Numerical Matrix Analysis

Notes #22 — Eigenvalues
Computing the Singular Value Decomposition

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Outline

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.

Ref: Watkins, D.S., 2008. *The QR Algorithm Revisited.* SIAM review, 50(1), pp.133-145.

The Core QR-Algorithm with Wilkinson Shift

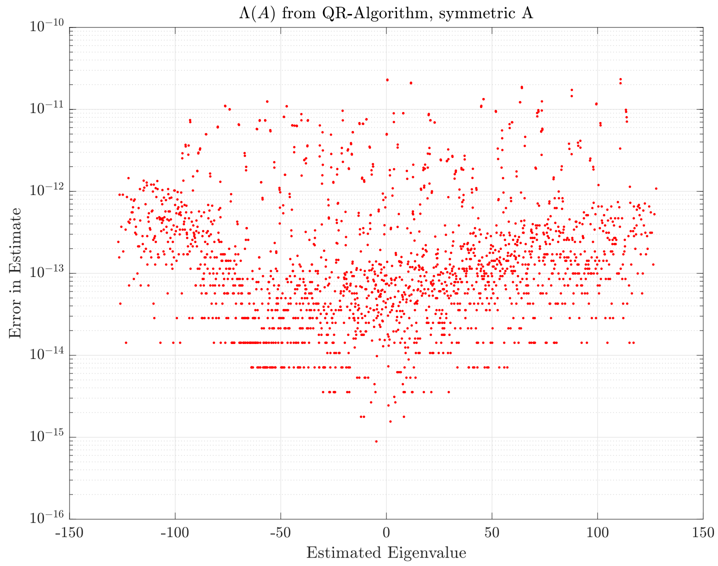
Algorithm (The QR-Algorithm with Wilkinson Shifts)

$\mathbf{A^{(0)}} = \texttt{hessenberg\_form}(\mathbf{A})$
`for k = 1:...`
  `Select` $\mu_{\mathtt{W}}^{(k)} = a_m - \frac{\text{sign}(\delta) b_{m-1}^2}{|\delta| + \sqrt{\delta^2 + b_{m-1}^2}}, \quad \delta = \frac{a_{m-1} - a_m}{2}$
  $\left[\mathbf{Q^{(k)}}, \mathbf{R^{(k)}}\right] = \texttt{qr}\left(\mathbf{A^{(k-1)}} - \mu_{\mathtt{W}}^{(\mathbf{k})}\mathbf{I}\right)$
  $\mathbf{A^{(k)}} = \mathbf{R^{(k)}}\mathbf{Q^{(k)}} + \mu_{\mathtt{W}}^{(\mathbf{k})}\mathbf{I}$
`endfor`

Where,

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

Result for Symmetric $A \in \mathbb{R}^{2048\times 2048}$ "Peel-Off Deflation"



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

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

Since A^*A and $\mathrm{diag}(\sigma_1^2, \ldots, \sigma_n^2)$ 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`

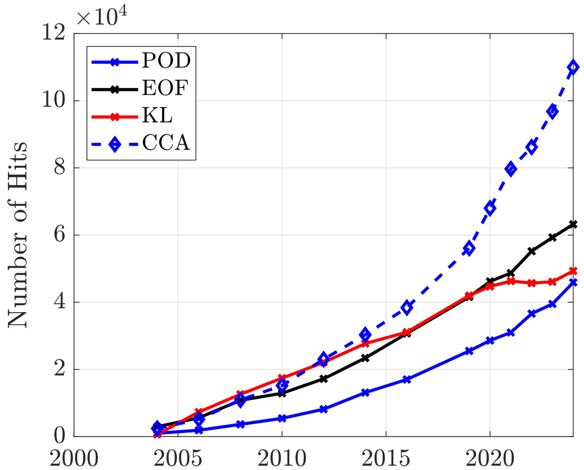


Figure: The many names, faces, and close relatives of the Singular Value Decomposition... Number of hits for "`Proper.Orthogonal.Decomposition`", "`Empirical.Orthogonal.(Function|Functions)`", "`Karhunen.Loeve`", "`Canonical.Correlation.Analysis`"

Flashback
The Big Prize — Computing the SVD
The Computation, Phase 1
The Computation, Phase 2
$\sigma(A)$ and $\lambda(A^*A)$
Stable Approach for $\sigma(A)$

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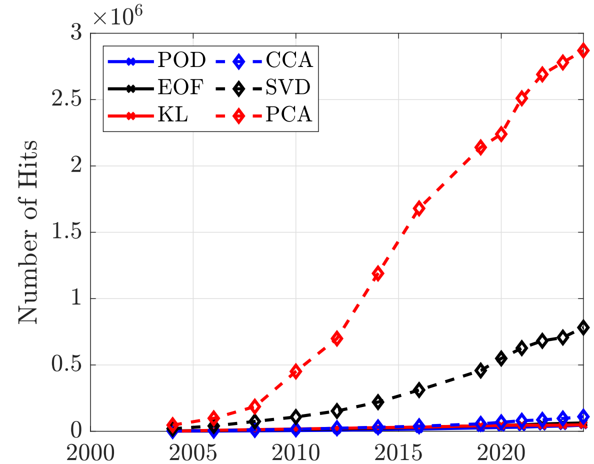

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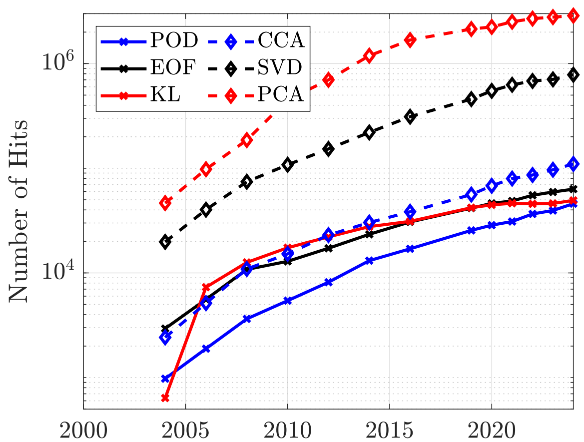

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Singular Values of A and Eigenvalues of A^*A 3 of 5

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!!!**

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

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

which implies

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

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

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

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

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

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

$$H = \left[\begin{array}{c:c} 0 & A^* \\ \hdashline A & 0 \end{array}\right] = \left[\begin{array}{c:c} 0 & V\Sigma U^* \\ \hdashline U\Sigma V^* & 0 \end{array}\right].$$

We can now write the eigenvalue decomposition of H

$$\left[\begin{array}{c:c} 0 & A^* \\ \hdashline A & 0 \end{array}\right] \left[\begin{array}{c:c} V & V \\ \hdashline U & -U \end{array}\right] = \left[\begin{array}{c:c} V & V \\ \hdashline U & -U \end{array}\right] \left[\begin{array}{c:c} \Sigma & 0 \\ \hdashline 0 & -\Sigma \end{array}\right].$$

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)

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

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

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

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. $A \to Q^* A \to U^* Q^* A V$. 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

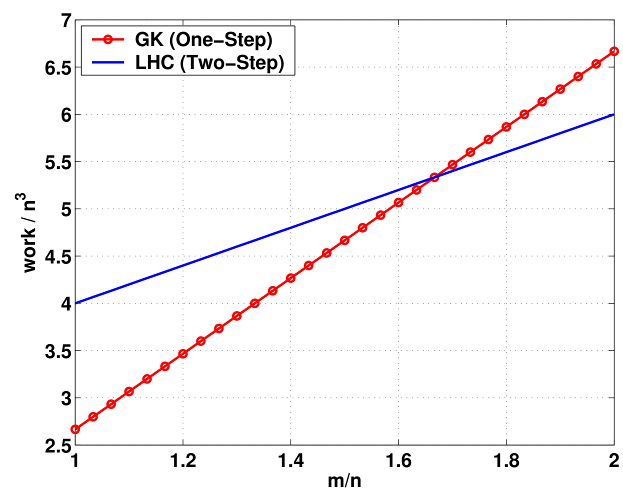
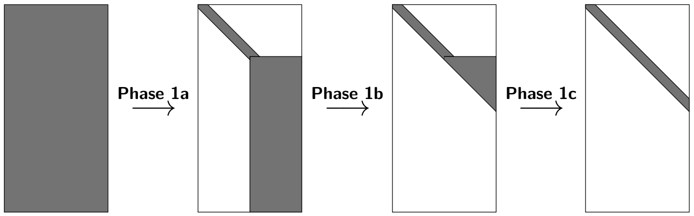


Figure: Comparing the work for Golub-Kahan and Lawson-Hanson-Chan bidiagonalization. The break-even point is $\frac{m}{n} = \frac{5}{3}$.

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

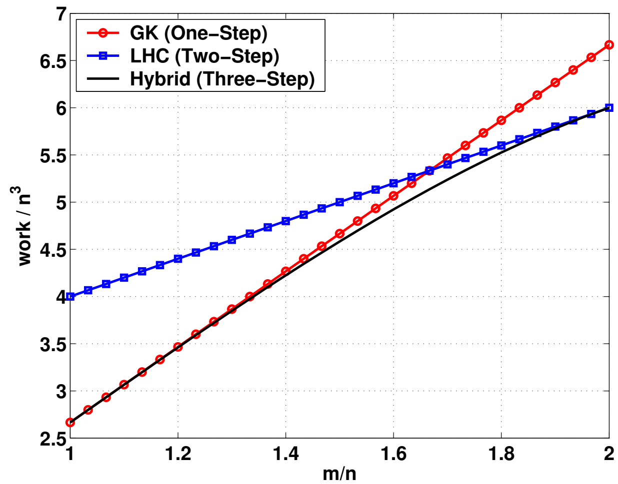


Figure: The work for the hybrid method is $\sim \left(4mn^2 - \frac{4}{3}n^3 - \frac{2}{3}(m-n)^3\right)$, and provides a small improvement in the range $n < m < 2n$.

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. *E.g.* Lapack's `sgesvd`, `cgesvd`, `dgesvd`, and `zgesvd`.

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

For instance Lapack's `sgesdd`, `cgesdd`, `dgesdd`, 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. Implementations in *e.g.* ScaLAPACK, cuSOLVER.

Old-school computing: Variable names in Fortran-77 consist of 1-6 characters chosen from the letters a-z and the digits 0-9. The first character must be a letter. Fortran-77 does not distinguish between upper and lower case, in fact, it assumes all input is upper case.

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.
- The implementations in the referenced libraries: Lapack, ScaLAPACK, and cuSOLVER are thousands of lines long.

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 University 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