Numerical Analysis for Machine Learning

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Chapter 1

Numerical Linear Algebra tools

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1.1 Introduction: Recap of Linear Algebra

In this section we will review some basic concepts of Linear Algebra that will be useful for the rest of the course.

1.1.1 Matrix-vector multiplication

Given a matrix $A \in \mathbb{R}^{m \times n}$ and a vector $x \in \mathbb{R}^n$, the matrix-vector multiplication $y = Ax$ is defined as:

$$y_i = \sum_{j=1}^{n} A_{ij} x_j \tag{1.1}$$

A matrix-vector multiplication can be considered as a linear combination of the columns of the matrix A. Lets see an example:

$$\begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} x_1 + \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} x_2 \tag{1.2}$$

1.1.2 Column space of a matrix

The column space of a matrix $A \in \mathbb{R}^{m \times n}$ is the subspace of $\mathbb{R}^m$ spanned by the columns of A. In other words, it is the set of all possible linear combinations of the columns of A. The column space of a matrix is denoted as $C(A)$.

If the columns of A are linearly independent, then the column space of A is the entire $\mathbb{R}^m$. If the columns of A are linearly dependent, then the column space of A is a subspace of $\mathbb{R}^m$ with dimension equal to the rank of A.

The rank of a matrix A is is the size of the largest set of linearly independent columns of A. It is denoted as $rank(A)$. Note that $rank(A) = rank(A^T)$.

1.1.3 System of linear equations

A system of linear equations is a set of m equations with n unknowns of the form:

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n &= b_2 \\
&\vdots \\
a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_n &= b_m
\end{aligned}
\tag{1.3}
$$

This system can be written in matrix form as $Ax = b$, where $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^n$ and $b \in \mathbb{R}^m$.

The system $Ax = b$ has a solution if and only if $b \in C(A)$. If $b \in C(A)$, then the system has a unique solution if and only if $rank(A) = n$. If $rank(A) < n$, then the system has infinitely many solutions.

1.1.4 CR factorization

The CR factorization of a matrix $A \in \mathbb{R}^{m \times n}$, with $m \geq n$, is a factorization of A as $A = CR$, where $C \in \mathbb{R}^{m \times r}$ is a matrix with the linearly independent columns of A and $R \in \mathbb{R}^{r \times n}$ is obtained by determining the coefficients of the linear combination of the columns of C that give the columns of A. In this factorization, $r = rank(A)$.

Lets see an example:

$$
A = \begin{bmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix} \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 2 \end{bmatrix} = CR
\tag{1.4}
$$

The matrix C is also called the Row Reduced Echelon Form of A.

1.1.5 Matrix-matrix multiplication

Given two matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times p}$, the matrix-matrix multiplication $C = AB$ is defined as:

$$
C_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj}
\tag{1.5}
$$

A matrix-matrix multiplication can be considered as the outer product of the columns of A and the rows of B. Lets see an example:

$$
\begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \end{bmatrix} + \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} \begin{bmatrix} 3 & 4 \end{bmatrix}
\tag{1.6}
$$

Note that each outer product generates a matrix of the same size as the result matrix, but always with rank 1. So the matrix-matrix multiplication can be considered as a sum of rank 1 matrices, obtained by the outer products of the columns of A and the rows of B.

1.1.6 Null space of a matrix

The null space of a matrix $A \in \mathbb{R}^{m \times n}$ is the set of all vectors $x \in \mathbb{R}^n$ such that $Ax = 0$. The null space of a matrix is denoted as $N(A)$. It is also called the kernel of A, denoted as $ker(A)$.

Formally, we have that:

$$N(A) = \{x \in \mathbb{R}^n : Ax = 0\} \tag{1.7}$$

The null space of a matrix is a subspace of $\mathbb{R}^n$. The dimension of the null space of a matrix is called the nullity of the matrix.

1.1.7 Fundamental subspaces of a matrix

Given a matrix $A \in \mathbb{R}^{m \times n}$, we can define four fundamental subspaces:

- The column space of A, denoted as $C(A)$
- The row space of A, denoted as $C(A^T)$
- The null space of A, denoted as $N(A)$
- The left null space of A, denoted as $N(A^T)$

These subspaces are related by the following properties:

$$\begin{aligned} C(A) &\perp N(A^T) \\ C(A^T) &\perp N(A) \end{aligned} \tag{1.8}$$

They also satisfy the following dimensions properties:

$$\begin{aligned} dim(C(A)) + dim(N(A)) &= n \\ dim(C(A^T)) + dim(N(A^T)) &= m \end{aligned} \tag{1.9}$$

This is known as the Rank-Nullity Theorem.

1.1.8 Orthogonal matrices

An orthogonal matrix is a square matrix $Q \in \mathbb{R}^{n \times n}$ such that $Q^T Q = I$, where I is the identity matrix. This implies that $Q^T = Q^{-1}$.

Now, consider that Q is an orthogonal matrix, and set $w = Q^T x$. Then we have that:

$$\begin{aligned} \|w\|^2 = w^T w &= x^T Q Q^T x \\ &= x^T x = \|x\|^2 \end{aligned} \tag{1.10}$$

This means that the norm of a vector is preserved under an orthogonal transformation. This is called an isometry. It is a useful property for numerical algorithms, as it helps to avoid numerical instability.

There are two main types of orthogonal transformations that we are interested:

Rotation matrices

A rotation matrix is an orthogonal matrix that represents a rotation in $\mathbb{R}^2$ or $\mathbb{R}^3$. In $\mathbb{R}^2$, a rotation matrix is of the form:

$$Q(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \tag{1.11}$$

Reflection matrices

A reflection matrix is an orthogonal matrix that represents a reflection with respect to a hyperplane. If n denotes the unit normal vector to the hyperplane, then the reflection matrix is of the form:

$$Q = I - 2nn^T \tag{1.12}$$

Note that the inverse of this matrix is itself, as $Q^T = Q^{-1}$ and in this case, Q is symmetric $(Q = Q^T)$.

1.1.9 QR factorization

The QR factorization of a matrix $A \in \mathbb{R}^{m \times n}$, with $m \geq n$, is a factorization of A as $A = QR$, where $Q \in \mathbb{R}^{m \times n}$ is an orthogonal matrix and $R \in \mathbb{R}^{n \times n}$ is an upper triangular matrix.

Gram-Schmidt process

The Gram-Schmidt process is a method to compute the QR factorization of a matrix. Given a matrix $A \in \mathbb{R}^{m \times n}$, the Gram-Schmidt process computes an orthonormal basis for the column space of A, as follows:

$$q_1 = \frac{a_1}{\|a_1\|}$$
$$q_i = a_i - \sum_{j=1}^{i-1} (q_j^T a_i) q_j \quad \forall i = 2, \dots, n \tag{1.13}$$

where a_i denotes the i-th column of A. The matrix Q is obtained by stacking the vectors q_i as columns. The matrix R is obtained by computing the coefficients of the linear combination of the columns of Q that give the columns of A.

1.1.10 Eigenvalues and eigenvectors

Given a square matrix $A \in \mathbb{R}^{n \times n}$, a scalar λ is called an eigenvalue of A if there exists a vector $v \in \mathbb{R}^n$ such that:

$$Av = \lambda v \tag{1.14}$$

The vector v is called an eigenvector of A associated with the eigenvalue λ.

Let P be the matrix whose columns are the eigenvectors of A, and Λ be the diagonal matrix whose diagonal elements are the eigenvalues of A. Then we have that:

$$A = P\Lambda P^{-1} \tag{1.15}$$

This is called the eigendecomposition of A.

The eigenvalues of a matrix are the roots of the characteristic polynomial of A, which is defined as:

$$det(A - \lambda I) = 0 \tag{1.16}$$

1.1.11 Similar matrices

Two square matrices A and B are called similar if there exists a non-singular matrix M such that:

$$B = M^{-1}AM \tag{1.17}$$

Similar matrices have the same eigenvalues, but not necessarily the same eigenvectors. Let (λ, y) be an eigenpair of B, then we have:

$$By = \lambda y \Rightarrow M^{-1}AMy = \lambda y \Rightarrow A(My) = \lambda(My) \tag{1.18}$$

This means that My is an eigenvector of A associated with the eigenvalue λ. So, to obtain the eigenvectors of A from the eigenvectors of B, we need to multiply the eigenvectors of B by M.

This property can be useful. For example, if we want to compute the eigenvalues of a matrix A, we can find some transformation M such that $M^{-1}AM = B$ is a simpler matrix to work with, usually a lower triangular matrix. Then we can compute the eigenvalues of B and obtain the eigenvalues of A. M is obtained by the permutation matrices to get from A to B. The Givens and Householder transformations are examples of such method.

1.2 Power method

The power method is an iterative algorithm to compute the dominant eigenvalue of a matrix (i.e., the eigenvalue with the largest magnitude). The algorithm is as follows:

Algorithm 1 Power method

1: Choose a random vector $x^{(0)}$, s.t. $\|x^{(0)}\| = 1$
2: **for** $k = 1, 2, \ldots$ **do**
3:     $y^{(k)} = Ax^{(k-1)}$
4:     $x^{(k)} = \frac{y^{(k)}}{\|y^{(k)}\|}$
5:     $\lambda^{(k)} = x^{(k)T}Ax^{(k)}$
6: **end for**

The convergence rate is determined by the ratio of the largest eigenvalue to the second largest eigenvalue.

1.2.1 Rayleigh quotient

The Rayleigh quotient is the base of the power method algorithm. Given a matrix $A \in \mathbb{R}^{n \times n}$ and a vector $x \in \mathbb{R}^n$, the Rayleigh quotient is defined as:

$$R(x) = \frac{x^T A x}{x^T x} \tag{1.19}$$

For every eigenpair (λ, v) of A, we have that:

$$R(v) = \frac{v^T A v}{v^T v} = \frac{v^T \lambda v}{v^T v} = \lambda \tag{1.20}$$

This means that the Rayleigh quotient is equal to the eigenvalue associated with the eigenvector v. This property is used in the power method to compute the dominant eigenvalue of a matrix.

1.2.2 Proof of convergence for the power method

The power method converges to the dominant eigenvalue of a matrix. The sketch proof is as follows:

Let $x^{(0)}$ be our initial vector, and let $\{v_1, \ldots, v_n\}$ be the eigenvectors of A. We can write $x^{(0)}$ as a linear combination of the eigenvectors of A (since the eigenvectors of A form a basis of $\mathbb{R}^n$):

$$x^{(0)} = \sum_{i=1}^{n} \alpha_i v_i \tag{1.21}$$

Then we have that:

$$A x^{(0)} = \sum_{i=1}^{n} \alpha_i A v_i = \sum_{i=1}^{n} \alpha_i \lambda_i v_i \tag{1.22}$$

Since in every iteration k of the power method we apply the matrix A to the vector $x^{(k-1)}$, we have that:

$$A x^{(k-1)} = A^k x^{(0)} = \sum_{i=1}^{n} \alpha_i \lambda_i^k v_i \tag{1.23}$$

Now, let us factorize the previous equation by the dominant eigenvalue $(\lambda_1)^k$:

$$A^k x^{(0)} = (\lambda_1)^k \left(\alpha_1 v_1 + \sum_{i=2}^{n} \alpha_i \left(\frac{\lambda_i}{\lambda_1} \right)^k v_i \right) \tag{1.24}$$

Note that the term inside the parenthesis converges to zero as $k \to \infty$, since the ratio of the other eigenvalues to the dominant eigenvalue is less than 1. This means that $x^{(}k)$ converges to the direction of the dominant eigenvector v_1. When it is normalized, its Rayleigh quotient converges to the dominant eigenvalue λ_1.

1.2.3 Inverse power method

The inverse power method is an iterative algorithm to compute the eigenvalue with the smalles magnitude of a matrix. Note that the smallest eigenvalue of a matrix is the largest eigenvalue of its inverse, since:

$$Ax = \lambda x \Rightarrow A^{-1}x = \frac{1}{\lambda}x \tag{1.25}$$

The algorithm is similar to the power method, but instead of applying the matrix A to the vector x, we apply the inverse of the matrix A:

Algorithm 2 Inverse power method

1: Choose a random vector $x^{(0)}$, s.t. $\|x^{(0)}\| = 1$
2: **for** $k = 1, 2, \ldots$ **do**
3:     $y^{(k)} = A^{-1}x^{(k-1)}$
4:     $x^{(k)} = \frac{y^{(k)}}{\|y^{(k)}\|}$
5:     $\lambda^{(k)} = x^{(k)T}Ax^{(k)}$
6: **end for**

In practice, we normally don't compute the inverse of the matrix A, but instead solve the linear system $Ax = y^{(k)}$ in each iteration.

1.2.4 Shifted inverse power method

The shifted inverse power method is an iterative algorithm to compute the eigenvalue with the smalles magnitude of a matrix, but with a shift μ added to the matrix A. The algorithm is as follows:

Algorithm 3 Shifted inverse power method

1: Choose a random vector $x^{(0)}$, s.t. $\|x^{(0)}\| = 1$
2: **for** $k = 1, 2, \ldots$ **do**
3:     $y^{(k)} = (A - \mu I)^{-1}x^{(k-1)}$
4:     $x^{(k)} = \frac{y^{(k)}}{\|y^{(k)}\|}$
5:     $\lambda^{(k)} = x^{(k)T}Ax^{(k)}$
6: **end for**

Note that with this algorithm, we are computing the eigenvalue of A that is closest to the shift μ. This can be useful to compute the eigenvalues of a matrix that are close to a given value.

1.3 Symmetric matrices

A matrix $A \in \mathbb{R}^{n \times n}$ is called symmetric if $A = A^T$. Symmetric matrices have important properties:

- The eigenvectors of a symmetric matrix form an orthonormal basis of $\mathbb{R}^n$.

- All the eigenvalues of a symmetric matrix are real.

Let us prove the first property:

Let A be a symmetric matrix, and let $\lambda_1, \ldots, \lambda_n$ be its eigenvalues. Let $v_1, \ldots, v_n$ be the eigenvectors associated with the eigenvalues $\lambda_1, \ldots, \lambda_n$. Let us take two eigenvectors v_i and v_j, such that $i \neq j$. Then we have that:

$$Av_i = \lambda_i v_i \quad \text{and} \quad Av_j = \lambda_j v_j \tag{1.26}$$

Then we have that:

$$(A - \lambda_i I)v_i = 0 \quad \text{and} \quad (A - \lambda_i I)v_j = (\lambda_j - \lambda_i)v_j$$

$$\Rightarrow v_i \in N(A - \lambda_i I) \quad \text{and} \quad v_j \in C(A - \lambda_i I) \tag{1.27}$$

Since A is symmetric, we have that $A - \lambda_i I$ is also symmetric. Then we have that:

$$N(A - \lambda_i I) = N((A - \lambda_i)^T) \perp C(A - \lambda_i I) \tag{1.28}$$

Concluding that v_i and v_j are orthogonal. Since this holds for all pairs of eigenvectors, we have that the eigenvectors of a symmetric matrix form an orthonormal basis of $\mathbb{R}^n$.

Now, let us prove the second property:

Since A is symmetric, we have that $A = A^T$. Then we have that:

$$\begin{aligned} Ax &= \lambda x \\ A\bar{x} &= \bar{\lambda}\bar{x} \end{aligned} \tag{1.29}$$

Then we have that:

$$\begin{aligned} \bar{x}^T A x &= \lambda x^T x = \lambda \|x\|^2 \\ x^T A \bar{x} &= \bar{\lambda} x^T \bar{x} = \bar{\lambda} \|x\|^2 \end{aligned} \tag{1.30}$$

Since $A = A^T$, we have that:

$$\bar{x}^T A x = (Ax)^T \bar{x} = x^T A^T \bar{x} = x^T A \bar{x} \tag{1.31}$$

Then we have that:

$$\lambda \|x\|^2 = \bar{\lambda} \|x\|^2 \Rightarrow \lambda = \bar{\lambda} \tag{1.32}$$

This means that the eigenvalues of a symmetric matrix are real.

1.3.1 Symmetric positive definite matrices

A matrix $A \in \mathbb{R}^{n \times n}$ is called symmetric positive definite if it is symmetric and if for every vector $x \in \mathbb{R}^n$ we have that:

$$x^T A x > 0 \quad \forall x \neq 0 \tag{1.33}$$

Symmetric positive definite matrices have important properties:

- All the eigenvalues of a symmetric positive definite matrix are positive.

- The Cholesky factorization of a symmetric positive definite matrix exists and is unique:

$$A = L^T L \tag{1.34}$$

In fact, a symmetric matrix is positive definite if and only if all its eigenvalues are positive, so:

$$x^T A x > 0 \quad \forall x \neq 0 \quad \Leftrightarrow \quad \lambda_i > 0 \quad \forall i \tag{1.35}$$

Note that the quantity $x^T A x$ is called the energy of the vector x with respect to the matrix A. This quantity is always positive for a symmetric positive definite matrix.

1.4 Singular Value Decomposition (SVD)

The Singular Value Decomposition (SVD) is a factorization of a matrix $A \in \mathbb{R}^{m \times n}$ as:

$$A = U \Sigma V^T \tag{1.36}$$

where $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ are orthogonal matrices, and $\Sigma \in \mathbb{R}^{m \times n}$ is a quasi-diagonal matrix with the singular values of A. The singular values of A are the square roots of the eigenvalues of $A^T A$.

Note that if $rank(A) = r$, then the matrix Σ has r non-zero singular values, and the remaining singular values are zero. Assume that the singular values of A are $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0$. Then we have that:

$$\begin{aligned} Av_i = \sigma_i u_i \quad &\forall i = 1, \ldots, r \\ Av_i = 0 \quad &\forall i = r+1, \ldots, n \end{aligned} \tag{1.37}$$

where u_i and v_i are the columns of U and V, respectively. The vectors u_i and v_i are called the left and right singular vectors of A, respectively.

The SVD can also be written as:

$$A = \sum_{i=1}^{r} \sigma_i u_i v_i^T \tag{1.38}$$

1.4.1 Economy SVD

The economy SVD is a factorization of a matrix $A \in \mathbb{R}^{m \times n}$ as:

$$A = U_r \Sigma_r V_r^T \tag{1.39}$$

where $U \in \mathbb{R}^{m \times r}$, $V \in \mathbb{R}^{n \times r}$ and $\Sigma \in \mathbb{R}^{r \times r}$, with $r = rank(A)$.

The economy SVD is useful when we are only interested in the first r singular values of A, which are the non-zero singular values.

1.4.2 Low-rank approximation

The SVD can be used to compute a low-rank approximation of a matrix $A \in \mathbb{R}^{m \times n}$. Given a rank k, with $k < r = rank(A)$, the low-rank approximation of A is given by:

$$A_k = U_k \Sigma_k V_k^T = \sum_{i=1}^{k} \sigma_i u_i v_i^T \tag{1.40}$$

where $U_k \in \mathbb{R}^{m \times k}$, $V_k \in \mathbb{R}^{n \times k}$ and $\Sigma_k \in \mathbb{R}^{k \times k}$, with $k < r = rank(A)$.

Because the singular values of A are sorted in decreasing order, the low-rank approximation only considers the first k singular values of A, as they are the components of A with the largest contribution.

The low-rank approximation of a matrix is useful for data compression, as it allows to represent a matrix with a smaller number of parameters. Note that the low-rank approximation of a matrix is the best rank-k approximation of the matrix in the Frobenius norm. This is called the Eckart-Young theorem.

1.4.3 Existance of the SVD

The SVD of a matrix $A \in \mathbb{R}^{m \times n}$ always exists. The proof is as follows:

Let $A \in \mathbb{R}^{m \times n}$ be a matrix. Then we have that $A^T A \in \mathbb{R}^{n \times n}$. We have that $A^T A$ is symmetric and positive semidefinite. In fact:

- $A^T A$ is symmetric: $(A^T A)^T = A^T (A^T)^T = A^T A$

- $A^T A$ is positive semidefinite: $x^T A^T A x = (Ax)^T Ax = \|Ax\|^2 \geq 0$

Therefore, $A^T A$ has an eigendecomposition:

$$A^T A = V \Lambda V^T \quad \text{s.t. } V^T V = I$$

Let us show now that $rank(A) = rank(A^T A)$. We can prove this by showing that the null space of A is the same as the null space of $A^T A$. Let $x \in N(A)$, then we have that:

$$Ax = 0 \Rightarrow A^T Ax = 0$$

This means that $N(A) \subseteq N(A^T A)$. Now, let $x \in N(A^T A)$, then we have that:

$$A^T Ax = 0 \Rightarrow x^T A^T Ax = 0 \Rightarrow \|Ax\|^2 = 0 \Rightarrow Ax = 0$$

This means that $N(A^T A) \subseteq N(A)$. Therefore, $N(A) = N(A^T A)$, and we have that $rank(A) = rank(A^T A)$.

Now, let us consider the eigenpairs (λ_i, v_i) of $A^T A$. Then let us define u_i as:

$$u_i = \frac{1}{\sqrt{\lambda_i}} A v_i$$

We will prove that each u_i is a unitary vector, and that the vectors u_i are mutually orthogonal. Let us first show that each u_i is a unitary vector:

$$\|u_i\|^2 = \left\| \frac{1}{\sqrt{\lambda_i}} A v_i \right\|^2 = \frac{1}{\lambda_i} v_i^T A^T A v_i = \frac{1}{\lambda_i} \lambda_i = 1$$

Now, let us show that the vectors u_i are mutually orthogonal. Let $i \neq j$, then we have that:

$$u_i^T u_j = \frac{1}{\sqrt{\lambda_i}} v_i^T A^T \frac{1}{\sqrt{\lambda_j}} A v_j = \frac{1}{\sqrt{\lambda_i \lambda_j}} v_i^T A^T A v_j$$

$$= \frac{1}{\sqrt{\lambda_i \lambda_j}} \lambda_j v_i^T v_j = 0$$

Now, we can show that the vectors u_i are the eigenvectors of AA^T, with eigenvalues λ_i:

$$AA^T u_i = AA^T \frac{1}{\sqrt{\lambda_i}} A v_i =$$

$$\frac{1}{\sqrt{\lambda_i}} AA^T A v_i = \frac{1}{\sqrt{\lambda_i}} A \lambda_i v_i = \lambda_i u_i$$

Therefore, we have that $AA^T = U \Lambda U^T$, where U is the matrix whose columns are the vectors u_i. Now, let us define Σ as the diagonal matrix whose diagonal elements are the square roots of the eigenvalues of $A^T A$:

$$\Sigma = \begin{bmatrix} \sqrt{\lambda_1} & 0 & \dots & 0 \\ 0 & \sqrt{\lambda_2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sqrt{\lambda_n} \end{bmatrix}$$

Then we have that:

$$A = U \Sigma V^T$$

where V is the matrix whose columns are the eigenvectors of $A^T A$. Therefore, the SVD of A exists.

1.4.4 Computation of the SVD

The SVD of a matrix can be computed using the following steps:

1. Compute the eigendecomposition of $A^T A$.

2. Compute the singular values of A as the square roots of the eigenvalues of $A^T A$.

3. Compute the right singular vectors of A as the eigenvectors of $A^T A$.

4. Compute the left singular vectors of A as $u_i = \frac{1}{\sqrt{\lambda_i}} A v_i$.

1.4.5 Geometrical interpretation of the SVD

The SVD of a matrix $A \in \mathbb{R}^{m \times n}$ can be interpreted geometrically as a composition of three transformations:

- The matrix V represents a rotation in $\mathbb{R}^n$.

- The matrix Σ represents a scaling in $\mathbb{R}^{m \times n}$.

- The matrix U represents a rotation in $\mathbb{R}^m$.

In $\mathbb{R}^2$, the SVD of a matrix A can be interpreted as a rotation of the unit circle, followed by a scaling along the axes, followed by another rotation. So this transformation can be represented with 4 parameters: two angles and two scaling factors. In $\mathbb{R}^3$, its the same idea, but with 6 parameters: three angles and three scaling factors.

1.4.6 Polar decomposition

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix. The polar decomposition of A is a factorization of A as:

$$A = QS \tag{1.41}$$

where Q is an orthogonal matrix and S is a symmetric positive definite matrix. The polar decomposition can be derived from the SVD of A as:

$$A = U\Sigma V^T = (UV^T)(V\Sigma V^T) = QS \tag{1.42}$$

where $Q = UV^T$ and $S = V\Sigma V^T$. So, the polar decomposition of a symmetric matrix always exists.

1.4.7 Eckart-Young theorem

The Eckart-Young theorem states that the best rank-k approximation of a matrix $A \in \mathbb{R}^{m \times n}$ in the Frobenius norm is given by the low-rank approximation of A, denoted as A_k:

$$\min_{rank(B)=k} \|A - B\|_F = \|A - A_k\|_F \tag{1.43}$$

This also applies to the spectral norm $\| \cdot \|_2$. To prove this, let us define the mentioned norms:

Frobenius norm

The Frobenius norm of a matrix $A \in \mathbb{R}^{m \times n}$ is defined as:

$$\|A\|_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij}^2} \tag{1.44}$$

The Frobenius norm is the Euclidean norm of the vector obtained by stacking the columns of A. It is also equal to:

$$\|A\|_F = \sqrt{tr(A^T A)} \tag{1.45}$$

It has 3 important properties:

1. $\|A\|_F = \|A^T\|_F$

2. It is invariant under orthogonal transformations: $\|QA\|_F = \|A\|_F$

3. It is equal to the square root of the sum of the squared singular values of A:

$$\|A\|_F = \sqrt{\sum_{i=1}^{r} \sigma_i^2} \tag{1.46}$$

Spectral norm

The spectral norm of a matrix $A \in \mathbb{R}^{n \times n}$ is defined as:

$$\|A\|_2 = \sup_{\|x\|_2=1} \|Ax\|_2 \tag{1.47}$$

It is equal to the largest singular value of A. This is denoted as:

$$\|A\|_2 = \sigma_1 \tag{1.48}$$

Proof of the Eckart-Young theorem

For both norms $\|\cdot\|_F$ and $\|\cdot\|_2$, we will prove that:

$$\|A - A_k\| \leq \|A - B\| \quad \forall B \in \mathbb{R}^{m \times n} \quad \text{s.t.} \quad rank(B) = k$$

Let $B \in \mathbb{R}^{m \times n}$ be a matrix such that $rank(B) = k$. Then we have that:

$$dim(N(B)) = n - k$$

Let us consider the matrix V_{k+1} whose columns are the vectors $v_1, \ldots, v_{k+1}$ from the SVD of A. Then we have that:

$$rank(V_{k+1}) = k + 1 \Rightarrow dim(C(V_{k+1})) = k + 1$$
$$\Rightarrow dim(N(B)) + dim(C(V_{k+1})) = n - k + k + 1 = n + 1$$

This means that $N(B) \cap C(V_{k+1}) \neq \emptyset$. Let $w \in N(B) \cap C(V_{k+1})$, such that $\|w\| = 1$. Then we have that, for coefficients α_i:

$$w = \sum_{i=1}^{k} \alpha_i v_i \quad \wedge \quad Bw = 0$$

Since $\|w\| = 1$, then $\sum_{i=1}^{k} \alpha_i^2 = 1$. Now, we have that, for the spectral norm:

$$\|A - B\|_2^2 \geq \|(A - B)w\|_2^2 = \|Aw\|_2^2 = w^T A^T A w$$

$$= w^T V \Sigma^2 V^T w = \sum_{i=1}^{k} \sigma_i^2 \alpha_i^2 \geq$$

$$\geq \sigma_{k+1}^2 \sum_{i=1}^{k} \alpha_i^2 = \sigma_{k+1}^2$$

$$= \|A - A_k\|_2^2$$

Therefore:

$$\|A - A_k\|_2 \leq \|A - B\|_2 \quad \forall B \in \mathbb{R}^{m \times n} \quad \text{s.t.} \quad rank(B) = k$$

For the Frobenius norm, we need to use the Weyl's inequality:

$$\sigma_{i+j-1}(X + Y) \leq \sigma_i(X) + \sigma_j(Y) \tag{1.49}$$

where $\sigma_i(X)$ denotes the i-th singular value of a matrix X. Using this inequality, let us define $X = A - B$ and $Y = B$. Then we have that:

$$\sigma_{i+k}(A) \leq \sigma_i(A - B) + \sigma_{k+1}(B)$$

Note that $\sigma_{k+1}(B) = 0$, since B has rank k. Therefore:

$$\sigma_{i+k}(A) \leq \sigma_i(A - B)$$

Then, we have that:

$$\|A - A_k\|_F^2 = \sum_{i=k+1}^{r} \sigma_i^2(A) = \sum_{i=1}^{r-k} \sigma_{i+k}^2(A) \leq$$

$$\leq \sum_{i=1}^{r-k} \sigma_i^2(A - B) \leq \sum_{i=1}^{n} \sigma_i^2(A - B) = \|A - B\|_F^2$$

Therefore:

$$\|A - A_k\|_F \leq \|A - B\|_F \quad \forall B \in \mathbb{R}^{m \times n} \quad \text{s.t.} \quad rank(B) = k$$

This completes the proof.