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Numerical Analysis for Machine Learning

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Chapter 1

Numerical Linear Algebra tools

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:

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

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.