



Classical Numerical Analysis, Chapter 02

Abner J. Salgado and Steven M. Wise

asalgad1@utk.edu swise1@utk.edu
University of Tennessee



Chapter 02

Singular Value Decomposition



Why is the Singular Value Decomposition (SVD) of Interest?

If $A \in \mathbb{C}^{n \times n}$ is Hermitian, then it is unitarily diagonalizable, i.e., there is a diagonal matrix $D \in \mathbb{R}^{n \times n}$ and a unitary matrix $U \in \mathbb{C}^{n \times n}$ such that

$$A = UDU^H.$$

This gives us, at least for this class of matrices, a nice geometric interpretation of the action of a matrix on a vector.

- 1 Since U^H is unitary and $\|U^H \mathbf{x}\|_2 = \|\mathbf{x}\|_2$, the action of U^H is *essentially* that of a rotation/reflection (it does not change the magnitude of the vector).
- 2 The matrix D is diagonal; its action is a (signed) dilation in each coordinate direction.
- 3 Finally, $U = (U^H)^{-1}$ reverses the rotation/reflection implemented by U^H .

Unfortunately, this decomposition only holds for Hermitian matrices. Can we somehow generalize unitary diagonalization for general matrices, even non-square matrices?



Reduced and Full SVDs



Definition of the (Full) Singular Value Decomposition

Definition (SVD)

Let $A \in \mathbb{C}^{m \times n}$. A **singular value decomposition** (SVD) of the matrix A is a factorization of the form

$$A = U \Sigma V^H,$$

where $U \in \mathbb{C}^{m \times m}$ and $V \in \mathbb{C}^{n \times n}$ are unitary, $\Sigma \in \mathbb{R}^{m \times n}$ is diagonal — meaning that $[\Sigma]_{i,j} = 0$, for $i \neq j$ — and the diagonal entries $[\Sigma]_{i,i} = \sigma_i$ are nonnegative and in non-increasing order: $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_p \geq 0$ with $p = \min(m, n)$.

The elements of the Σ are called the **singular values of A** . The columns of U and V are called the **left** and **right singular vectors**, respectively.



Full SVD to Reduced SVD

Let us, for the sake of definiteness, assume that $m \geq n$. If $A \in \mathbb{C}^{m \times n}$ has an SVD, then we can write

$$A\mathbf{v}_j = \sigma_j \mathbf{u}_j, \quad j = 1, \dots, n,$$

or, equivalently,

$$A \begin{bmatrix} | & & | \\ \mathbf{v}_1 & \cdots & \mathbf{v}_n \\ | & & | \end{bmatrix} = \begin{bmatrix} | & & | \\ \mathbf{u}_1 & \cdots & \mathbf{u}_n \\ | & & | \end{bmatrix} \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{bmatrix}.$$

In other words, we have obtained the representation

$$AV = \hat{U}\hat{\Sigma},$$

where (i) $\hat{\Sigma} \in \mathbb{R}^{n \times n}$ is square and diagonal, with non-negative diagonal entries; (ii) $\hat{U} \in \mathbb{C}^{m \times n}$ has orthonormal columns; and (iii) $V \in \mathbb{C}^{n \times n}$ is unitary. Thus, we have the **reduced SVD**,

$$A = \hat{U}\hat{\Sigma}V^H.$$



Reduced SVD to Full SVD

Now, assume that $m > n$. Suppose that we know (somehow) that $A \in \mathbb{C}^{m \times n}$ has the reduced SVD

$$A = \hat{U} \hat{\Sigma} V^H,$$

where (i) $\hat{\Sigma} \in \mathbb{R}^{n \times n}$ is square and diagonal, with non-negative diagonal entries; (ii) $\hat{U} \in \mathbb{C}^{m \times n}$ has orthonormal columns; and (iii) $V \in \mathbb{C}^{n \times n}$ is unitary. Use basis completion and the Gram-Schmidt process to add orthonormal vectors onto the columns of \hat{U} . Define

$$U = \left[\begin{array}{c|ccc|ccc} | & & | & | & & | \\ \mathbf{u}_1 & \cdots & \mathbf{u}_n & \mathbf{u}_{n+1} & \cdots & \mathbf{u}_m \\ | & & | & | & & | \end{array} \right],$$

where $\mathbf{u}_{n+1}, \dots, \mathbf{u}_m$ are the added orthonormal columns. The matrix $U \in \mathbb{C}^{m \times m}$ is unitary.



Reduced SVD to Full SVD, Cont.

Next, define

$$\Sigma = \begin{bmatrix} \hat{\Sigma} \\ \mathbf{O} \end{bmatrix} \in \mathbb{R}^{m \times n},$$

where $\mathbf{O} \in \mathbb{R}^{(m-n) \times n}$ is a matrix all of whose entries are zero.

Now, it follows that

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^H,$$

because the added columns of \mathbf{U} are nullified by the added zeros in Σ .
Essentially, no new information has been added.

We have show that, if \mathbf{A} has a full SVD, it has a reduced SVD, and *vice versa*.



Theorem (existence of SVD)

Every matrix $A \in \mathbb{C}^{m \times n}$ has a singular value decomposition. The singular values are unique and

$$\{\sigma_i^2\}_{i=1}^p = \begin{cases} \sigma(A^H A) & \text{if } m \geq n, \\ \sigma(AA^H) & \text{if } m \leq n, \end{cases}$$

where $p = \min(m, n)$. Recall, the symbol $\sigma(B)$ stands for the spectrum of the square matrix B .

Proof.

Assume, WLOG, that $m > n$. Clearly, $A^H A$ and AA^H are Hermitian. Let $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{y} \in \mathbb{R}^m$ be arbitrary. Then

$$\mathbf{x}^H A^H A \mathbf{x} = \|A\mathbf{x}\|_2^2 \geq 0 \quad \text{and} \quad \mathbf{y}^H A A^H \mathbf{y} = \|A^H \mathbf{y}\|_2^2 \geq 0.$$

This proves that eigenvalues of $A^H A$ and AA^H are non-negative. (Exercise.) Furthermore, $A^H A$ and AA^H share the same non-zero eigenvalues. (Exercise.)



Proof, Cont.

By the spectral decomposition theorem, there are unitary matrices $U \in \mathbb{C}^{m \times m}$ and $V \in \mathbb{C}^{n \times n}$ such that

$$AA^H = U\Lambda_1 U^H \quad \text{and} \quad A^H A = V\Lambda_2 V^H,$$

where

$$\Lambda_1 = \text{diag}(\lambda_1, \dots, \lambda_n, 0, \dots, 0) \in \mathbb{R}^{m \times m} \quad \text{and} \quad \Lambda_2 = \text{diag}(\lambda_1, \dots, \lambda_n) \in \mathbb{R}^{n \times n}.$$

Without loss of generality, we may assume that the eigenvalues are ordered so that

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \geq 0.$$

Now, we define

$$\sigma_i := \sqrt{\lambda_i}, \quad i = 1, \dots, n,$$

and

$$\Sigma := \text{diag}(\sigma_1, \dots, \sigma_n) \in \mathbb{C}^{m \times n}.$$

Then,

$$\Sigma \Sigma^H = \Lambda_1 \in \mathbb{R}^{m \times m} \quad \text{and} \quad \Sigma^H \Sigma = \Lambda_2 \in \mathbb{R}^{n \times n}.$$



Proof, Cont.

Now, let us examine the decomposition

$$A^H A = V \Sigma^T \Sigma V^H,$$

as given above. It follows that

$$A^H A \mathbf{v}_i = \sigma_i^2 \mathbf{v}_i, \quad i = 1, \dots, n,$$

where \mathbf{v}_k is the k^{th} column of V . Let $r \in \{1, \dots, n\}$ be the unique index satisfying

$$\sigma_r > 0 \quad \text{and} \quad \sigma_{r+1} = 0.$$

Except for the trivial case, there must be such an r . Define

$$\mathbf{u}_k = \frac{A \mathbf{v}_k}{\sigma_k}, \quad k = 1, \dots, r.$$



Proof, Cont.

Then

$$AA^H \mathbf{u}_k = A \left(\frac{A^H A \mathbf{v}_k}{\sigma_k} \right) = A (\sigma_k \mathbf{v}_k) = \sigma_k^2 \mathbf{u}_k, \quad k = 1, \dots, r.$$

Thus the constructed vectors \mathbf{u}_k can be identified as eigenvectors of AA^H . They are also orthonormal: for $i, j \in \{1, \dots, r\}$,

$$\mathbf{u}_i^H \mathbf{u}_j = \frac{\mathbf{v}_i^H A^H A \mathbf{v}_j}{\sigma_i \sigma_j} = \frac{\sigma_j}{\sigma_i} \mathbf{v}_i^H \mathbf{v}_j = \delta_{ij}.$$

Therefore, the constructed vectors \mathbf{u}_k can be identified as the first r columns of the matrix U that we found earlier. The remaining vectors $\mathbf{u}_{r+1}, \dots, \mathbf{u}_m$ can be obtained, via basis completion, so that

$$U = [\mathbf{u}_1, \dots, \mathbf{u}_m] \in \mathbb{C}^{m \times m}$$

is unitary, as desired. We have, finally,

$$A = U \Sigma V^H.$$





Uniqueness of Singular Vectors

Theorem

Suppose that $A \in \mathbb{C}^{m \times n}$ with $m \geq n$. If

$$A = U_1 \Sigma_1 V_1^H = U_2 \Sigma_2 V_2^H$$

are two SVDs for A , then $\Sigma_1 = \Sigma_2$, the columns of V_1 and V_2 form an orthonormal basis of eigenvectors of $A^H A$, and, if $A^H A$ has n distinct eigenvalues, then

$$V_1 = V_2 D,$$

for some $D = \text{diag}[e^{i\theta_1}, \dots, e^{i\theta_n}]$, with angles $\theta_i \in \mathbb{R}$, $i = 1, \dots, n$. Finally, if $\text{rank}(A) = n$ (A has full rank), and

$$A = U_1 \Sigma V^H = U_2 \Sigma V^H$$

are two SVDs for A , then the first n columns of U_1 and U_2 are equal.



Further Properties of the SVD



SVD and Rank

Theorem

Let $A \in \mathbb{C}^{m \times n}$, then $\text{rank}(A)$ coincides with the number of nonzero singular values.

Proof.

We write the SVD: $A = U\Sigma V^H$. Since U and V are unitary they are full rank. By a theorem, the rank is unchanged by multiplying by invertible (square, full rank) matrices. Thus, $\text{rank}(A) = \text{rank}(\Sigma)$ and since Σ is diagonal the assertion follows. □



Range and Kernel Through SVD

Theorem

Let $A \in \mathbb{C}^{m \times n}$ with $\text{rank}(A) = r$. Suppose an SVD for A is given by $A = U\Sigma V^H$, where $\mathbf{u}_1, \dots, \mathbf{u}_m$ denote the columns of U and $\mathbf{v}_1, \dots, \mathbf{v}_n$ denote the columns of V . Then

$$\langle \mathbf{u}_1, \dots, \mathbf{u}_r \rangle = \text{im}(A) \quad \text{and} \quad \langle \mathbf{v}_{r+1}, \dots, \mathbf{v}_n \rangle = \ker(A).$$

Proof.

(\subseteq): From the SVD one can easily write $A\mathbf{v}_i = \sigma_i\mathbf{u}_i$, for $i = 1, \dots, r$. This proves immediately that $\mathbf{u}_i \in \text{im}(A)$, for $i = 1, \dots, r$. Since $\text{im}(A)$ is a subspace of \mathbb{C}^m , any linear combination of $\mathbf{u}_1, \dots, \mathbf{u}_r$ is in $\text{im}(A)$. Hence $\langle \mathbf{u}_1, \dots, \mathbf{u}_r \rangle \subseteq \text{im}(A)$.



Proof, Cont.

(\supseteq): Let $\mathbf{y} \in \text{im}(A)$. Then $\exists \mathbf{x} \in \mathbb{C}^n$ such that $A\mathbf{x} = \mathbf{y}$. This implies that $U\Sigma V^H \mathbf{x} = \mathbf{y}$ for some \mathbf{x} . Let $\mathbf{x}' = V^H \mathbf{x}$. Then for some $\mathbf{x}' \in \mathbb{C}^n$, $U\Sigma \mathbf{x}' = \mathbf{y}$. Set $\mathbf{x}'' = \Sigma \mathbf{x}'$. Note that $\mathbf{x}'' \in \mathbb{C}^m$ and $x''_{r+1} = \cdots = x''_m = 0$. Hence for some $\mathbf{x}'' \in \mathbb{C}^m$, $U\mathbf{x}'' = \mathbf{y}$. Now we write

$$\mathbf{y} = U\mathbf{x}'' = \sum_{j=1}^m x''_j \mathbf{u}_j = \sum_{j=1}^r x''_j \mathbf{u}_j \in \langle \mathbf{u}_1, \dots, \mathbf{u}_r \rangle .$$

This proves that $\langle \mathbf{u}_1, \dots, \mathbf{u}_r \rangle \supseteq \text{im}(A)$, and we are done.

(\subseteq): From the SVD one can easily write $A\mathbf{v}_i = \mathbf{0}$, for $i = r+1, \dots, n$. This proves immediately that $\mathbf{v}_i \in \ker(A)$, for $i = r+1, \dots, n$. Since $\ker(A)$ is subspace of \mathbb{C}^n , any linear combination of $\mathbf{v}_{r+1}, \dots, \mathbf{v}_n$ is in $\ker(A)$. Hence $\langle \mathbf{v}_{r+1}, \dots, \mathbf{v}_n \rangle \subseteq \ker(A)$.



Proof, Cont.

(\supseteq): Let $\mathbf{x} \in \ker(A)$. Then $A\mathbf{x} = \mathbf{0}$. This implies that $U\Sigma V^H \mathbf{x} = \mathbf{0}$. Let $\mathbf{x}' = V^H \mathbf{x}$. This implies that $\mathbf{x} = V\mathbf{x}'$ and $U\Sigma \mathbf{x}' = \mathbf{0}$. Since U is invertible, this implies that $\Sigma \mathbf{x}' = \mathbf{0}$. This homogeneous system always has a solution of the form

$$\mathbf{x}' = \begin{bmatrix} x'_1 = 0 \\ \vdots \\ x'_r = 0 \\ x'_{r+1} = \alpha_{r+1} \\ \vdots \\ x'_n = \alpha_n \end{bmatrix}$$

where $\alpha_{r+1}, \dots, \alpha_n$ are arbitrary. But this shows that

$$\mathbf{x} = V\mathbf{x}' = \sum_{j=1}^n x'_j \mathbf{v}_j = \sum_{j=r+1}^n \alpha_j \mathbf{v}_j \in \langle \mathbf{v}_{r+1}, \dots, \mathbf{v}_n \rangle .$$

This proves that $\langle \mathbf{v}_{r+1}, \dots, \mathbf{v}_n \rangle \supseteq \ker(A)$, and we are done. □



Rank–Plus–Nullity Theorem

Corollary

Suppose that $A \in \mathbb{C}^{m \times n}$. Then,

$$\text{rank}(A) + \text{nullity}(A) = \dim(\text{im}(A)) + \dim(\ker(A)) = n.$$

Proof.

Set $r = \text{rank}(A)$. The last theorem guarantees that

$$\langle \mathbf{u}_1, \dots, \mathbf{u}_r \rangle = \text{im}(A) \quad \text{and} \quad \langle \mathbf{v}_{r+1}, \dots, \mathbf{v}_n \rangle = \ker(A).$$





When is $A^H A$ is Nonsingular?

Theorem

Suppose $A \in \mathbb{C}^{m \times n}$ with $m \geq n$. $A^H A$ is nonsingular iff $\text{rank}(A) = n$.

Proof.

Let $A = U \Sigma V^H$ be an SVD for A . Then $A^H A = V \Sigma^T \Sigma V^H$ yields a unitary diagonalization of $A^H A$. Note that

$$\Sigma^T \Sigma = \text{diag} [\sigma_1^2, \dots, \sigma_n^2] ,$$

where $\sigma_1, \dots, \sigma_n$ are the singular values of A , some of which may be zero. It is clear that $\text{rank}(A) = r$, where r is the number of nonzero singular values. Of course, it must be that $r \leq n$. Likewise, $\text{rank}(A^H A)$ is the number of nonzero elements on the diagonal of $\Sigma^H \Sigma$. This number must also be r . In other words,

$$\text{rank}(A) = r = \text{rank}(A^H A),$$

which proves the result. □



Some Further Properties

Theorem (SVD and norms)

Let $A \in \mathbb{C}^{m \times n}$, then $\|A\|_2 = \sigma_1$ and $\|A\|_F^2 = \sum_{i=1}^r \sigma_i^2$.

Theorem (SVD and self-adjoint matrices)

If A is Hermitian, that is, $A^H = A$, then the singular values of A are the absolute values of its eigenvalues. If A is Hermitian with non-negative eigenvalues, then the eigenvalues and the singular values coincide.

Theorem (SVD and determinants)

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

$$|\det(A)| = \prod_{i=1}^n \sigma_i.$$



Low Rank Approximations



Rank–One Matrices

Definition

Given $\mathbf{u} \in \mathbb{C}_*^m$, $\mathbf{v} \in \mathbb{C}_*^n$ and $\sigma \in \mathbb{C}_*$, the matrix $A \in \mathbb{C}^{m \times n}$ defined via

$$A = \sigma \mathbf{u} \mathbf{v}^H = \sigma \mathbf{u} \otimes \mathbf{v},$$

is called a **rank–one matrix**.

For every $\mathbf{x} \in \mathbb{C}^n$, the rank–one matrix A , defined above, acts as

$$A\mathbf{x} = \sigma \left(\mathbf{v}^H \mathbf{x} \right) \mathbf{u} \in \text{span}\{\mathbf{u}\}.$$

The rank of such a matrix is exactly equal to one. This justifies the name. The question we want to address now is whether *every* matrix can be represented (or at least approximated) by linear combinations of rank–one matrices.



Rank–One Decomposition Theorem

Theorem

Let $A \in \mathbb{C}^{m \times n}$ be such that $r = \text{rank}(A)$ and $A = U\Sigma V^H$ be a SVD. Then A is a linear combination of r rank–one matrices:

$$A = \sum_{j=1}^r \sigma_j \mathbf{u}_j \otimes \mathbf{v}_j.$$

Proof.

It suffices to write Σ as the sum of matrices of the form

$$\Sigma_j = \text{diag}[0, \dots, 0, \sigma_j, 0, \dots, 0],$$

where the element σ_j is in the j –th entry. The rest of the details are left as an exercise. □

Eckart–Young Theorem



Theorem

Let $A \in \mathbb{C}^{m \times n}$ be such that $r = \text{rank}(A)$. Let $A = U\Sigma V^H$ be an SVD of A . For $k < r$ define $A_k = \sum_{j=1}^k \sigma_j \mathbf{u}_j \otimes \mathbf{v}_j$. Let us denote by \mathcal{C}_k the collection of all matrices $B \in \mathbb{C}^{m \times n}$ such that $\text{rank}(B) \leq k$. Then, A_k is of rank k , and

$$\|A - A_k\|_2 = \sigma_{k+1} = \inf_{B \in \mathcal{C}_k} \|A - B\|_2.$$

Furthermore,

$$\|A - A_k\|_F = \sqrt{\sum_{j=k+1}^r \sigma_j^2} = \inf_{B \in \mathcal{C}_k} \|A - B\|_F.$$



Example

Consider the 7×7 matrix

$$A = \begin{bmatrix} 2.9057 & 6.5457 & 3.8587 & 4.6737 & 2.4171 & 3.8703 & 0.9922 \\ 2.6460 & 0.8889 & 3.2542 & 1.7574 & 6.8099 & 1.4357 & 6.2114 \\ 2.1268 & 3.4270 & 2.6255 & 2.6030 & 3.0228 & 2.1093 & 2.2459 \\ 2.1686 & 2.6778 & 3.8653 & 3.6416 & 3.6917 & 3.3553 & 2.2689 \\ 3.8927 & 6.6301 & 6.4863 & 6.8192 & 5.0281 & 6.0910 & 2.5521 \\ 4.0461 & 6.2798 & 3.1713 & 2.7880 & 6.1632 & 1.6456 & 5.8120 \\ 2.9612 & 1.9820 & 6.1018 & 5.1754 & 6.4646 & 5.0316 & 4.2031 \end{bmatrix}.$$

The singular values are, to 13 decimal digits of precision,

$$\sigma_1 = 27.7754505112764,$$

$$\sigma_2 = 08.0248423105149,$$

$$\sigma_3 = 05.2245562622115,$$

$$\sigma_4 = 00.0001965858656,$$

$$\sigma_5 = 00.0000856660061,$$

$$\sigma_6 = 00.0000628919629,$$

$$\sigma_7 = 00.0000071697992.$$



Example (Example, Cont.)

This matrix is very nearly singular and is well approximated by the rank-3 (compressed) matrix

$$A_3 = \sum_{i=1}^3 \sigma_i \mathbf{u}_i \mathbf{v}_i^T,$$

where $\mathbf{u}_i, \mathbf{v} \in \mathbb{R}^7$ are the singular vectors, which are suppressed for brevity. In other words, to a good approximation, there are really only 3 important components of A — namely, $\sigma_i \mathbf{u}_i \mathbf{v}_i^T$, $i = 1, 2, 3$ — that express its action. In particular, according to the Eckart–Young Theorem 3.3, the relative error in the compressed matrix is relatively small,

$$\frac{\|A - A_3\|_2}{\|A\|_2} = \frac{\sigma_4}{\sigma_1} = 7.07768 \times 10^{-06}.$$