to Q^*A \to U^*Q^*AV$. This is known as the Lawson-Hanson-Chan bidiagonalization, and it requires

$$\texttt{Work} \sim \left(2mn^2 + 2n^3\right).$$

Golub-Kahan vs. Lawson-Hanson-Chan Bidiagonalization

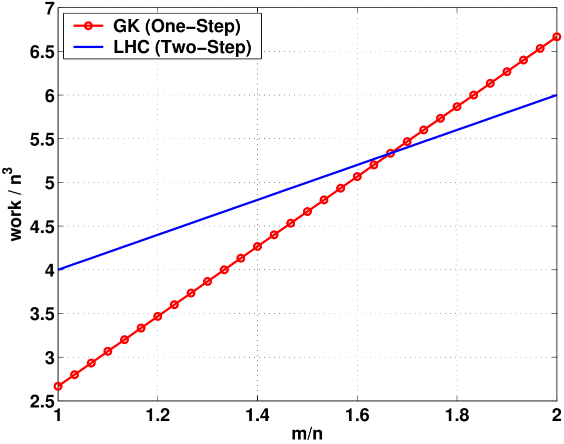
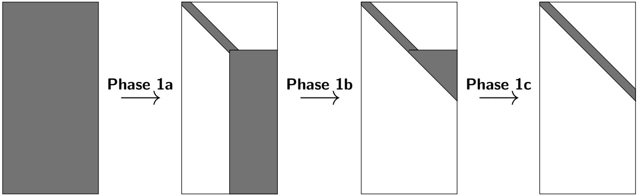


Figure: Comparing the work for Golub-Kahan and Lawson-Hanson-Chan bidiagonalization. The break-even point is $\frac{m}{n} = \frac{5}{3}$.

A Hybrid 3-Step Method

It is possible to define a hybrid algorithm, which switches from Golub-Kahan to Lawson-Hanson-Chan bidiagonalization at the optimal point. We end up with a 3-step method, pictorially defined by



We perform Golub-Kahan bidiagonalization for k steps, until $\frac{m-k}{n-k} = 2$, and then perform Lawson-Hanson-Chan bidiagonalization to the remaining, non-diagonalized part of the matrix.

Hybrid Golub-Kahan / Lawson-Hanson-Chan Bidiagonalization

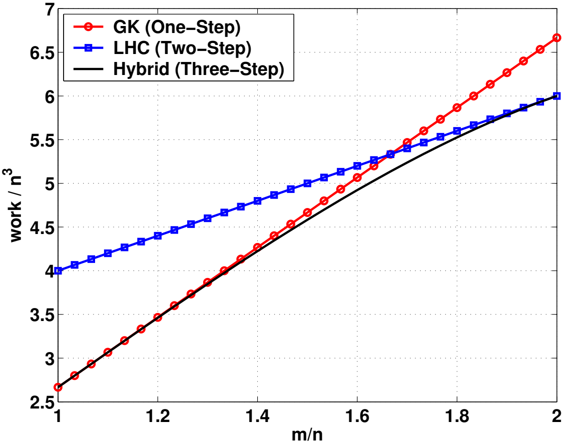


Figure: The work for the hybrid method is $\sim \left(4mn^2 - \frac{4}{3}n^3 - \frac{2}{3}(m-n)^3\right)$, and provides a small improvement in the range $n < m < 2n$.

Computing the SVD: Phase 2

Until recently (1990's), the standard approach to Phase 2 was a variant of the QR-algorithm, applied to the bidiagonal matrix generated during phase 1.

More recently, **divide-and-conquer** algorithms, based on subdivision into smaller subproblems have gained favor in the computational community.

For instance Lapack's `cgesdd`, `dgesdd`, `sgesdd`, and `zgesdd` algorithms are based on this paradigm.

One main advantage of this approach is that it can be parallelized, and thus phase 2 can be computed very rapidly in a multi-core environment.

Divide-and-Conquer: Vigorous Hand-waving

In essence divide-and-conquer works like this: We want to compute the diagonalization of B, which we decompose into three parts $B = B_1 + B_2 + \delta B$, where $\mathrm{rank}(\delta B) = 1$:

$$
\left[\begin{array}{ccc|ccc}
* & * & & & & \\
& * & * & & & \\
& & * & * & & \\
\hline
& & & * & * & \\
& & & & * & * \\
& & & & & *
\end{array}\right]
=
\left[\begin{array}{c|c}
B_1 & \\
\hline
& B_2
\end{array}\right]
+
\left[\begin{array}{c|c}
& * \\
\hline
&
\end{array}\right]
$$

Now, the diagonalization of the B_1 and B_2 blocks are computed (using the same strategy), then we (iteratively) correct for the rank-1 perturbation

$$
\left[\begin{array}{c|c}
\Sigma(B_1) & * \\
\hline
& \Sigma(B_2)
\end{array}\right]
\longrightarrow
\left[\begin{array}{c}
\Sigma(B)
\end{array}\right].
$$

Phase 2 Implementations

We leave phase 2 implementations as suggested projects.

- Phase 2 implementation based on the QR-algorithm is quite straight-forward.
- Phase 2 implementation based on the divide-and-conquer paradigm requires careful consideration of all the "book-keeping" details. While not necessarily more difficult in a mathematical sense, the practical implementation of this approach is more challenging.

Phase 2 Implementations in the "Wild"

- LAPACK's `dbdsqr`/`zbdsqr` implements an iterative variant of the QR algorithm
  - *"Calculating the Singular Values and Pseudo-Inverse of a Matrix"*, G. Golub and W. Kahan, Journal of the Society for Industrial and Applied Mathematics Series B Numerical Analysis, Volume 2, Issue 2, pp.205–224. (1964). `https://doi.org/10.1137/0702016`
  - *"Accurate Singular Values of Bidiagonal Matrices"*, James Demmel and W. Kahan, SIAM Journal on Scientific and Statistical Computing, Volume 11, Issue 5, pp.873–912. (1990). `https://doi.org/10.1137/0911052`

SOURCE: `https://en.wikipedia.org/wiki/Singular_value_decomposition#Numerical_approach`
REFERENCE: `http://www.netlib.org/lapack/explore-html/d0/da6/group__complex16_o_t_h_e_rcomputational_gae7f455622680c22921ba25be440a726f.html`

Phase 2 Implementations in the "Wild"

- The GNU Scientific Library (GSL) also implements an alternative approach: a one-sided Jacobi orthogonalization; the SVD of the bidiagonal matrix is obtained by solving a sequence of 2×2 SVD problems, similar to how the Jacobi eigenvalue algorithm solves a sequence of 2×2 eigenvalue methods
  - *"Matrix Computations"* 4th edition, Gene H. Golub and Charles F. Van Loan. Johns Hopkins Univeristy Press (2013). §8.6.3—"The SVD Algorithm"; §8.6.4—"Jacobi SVD Procedures"

SOURCE: `https://en.wikipedia.org/wiki/Singular_value_decomposition#Numerical_approach`