Computer Vision and Pattern Recognition

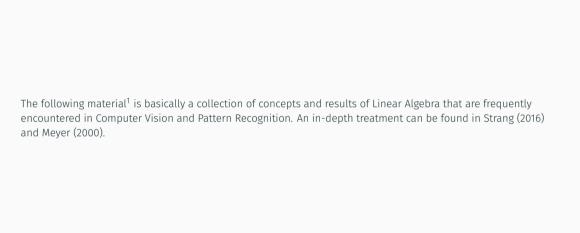
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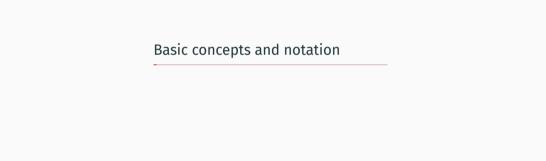
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¹ Part of which is taken from Kolter (2019). Felice Andrea Pellegrino



Sets of linear equations

Linear algebra deals with sets of linear equations.

Linear algebra provides a way to represent compactly the sets of linear equations, analyzing their properties and operating on them.

For example:

$$x_1 + 2x_2 = 5$$
$$-x_1 + x_2 = 2$$

is a set of two equations in two variables. It can be compactly represented as

$$Ax = b$$

where

$$A = \begin{bmatrix} 1 & 2 \\ -1 & 1 \end{bmatrix}, \qquad b = \begin{bmatrix} 5 \\ 2 \end{bmatrix}.$$

Basic notation

- By $A \in \mathbb{R}^{m \times n}$ we denote a matrix having m rows and n columns, whose entries are real numbers;
- by $x \in \mathbb{R}^n$ we denote a vector of n entries. We will treat an n-dimensional vector as a special case of a matrix, namely a matrix having n rows and 1 column (column vector). A row vector, i.e. a matrix having 1 row and n columns, will be typically denoted by x^\top ;
- the *i*th element of vector x is denoted by x_i :

$$x = \left[\begin{array}{c} x_1 \\ x_2 \\ \vdots \\ x_n \end{array} \right];$$

• we denote by a_{ij} (or, sometimes, A_{ij}) the entry of A in the ith row and jth column:

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix};$$

Basic notation (cont.)

• we denote by a_i the *j*th column of A:

$$A = \left[\begin{array}{cccc} a_1 & a_2 & \dots & a_n \end{array} \right];$$

• we denote by a_i^{\top} the *i*th row of A:

$$A = \left[\begin{array}{c} a_1^\top \\ a_2^\top \\ \vdots \\ a_m^\top \end{array} \right].$$

Notice that above notation is ambiguous (for example, a_1 and a_1^{\top} are not one the transpose² of the other), but the actual meaning of the symbols will be clear from the context.

²The transpose will be formally defined in the following. Felice Andrea Pellegrino



Product of two matrices

Definition

The product of two matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times p}$ is the matrix:

$$C = AB \in \mathbb{R}^{m \times p}$$

where

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}. \tag{1}$$

· Matrix multiplication is associative:

$$(AB)C = A(BC).$$

· Matrix multiplication is distributive:

$$A(B+C) = AB + AC.$$

• Matrix multiplication is, in general, not commutative. Indeed, in general, provided that both AB and BA exist, we have $AB \neq BA$. In the special case when AB = BA, we say that A and B commute.

Product of two matrices (cont.)

The matrix product expression (1) holds also for *block matrices* (or *partitioned matrices*), i.e. matrices whose rows and columns are grouped in such a way that each "entry" is actually a submatrix:

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} & \cdots & B_{1p} \\ B_{21} & B_{22} & \cdots & B_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ B_{n1} & B_{n2} & \cdots & B_{np} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & \cdots & C_{1p} \\ C_{21} & C_{22} & \cdots & C_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ C_{m1} & C_{m2} & \cdots & C_{mp} \end{bmatrix}$$

where

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

Of course, he columns of A and the rows of B must be partitioned consistently, meaning that, for all k, A_{ik} must have as many columns as the number of rows of B_{kj} .

Vector-vector products

Definition (Dot product)

Given two vectors $x, y \in \mathbb{R}^n$, the dot product (or inner product) of x and y is the scalar

$$x^{\top}y = \left[\begin{array}{ccc} x_1 & x_2 & \cdots & x_n \end{array}\right] \left[\begin{array}{c} y_1 \\ y_2 \\ \vdots \\ y_n \end{array}\right] = \sum_{i=1}^n x_i y_i \in \mathbb{R}.$$

By definition, we have $x^{\top}y = y^{\top}x$.

Vector-vector products (cont.)

Definition (Outer product)

Given two vectors $x \in \mathbb{R}^n$, $y \in \mathbb{R}^n$ the outer product of x and y is the matrix whose entries are given by $(xy^{\top})_{ij} = x_i y_i$, i.e.

$$xy^{\top} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} \begin{bmatrix} y_1 & y_2 & \cdots & y_n \end{bmatrix} = \begin{bmatrix} x_1y_1 & x_1y_2 & \cdots & x_1y_n \\ x_2y_1 & x_2y_2 & \cdots & x_2y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_my_1 & x_my_2 & \cdots & x_my_n \end{bmatrix} \in \mathbb{R}^{m \times n}.$$

By definition, we have $x^{\top} y = y^{\top} x$.

Matrix-vector products

Matrix multiplication can be looked at in different ways. We will examine some of them in the following, starting from the special case of matrix-vector products.

Given $A \in \mathbb{R}^{m \times n}$ and $x \in \mathbb{R}^n$, their product is the vector

$$y = Ax \in \mathbb{R}^m$$
.

A first way of interpreting Ax is a stack of dot products: by writing A by rows we get:

$$y = Ax = \begin{bmatrix} a_1^\top \\ a_2^\top \\ \vdots \\ a_m^\top \end{bmatrix} x = \begin{bmatrix} a_1^\top x \\ a_2^\top x \\ \vdots \\ a_m^\top x \end{bmatrix}.$$

In words, the *i*th entry of y is the dot product of the *i*th row of A and x, i.e. $y_i = a_i^\top x$.

Matrix-vector products (cont.)

Alternatively, by writing A column-wise we get:

$$y = Ax = \begin{bmatrix} a_1 & a_2 & \dots & a_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} a_1 \\ x_1 \end{bmatrix} x_1 + \begin{bmatrix} a_2 \\ x_2 \end{bmatrix} x_2 + \dots + \begin{bmatrix} a_n \\ x_n \end{bmatrix} x_n.$$

In other words, y is a linear combinations of the columns of A, where the coefficients are the entries of x.

Matrix-vector products (cont.)

If we multiply a matrix on the left by a row vector, we get a row vector $y^{\top} = x^{\top} A$, where $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^m$. $u \in \mathbb{R}^n$. The row vector u^{\top} can be expressed in two ways, as before. If we write A column-wise we have

$$y^{\top} = x^{\top} A = x^{\top} \begin{bmatrix} a_1 & a_2 & \dots & a_n \end{bmatrix} = \begin{bmatrix} x^{\top} a_1 & x^{\top} a_2 & \dots & x^{\top} a_n \end{bmatrix},$$

thus the ith entry of y^{\top} is the inner product of x and the ith column of A.

Conversely, if we write A row-wise we have:

$$y^{\top} = x^{\top} A = \begin{bmatrix} x_1 & x_2 & \cdots & x_m \end{bmatrix} \begin{bmatrix} a_1^{\top} \\ a_2^{\top} \\ \vdots \\ a_m^{\top} \end{bmatrix} = x_1 \begin{bmatrix} a_1^{\top} \\ \end{bmatrix} + x_2 \begin{bmatrix} a_2^{\top} \\ \end{bmatrix} + \cdots + x_m \begin{bmatrix} a_m^{\top} \\ \end{bmatrix}$$

this y^{\top} is a linear combination of the rows of A where the coefficients are the entries of x.

Matrix-matrix products

We now focus on the product C = AB and show four different ways it can be thought of.

1. By partitioning A row-wise and B column-wise we get

$$C = AB = \begin{bmatrix} a_1^\top \\ a_2^\top \\ \vdots \\ a_m^\top \end{bmatrix} \begin{bmatrix} b_1 & b_2 & \cdots & b_p \end{bmatrix} = \begin{bmatrix} a_1^\top b_1 & a_1^\top b_2 & \cdots & a_1^\top b_p \\ a_2^\top b_1 & a_2^\top b_2 & \cdots & a_2^\top b_p \\ \vdots & \vdots & \ddots & \vdots \\ a_m^\top b_1 & a_m^\top b_2 & \cdots & a_m^\top b_p \end{bmatrix}$$

thus the product C is a matrix whose (i, j)th entry is the dot product of the ith row of A and the jth column of B.

Matrix-matrix products (cont.)

2. By partitioning A column-wise and B row-wise we get

$$C = AB = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix} \begin{bmatrix} b_1^\top \\ b_2^\top \\ \vdots \\ b_n^\top \end{bmatrix} = \sum_{i=1}^n a_i b_i^\top$$

where the last equality follows from the generalization of the product matrix to partitioned matrices. Thus, the product AB is written as a sum of outer products $a_ib_i^{\perp}$, each of which is an $m \times p$ matrix.

3. By representing B by columns, and interpreting the matrix-matrix multiplication as a set of matrix-vector products, we get

$$C = AB = A \begin{bmatrix} b_1 & b_2 & \cdots & b_p \end{bmatrix} = \begin{bmatrix} Ab_1 & Ab_2 & \cdots & Ab_p \end{bmatrix},$$

thus the *i*th column of C is a column vector obtained as the product of A and the *i*th column of b: $c_i = Ab_i$.

Matrix-matrix products (cont.)

4. Finally, by representing A by rows we get:

$$C = AB = \begin{bmatrix} a_1^\top \\ a_2^\top \\ \vdots \\ a_m^\top \end{bmatrix} B = \begin{bmatrix} a_1^\top B \\ a_2^\top B \\ \vdots \\ a_m^\top B \end{bmatrix},$$

thus the *i*th row of C is the product of the *i*th row of A and B: $c_i^{\top} = a_i^{\top} B$.

Operations and properties

Identity matrix

Definition

The identity matrix of size n is the square matrix $I_n \in \mathbb{R}^{n \times n}$ with ones on the main diagonal and zeros elsewhere:

$$(I_n)_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}.$$

For example, the following are identity matrices:

$$I_{1} = \begin{bmatrix} 1 \end{bmatrix}, I_{2} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, I_{3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \dots, I_{n} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

For all $A \in \mathbb{R}^{m \times n}$ we have:

$$I_m A = A = A I_n$$
.

Transpose

Definition

Given a matrix $A \in \mathbb{R}^{m \times n}$, its transpose denoted by $A^{\top} \in \mathbb{R}^{n \times m}$ is the $n \times m$ matrix such that

$$\left(A^{\top}\right)_{ij} = A_{ji}.$$

For example:

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}, \qquad A^{\top} = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}.$$

The following properties hold:

$$\cdot (A^{\top})^{\top} = A$$

$$\cdot (AB)^{\top} = B^{\top}A^{\top}$$

$$\cdot (A+B)^{\top} = A^{\top} + B^{\top}$$

Symmetric matrices

Definition

A square matrix $A \in \mathbb{R}^{n \times n}$ is said to be symmetric if

$$A = A^{\top}$$
.

Definition

A square matrix $A \in \mathbb{R}^{n \times n}$ is said to be skew-symmetric or anti-symmetric if

$$A = -A^{\top}$$
.

For example, the following matrices are respectively symmetric and skew-symmetric:

$$\begin{bmatrix}
 1 & 3 & 5 \\
 3 & 5 & 7 \\
 5 & 7 & 9
 \end{bmatrix}
 \qquad
 \begin{bmatrix}
 0 & -1 & -2 \\
 1 & 0 & -1 \\
 2 & 1 & 0
 \end{bmatrix}$$

Symmetric matrices (cont.)

Any square matrix $A \in \mathbb{R}^{n \times n}$ can be written as the sum of a symmetric matrix and a skew-symmetric matrix, in view of the following identity:

$$A = \frac{1}{2} \left(A + A^{\top} \right) + \frac{1}{2} \left(A - A^{\top} \right).$$

For example:

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 3 & 5 \\ 3 & 5 & 7 \\ 5 & 7 & 9 \end{bmatrix} + \begin{bmatrix} 0 & -1 & -2 \\ 1 & 0 & -1 \\ 2 & 1 & 0 \end{bmatrix}.$$

Trace

Definition

The trace of a square matrix $A \in \mathbb{R}^{n \times n}$, denoted as tr(A) or tr(A) or tr(A) is the sum of the elements of the main diagonal:

$$\operatorname{tr} A = \sum_{i=1}^{n} a_{ii}.$$

The following properties hold:

·
$$\operatorname{tr} A = \operatorname{tr} A^{\top}$$

•
$$\operatorname{tr}(A+B) = \operatorname{tr} A + \operatorname{tr} B$$

$$tr(\alpha A) = \alpha tr A, \quad \forall \alpha \in \mathbb{R}$$

·
$$tr(AB) = tr(BA)$$

Inverse

Definition

Let A be an $n \times n$ square matrix: $A \in \mathbb{R}^{n \times n}$. If there exists a matrix B such that

$$AB = BA = I_n,$$

then B is called *inverse* of A, and denoted by A^{-1} .

The following properties hold true (in the identities below, we assume that all the inverses do exist):

- · the inverse, if it does exist, is unique:
- $(A^{-1})^{-1} = A$:
- $(A^{-1})^{\top} = (A^{\top})^{-1} \doteq A^{-\top}$
- $(AB)^{-1} = B^{-1}A^{-1}$.

For example:

$$B = \left[\begin{array}{cc} -1 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{array} \right] \quad \text{is the inverse of} \quad A = \left[\begin{array}{cc} 0 & 2 \\ 2 & 4 \end{array} \right].$$

Inverse (cont.)

Definition

A square matrix A is said to be invertible or non-singular if A^{-1} exists.

It is said to be non-invertible or singular otherwise.

In the following we will give necessary and sufficient conditions for a matrix being invertible.

The inverse can be used to solve a linear systems of equations. Let the system be Ax = b, where $A \in \mathbb{R}^{n \times n}$ and $x, b \in \mathbb{R}^n$. Then, provided that A is invertible, by multiplying both sides by A^{-1} we get

$$x = A^{-1}b.$$

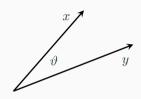
Geometric interpretation of the dot product

The dot product (or scalar product or inner product) between the vectors \boldsymbol{x} and \boldsymbol{y} has the following geometrical meaning:

$$x \cdot y = \|x\| \, \|y\| \cos \vartheta$$

where ϑ is the acute angle between the two arrows that represent x and y. When the vectors are treated as single-column matrices, the dot product is obtained by a matrix product as follows:

$$x \cdot y = x^{\top} y = y^{\top} x.$$



Definition

Two vectors x and y are said to be *orthogonal* if their dot product is zero:

$$x^\top y = 0.$$

If x and y are orthogonal, the arrows representing x and y are mutually perpendicular.

Norms

Definition (Vector norm)

A *norm* is any function $\|\cdot\|:\mathbb{R}^n\longrightarrow\mathbb{R}$ that satisfies the following properties:

- 1. ||x|| > 0, $\forall x \neq 0$ (positivity);
- 2. $||ax|| = |a| ||x||, \forall a \in \mathbb{R}$ (homogeneity);
- 3. $||x + y|| \le ||x|| + ||y||$ (triangle inequality).

Examples of norms are:

· Euclidean norm:

$$||x||_2 = \sqrt{\sum_{i=1}^n x_i^2}$$

• L_1 norm:

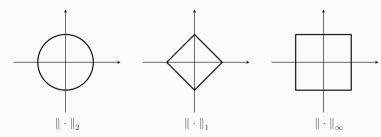
$$||x||_1 = \sum_{i=1}^n |x_i|$$

• L_{∞} norm (or max norm):

$$||x||_{\infty} = \max_{i} |x_i|$$

Norms (cont.)

The level surfaces of the previous norms are, respectively, spheres, diamonds and cubes.



The previous norms are a special case of the \mathcal{L}_p norm, defined as

$$||x||_p = \sqrt[p]{\sum_{i=1}^n |x_i|^p}$$

for $p \in \mathbb{R}$, $p \geq 1$.

Norms (cont.)

Any vector norm induces a corresponding matrix norm in the following way.

Definition (Induced matrix norm)

Let $\|\cdot\|$ be a vector norm. The corresponding induced matrix norm is defined as

$$\|A\| = \max_{\|x\|=1} \|Ax\|$$

Thus, we can define $||A||_1$, $||A||_2$, $||A||_{\infty}$.

Informally speaking, the induced L_p norm of A is a measure of the maximum "amplification" that a vector $x \in \mathbb{R}^n$ may incur when multiplied by A, when the length of the vectors are measured using the vector norm L_p .

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Norms (cont.)

Definition (Frobenius norm)

Given a matrix A, its Frobenius norm is defined as

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

Thus, the Frobenius norm is the Euclidean norm of a column vector obtained by stacking all the entries of A.

It can be easily checked that

$$\left\|A\right\|_F = \sqrt{\operatorname{tr}\left(A^\top A\right)}.$$

Determinant

Definition (Determinant)

Let $A \in \mathbb{R}^{n \times n}$. The *determinant* of A, denoted as $\det(A)$, $\det A$ or |A|, is a scalar defined, by either of the following recursions:

$$\begin{cases} \det(A) = \sum_{j=1}^n a_{ij} (-1)^{i+j} \det(A_{\backslash i, \backslash j}) & (i \text{ fixed}) \\ \det(a) = a \end{cases} \quad \text{or} \quad \begin{cases} \det(A) = \sum_{i=1}^n a_{ij} (-1)^{i+j} \det(A_{\backslash i, \backslash j}) & (j \text{ fixed}) \\ \det(a) = a \end{cases}$$

where $A_{\setminus i,\setminus j}$ is a matrix obtained from A by suppressing the ith row and the jth column. The determinant does not depend on fixed indices $1 \le i \le n$ and $1 \le j \le n$.

For example, the determinant of a 2×2 matrix takes the form:

$$\det\left(\left[\begin{array}{cc}a&b\\c&d\end{array}\right]\right)=ad-bc.$$

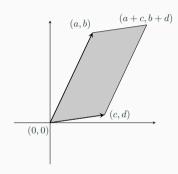
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Determinant (cont.)

The determinant of a 2×2 matrix has the following geometric meaning: its absolute value represents the area of the parallelogram defined by the rows of the matrix, as shown in the figure.

It represents also the area of a parallelogram (in general, different) defined by the columns.

The above geometrical meaning extends to three dimensional volume and n-dimensional volume.



Determinant (cont.)

The following properties hold, for $A \in \mathbb{R}^{n \times n}$:

- $\cdot \, \det(AB) = \det(A) \det(B)$
- $\cdot \det(\alpha A) = \alpha^n \det(A)$, where $\alpha \in \mathbb{R}$
- $\cdot \det(I) = 1$
- $\cdot \, \det(A^{-1}) = \frac{1}{\det(A)}$
- · A is invertible $\iff \det(A) \neq 0$
- if A is invertible, then the inverse can be written as

$$A^{-1} = \frac{1}{\det(A)} \operatorname{adj}(A)$$

where the adjoint matrix $\operatorname{adj}(A) \in \mathbb{R}^{n \times n}$ is such that $(\operatorname{adj}(A))_{ij} = (-1)^{i+j} \det(A_{\setminus j, \setminus i})$

Linear independence

Definition

The set of vectors $x_1, x_2, \ldots, x_m \in \mathbb{R}^n$ is said to be *linearly independent* if

$$\sum_{i=1}^{m} \alpha_i x_i = 0 \quad \Longrightarrow \quad \alpha_i = 0, \ \forall i$$

Equivalently, a set of vectors is linearly independent if no vector can be written as a linear combination of the remaining vectors. For example, the vectors

$$x_1 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \qquad x_2 = \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} \qquad x_3 = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}$$

are not linearly independent because $x_3 = -2x_1 + x_2$.

Orthogonal matrices

Recall that two vectors $x, y \in \mathbb{R}^n$ are orthogonal if $x^\top y = 0$.

Definition

A vector $x \in \mathbb{R}^n$ is normalized if $||x||_2 = 1$.

Definition

A square matrix $U \in \mathbb{R}^{n \times n}$ is orthogonal if all its columns are orthonormal, i.e.:

- 1. normalized, and
- 2. orthogonal to each other (mutually orthogonal).

It follows that

$$U^{\top}U = I = UU^{\top}.$$

thus the inverse of an orthogonal matrix is its transpose.

It can be shown that, if U is orthogonal, then

$$||Ux||_2 = ||x||_2$$

thus operating on a vector with an orthogonal matrix will not change its Euclidean norm.

Rank

Definition (Column rank)

The column rank of matrix $A \in \mathbb{R}^{m \times n}$ is the size of the largest subset of columns of A that constitute a linearly independent set.

Definition (Row rank)

The $row\ rank$ of matrix $A \in \mathbb{R}^{m \times n}$ is the size of the largest subset of rows of A that constitute a linearly independent set.

Proposition

For any $A \in \mathbb{R}^{m \times n}$ the column rank and the row rank are equal.

In view of the above Proposition, we can simply refer to the rank of a matrix A, denoted by rank(A) or rank(A)

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Rank (cont.)

The following properties hold:

- for $A \in \mathbb{R}^{m \times n}$, $\operatorname{rank}(A) \leq \min(m, n)$. If $\operatorname{rank}(A) = \min(m, n)$, then A is said to be full rank (more precisely, if the rank is n it is full column rank, if the rank is m it is full row rank).
- $\cdot \operatorname{rank}(A) = \operatorname{rank}(A^{\top})$
- $\cdot \operatorname{rank}(AB) \leq \min(\operatorname{rank}(A), \operatorname{rank}(B))$
- $\cdot \operatorname{rank}(A+B) \leq \operatorname{rank}(A) + \operatorname{rank}(B)$
- $A \in \mathbb{R}^{n \times n}$ is full rank $\iff \det(A) \neq 0$
- if B is invertible, then rank(AB) = rank(A)
- if B is invertible, then rank(BA) = rank(A)

Definition (Span of a set of vectors)

The span of a set of vectors $\{x_1, x_2, \dots, x_m\}$ is the set of all vectors that can be written as a linear combination of $\{x_1, x_2, \dots, x_m\}$:

$$\operatorname{span}\{x_1,x_2,\ldots,x_m\} = \left\{v: v = \sum_{i=1}^m \alpha_i x_i, \ \alpha_i \in \mathbb{R}\right\}$$

For example, the span of $\left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}$ is the whole \mathbb{R}^2 since any vector $v \in \mathbb{R}^2$ can be written as

$$v = \alpha_1 \left[\begin{array}{c} 1 \\ 0 \end{array} \right] + \alpha_2 \left[\begin{array}{c} 0 \\ 1 \end{array} \right]$$

for some α_1, α_2 .

Span (cont.)

Let $\{x_1, x_2, \dots, x_m\}$ be a set of vectors and suppose that x_i can be expressed a linear combination of the remaining vectors:

$$x_i = \sum_{j \neq i} \alpha_j x_j.$$

It is easy to prove that:

$$span(\{x_1, x_2, \dots, x_m\}) = span(\{x_1, x_2, \dots, x_m\} \setminus x_i).$$

As a consequence, the span of a set of vectors is equal to the span of the largest subset of independent vectors.

Subspaces

Definition (Subspace)

Let \mathcal{V} be a subset of \mathbb{R}^n : $\mathcal{V} \subseteq \mathbb{R}^n$. It is said to be a *subspace* of \mathbb{R}^n if it is closed with respect to linear combinations:

$$u, v \in \mathcal{V} \implies \alpha u + \beta v \in \mathcal{V}, \ \forall \alpha, \beta \in \mathbb{R}.$$

Clearly, \mathbb{R}^n is a subspace of itself. Moreover, the span of any set of vectors of \mathbb{R}^n is a subspace of \mathbb{R}^n . Conversely, any subspace of \mathbb{R}^n can be written as the span of a suitable set of vectors of \mathbb{R}^n .

Definition (Basis)

Let $\mathcal V$ be a subspace of $\mathbb R^n$. A set of vectors $\{v_1,\ldots,v_m\}$ is said to be a *basis* for $\mathcal V$ if both the following properties hold:

- $V = \mathsf{span}\{v_1, \ldots, v_m\}$ (\mathcal{V} is generated by $\{v_1, \ldots, v_m\}$)
- the set $\{v_1, \ldots, v_m\}$ is linearly independent.

Subspaces (cont.)

For example, the sets

$$\left\{ \left[\begin{array}{c} 1 \\ 0 \end{array}\right], \left[\begin{array}{c} 0 \\ 1 \end{array}\right] \right\} \qquad \text{and} \qquad \left\{ \left[\begin{array}{c} 1 \\ 2 \end{array}\right], \left[\begin{array}{c} -1 \\ 0 \end{array}\right] \right\}$$

are both basis of \mathbb{R}^2 . The set

$$\left\{ \left[\begin{array}{c} 1\\2 \end{array}\right], \left[\begin{array}{c} -1\\0 \end{array}\right], \left[\begin{array}{c} 5\\1 \end{array}\right] \right\}$$

is not a basis, because the set of vectors is not linearly independent. A subspace has an infinite number of different bases, nut they all share the same number of elements, as state by the following proposition.

Proposition

If
$$\{v_1,\ldots v_p\}$$
 and $\{w_1,\ldots,w_q\}$ are both bases of the same (sub)space $\mathcal V$, then $p=q$.

Thus we can formulate the following definition.

Definition (Dimension)

The dimension of a (sub)space \mathcal{V} , denoted by $\dim \mathcal{V}$, is the number of vectors of any basis of \mathcal{V} . The null subspace $\mathcal{V} = \{0\}$ has dimension zero.

Range and nullspace

Definition (Range of a matrix)

The range (or columnspace, or image) of a matrix $A \in \mathbb{R}^{m \times n}$, denoted by im A, is the subspace of \mathbb{R}^m given by the span of the columns of A:

$$\operatorname{im} A = \{ v \in \mathbb{R}^m : v = Ax, \ x \in \mathbb{R}^n \}.$$

Properties:

- $\cdot \dim (\operatorname{im} A) = \operatorname{rank}(A)$
- $\cdot \operatorname{im} A = \operatorname{im}(AA^{\top})$

Definition (Rowspace)

The span of the rows of $A \in \mathbb{R}^{m \times n}$ (a subset of \mathbb{R}^n) is said to be the *rowspace* of A and denoted by $\operatorname{im}(A^{\top})$. Its dimension is equal to the rank of A: $\operatorname{dim}(\operatorname{im}(A^{\top})) = \operatorname{rank}(A)$.

Range and nullspace (cont.)

Definition (Nullspace)

The nullspace (or kernel) of a matrix $A \in \mathbb{R}^{m \times n}$, denoted by ker A, is the set of all vectors of \mathbb{R}^n that equal 0 when multiplied by A:

$$\ker A = \{x \in \mathbb{R}^n : Ax = 0\}.$$

Since Au = 0, $Bv = 0 \Longrightarrow A(\alpha u + \beta v) = 0$, it follows that ker A is a subspace.

The following fundamental theorem establishes a relationship between dim(ker A) and dim(im A).

Theorem (Rank-nullity theorem)

Let $A \in \mathbb{R}^{m \times n}$. Then

$$n = \underbrace{\dim(\operatorname{im} A)}_{\operatorname{rank} A} + \dim(\ker A).$$

Range and nullspace (cont.)

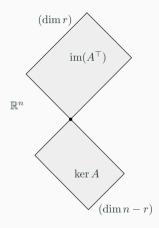
Another fundamental result is the following.

Theorem

For $A \in \mathbb{R}^{m \times n}$ we have

$$\left\{w: w=u+v, u\in \mathsf{im}(A^{ op}), v\in \ker A
ight\}=\mathbb{R}^n \quad \mathsf{and} \quad \mathsf{im}(A^{ op})\cap \ker A=\left\{0\right\}.$$

In other words, the rowspace and the nullspace of a matrix have trivial intersection and together span the whole \mathbb{R}^n . They are said to be *orthogonal complements*, denoted as $\operatorname{im}(A^\top) = \ker(A)^\perp$.



QR decomposition

Theorem (QR decomposition)

Every matrix $A \in \mathbb{R}^{m \times n}$ with linearly independent columns can be uniquely factored as

$$A = QR,$$

in which the columns of $Q \in \mathbb{R}^{m \times n}$ are an orthonormal basis for $\operatorname{im} A$ and $R \in \mathbb{R}^{n \times n}$ is an upper-triangular matrix with positive diagonal entries.

For example:

$$\begin{bmatrix} 0 & -20 & -14 \\ 3 & 27 & -4 \\ 4 & 11 & -2 \end{bmatrix} = \frac{1}{25} \begin{bmatrix} 0 & -20 & -15 \\ 15 & 12 & -16 \\ 20 & -9 & 12 \end{bmatrix} \begin{bmatrix} 5 & 25 & -4 \\ 0 & 25 & 10 \\ 0 & 0 & 10 \end{bmatrix}$$

Eigenvalues and eigenvectors

Definition

Given a square matrix $A \in \mathbb{R}^{n \times n}$, we say that $\lambda \in \mathbb{C}$ is an eigenvalue of A and $x \in \mathbb{C}^n$ is the corresponding eigenvector if

$$Ax = \lambda x, \quad x \neq 0. \tag{2}$$

The pair x, λ is sometimes referred to as an *eigenpair*.

Intuitively, the above definition means that multiplying A by an eigenvector x results is a vector having the same direction as x but scaled by a factor λ .

Eq. (2) is equivalent to

$$(\lambda I - A)x = 0, \quad x \neq 0.$$

But $(\lambda I - A)x = 0$ has a non-zero solution if and only if $(\lambda I - A)$ is not full rank, i.e. if and only if

$$\det(\lambda I - A) = 0.$$

Thus the eigenvalues are the roots of the nth degree polynomial

$$p(\lambda) = \det(\lambda I - A),$$

Eigenvalues and eigenvectors (cont.)

called the *characteristic polynomial*. As a consequence, an $n \times n$ matrix has n (not necessarily distinct) eigenvalues $\lambda_1, \ldots, \lambda_n$.

If $\bar{\lambda}$ is an eigenvalue, the set of the corresponding eigenvectors (whose union with $\{0\}$ is a subspace called eigenspace) is the set of non-zero solutions of the system

$$(\bar{\lambda}I - A)x = 0.$$

The following properties hold, for any $A \in \mathbb{R}^{n \times n}$.

- $\cdot \operatorname{tr} A = \sum_{i=1}^{n} \lambda_{i}$
- det $A = \prod_{i=1}^n \lambda_i$ (thus, a singular matrix has at least one zero eigenvalue);
- the rank of A is equal to the number of non-zero eigenvalues of A:
- if A is non-singular and (x, λ) is en eigenpair of A, then $(x, 1/\lambda)$ is an eigenpair of A^{-1} ;
- if A is triangular, its eigenvalues are the entries of main diagonal;
- if A is symmetric, then its eigenvalues are real:
- if A is symmetric, then its eigenvectors are orthogonal.

Eigenvalues and eigenvectors (cont.)

Theorem (Schur decomposition)

Any matrix $A \in \mathbb{R}^{n \times n}$ can be expressed as

$$QUQ^*$$
,

where U is an upper triangular matrix and Q is a unitary matrix (i.e. a matrix whose conjugate transpose Q^* is also its inverse).

Notice that, in general, both U and Q are complex valued.

Example (real eigenvalues):

$$\begin{bmatrix} 7 & -2 \\ 12 & -3 \end{bmatrix} = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 & -2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 3 & -14 \\ 0 & 1 \end{bmatrix} \frac{1}{\sqrt{5}} \begin{bmatrix} 1 & 2 \\ -2 & 1 \end{bmatrix}.$$

Example (complex eigenvalues):

$$\begin{bmatrix} 1 & 1 \\ -2 & 3 \end{bmatrix} = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1-j \\ 1+j & -1 \end{bmatrix} \begin{bmatrix} 2+j & -1+2j \\ 0 & 2-j \end{bmatrix} \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1-j \\ 1+j & -1 \end{bmatrix}.$$

Eigenvalues and eigenvectors (cont.)

Theorem (Schur diagonalization)

Any symmetric matrix $A \in \mathbb{R}^{n \times n}$, having eigenvalues $\lambda_1, \ldots, \lambda_n$, can be expressed as

$$A = T \Lambda T^{\top},$$

where $\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_n)$ and T is orthogonal. The columns $t_1 \dots t_n$ of T are eigenvectors of T associated to, respectively, $\lambda_1, \dots, \lambda_n$ (in other words, (λ_i, t_i) is an eigenpair).

Example:

$$\left[\begin{array}{cc} 1 & 2 \\ 2 & 1 \end{array}\right] = \left[\begin{array}{cc} -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{array}\right] \left[\begin{array}{cc} -1 & 0 \\ 0 & 3 \end{array}\right] \left[\begin{array}{cc} -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{array}\right].$$

Quadratic forms

Definition (Quadratic form)

Given a square matrix $A \in \mathbb{R}^{n \times n}$ and a vector $x \in \mathbb{R}^n$, the scalar value $x^\top A x$ is called a *quadratic form*:

$$x^{\top}Ax = \sum_{i=1}^{n} x_i (Ax)_i = \sum_{i=1}^{n} x_i (\sum_{j=1}^{n} a_{ij}x_j)_i = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}x_ix_j.$$

Since the transpose of a scalar is equal to the scalar itself we have

$$x^{\top}Ax = (x^{\top}Ax)^{\top} = x^{\top}A^{\top}x.$$

Moreover, by averaging the first and last member, which are equal, we get

$$x^{\top} A x = x^{\top} \underbrace{\left(\frac{A}{2} + \frac{A^{\top}}{2}\right)}_{\text{symmetric part of A}} x$$

thus only the symmetric part of A contributes to the quadratic form.

Definition (Positive definite matrix)

A matrix $A \in \mathbb{R}^{n \times n}$ is positive definite (denoted by $A \succ 0$) if

$$x^{\top} Ax > 0, \quad \forall x \neq 0, x \in \mathbb{R}^n.$$

Definition (Positive semidefinite matrix)

A matrix $A \in \mathbb{R}^{n \times n}$ is positive semidefinite (denoted by $A \succeq 0$) if

$$x^{\top} A x \ge 0, \quad \forall x \in \mathbb{R}^n.$$

The following matrices are, respectively positive definite and positive semidefinite:

$$A_1 = \left[\begin{array}{cc} 5 & 0 \\ 0 & 10 \end{array} \right], \qquad A_2 = \left[\begin{array}{cc} 0 & 0 \\ 0 & 10 \end{array} \right].$$

Indeed, the respective quadratic forms are $x^{\top}A_1x = 5x_1^2 + 10x_2^2 > 0$, $\forall x \neq 0$ and $x^{\top}A_2x = 10x_2^2 \geq 0$, $\forall x$. Notice that the definitions above imply that a positive definite matrix is also positive semidefinite.

Definition (Negative definite matrix)

A matrix $A \in \mathbb{R}^{n \times n}$ is negative definite (denoted by $A \prec 0$) if

$$x^{\top} Ax < 0, \quad \forall x \neq 0, x \in \mathbb{R}^n.$$

Definition (Negative semidefinite matrix)

A matrix $A \in \mathbb{R}^{n \times n}$ is negative semidefinite (denoted by $A \leq 0$) if

$$x^{\top} A x \le 0, \quad \forall x \in \mathbb{R}^n.$$

Recall that all eigenvalues of a symmetric matrix are real. The following results are useful.

Lemma

A symmetric matrix A is positive (negative) definite if and only if all its eigenvalues are strictly positive (negative):

$$A \succ 0 \iff \lambda_i > 0, \quad i = 1, \dots, n$$

where λ_i denotes the *i*-th eigenvalue of A.

Lemma

A symmetric matrix A is positive (negative) semidefinite if and only if all its eigenvalues are non-negative (non-positive):

$$A \succeq 0 \qquad \Longleftrightarrow \qquad \lambda_i \geq 0, \quad i = 1, \dots, n$$

Observe that, for non-symmetric matrices, the eigenvalue check must be carried out on the symmetric part.

The following properties are useful:

- for any $A \in \mathbb{R}^{m \times n}$, the matrices $(A^{\top}A) \in \mathbb{R}^{n \times n}$ and $(AA^{\top}) \in \mathbb{R}^{m \times m}$ are both positive semidefinite;
- the gradient ∇ (regarded as a column vector) of a quadratic form is:

$$\nabla x^{\top} A x = 2Ax$$
 (if A is symmetric);

• the Hessian matrix $H(\cdot)$ of a quadratic form is:

$$H(x^{\top}Ax) = 2A$$
 (if A is symmetric).

Theorem (Cholesky)

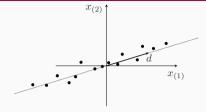
Any real symmetric and positive definite matrix *A* can be decomposed uniquely as the product of lower triangular matrix having strictly positive eigenvalues and its transpose:

$$A = LL^{\top}$$
.

For example:

$$\begin{bmatrix} 4 & 12 & -16 \\ 12 & 37 & -43 \\ -16 & -43 & 98 \end{bmatrix} = \begin{bmatrix} 2 & 0 & 0 \\ 6 & 1 & 0 \\ -8 & 5 & 3 \end{bmatrix} \begin{bmatrix} 2 & 6 & -8 \\ 0 & 1 & 5 \\ 0 & 0 & 3 \end{bmatrix}.$$

Principal Component Analysis (PCA)



An important application of Schur diagonalization is the Principal Component Analysis (PCA). The PCA has many motivations and interpretations. The most common is "find the direction along which the data varies the most".

Suppose we are given a set of n points $x_1, \ldots, x_n \in \mathbb{R}^m$. Assume that the set has zero mean:

$$\mu \doteq \frac{1}{n} \sum_{i=1}^{n} x_i = 0.$$

(If the set has nonzero mean, we can subtract μ to all the vectors). Let a direction in \mathbb{R}^m be represented by a unit vector $d \in \mathbb{R}^m$. The component of x_i along the direction d is thus given by the dot product $d^{\top}x_i$. The amount of "variation of the data set along d" can be quantified as the empirical variance of the components, i.e.

$$\frac{1}{n} \sum_{i=1}^{n} \left(d^{\top} x_i \right)^2.$$

Finding the direction of maximal variance amounts to solving the following optimization problem:

$$\underset{\|d\|_2=1}{\operatorname{argmax}} \sum_{i=1}^n \left(d^\top x_i \right)^2 = \underset{\|d\|_2=1}{\operatorname{argmax}} \sum_{i=1}^n \left(d^\top x_i \right) \left(x_i^\top d \right),$$

where the division by n has been omitted since the minimizer is the same.

By collecting the data in the matrix

$$X = \left[\begin{array}{ccc} x_1 & x_2 & \dots & x_n \end{array} \right]$$

we have

$$d^{\top}X = \begin{bmatrix} d^{\top}x_1 & d^{\top}x_2 & \dots & d^{\top}x_n \end{bmatrix} \quad \text{and} \quad X^{\top}d = \begin{bmatrix} x_1^{\top}d \\ x_2^{\top}d \\ \vdots \\ x_n^{\top}d \end{bmatrix}$$

thus the objective function can be written more compactly and the problem becomes

$$\underset{\|d\|_2=1}{\operatorname{argmax}} \ d^\top X X^\top d.$$

The matrix XX^{\top} is called *covariance matrix* and is symmetric and positive semidefinite by construction. Thus, according to the Schur's diagonalization theorem, it can be diagonalized by an orthogonal transform:

$$XX^{\top} = T \Lambda T^{\top} = T \begin{bmatrix} \lambda_1 & 0 & \dots & \\ 0 & \lambda_2 & 0 & \dots \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \lambda_m \end{bmatrix} T^{\top}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m \geq 0$. Thus, the objective function becomes

$$d^{\top} T \Lambda T^{\top} d$$
,

and we search for the maximizing unit vector d. By letting

$$y = T^{\top} d,$$

and observing that $||y||_2 = 1 \Leftrightarrow ||d||_2 = 1$, the problem becomes

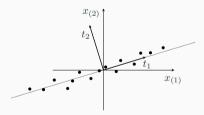
$$\underset{\|y\|_2=1}{\operatorname{argmax}} y^{\top} \Lambda y,$$

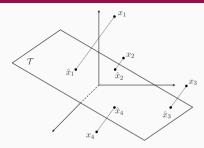
whose solution, since the eigenvalues appear in decreasing order, is $y = [1 \ 0 \ \dots \ 0]^{\top}$. Thus, the maximizing d is

$$d = Ty = t_1,$$

i.e. the first column of T, corresponding to an eigenvector associated to the largest eigenvalue.

From the above, it should be clear that the subsequent columns of T, i.e. $t_2, t_3 \ldots$ represent directions, orthogonal to each other and to t_1 , exhibiting a decreasing variance.





The PCA can be used for dimensionality reduction, by projecting the original data in the subspace spanned by the first k < m columns of T. If $x \in \mathbb{R}^m$ is a vector of the original set, its projection onto the subspace \mathcal{T} spanned by $\{t_1, t_2, \ldots, t_k\}$ is the vector $\hat{x} \in \mathbb{R}^m$:

$$\hat{x} = DD^{\top}x$$
, where $D = [t_1 \ t_2 \ \dots \ t_k]$.

The coordinates of \hat{x} with respect to the basis of $\{t_1, , t_2, \dots, t_k\}$ of \mathcal{T} are given by the vector

$$z = D^{\top} x$$

and are called the first k principal components of x.

equations

Solutions to linear systems of

Solutions to linear systems of equations

Consider the linear system of equations:

$$Ax = b. (3)$$

where $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^n$ and $b \in \mathbb{R}^m$.

For b=0 the system is said to be homogeneous and (3) becomes

$$Ax = 0.$$

From the definition of nullspace, the set of the solutions is thus ker(A). Two cases may occur:

- 1. rank A = n (i.e. A is full column rank): in that case by the rank-nullity theorem, $\dim(\ker(A)) = 0$. Thus $\ker(A) = \{0\}$ and the trivial solution x = 0 is the only solution;
- 2. rank A < n: there exist infinite solutions, precisely the set of solutions is a subspace of \mathbb{R}^n of dimension

$$\dim(\ker(A)) = n - \operatorname{rank}(A) \ge 1.$$

Solutions to linear systems of equations (cont.)

For $b \neq 0$ the system Ax = b is said to be non-homogeneous. The following theorem provides a necessary and sufficient condition for the existence of solutions.

Theorem

Consider the system

$$Ax = b$$

where $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^n$ and $b \in \mathbb{R}^m$. Then,

the system admits a solution
$$\iff$$
 rank $(A) = \text{rank}(A \mid b \mid)$.

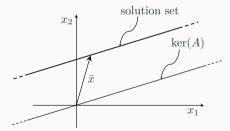
Moreover, if it admits a solution, and denoting by \bar{x} any specific solution to Ax = b, the entire solution set can be described as

$$\{x: x = x_0 + \bar{x} \quad \text{where} \quad x_0 \in \ker(A)\}. \tag{4}$$

Solutions to linear systems of equations (cont.)

Observe that:

- the condition rank(A) = rank(A) = rank(A) is equivalent to $b \in im(A)$;
- if rank(A) = n and the system admits a solution, then the solution is unique;
- if A is square and full rank, the condition is certainly satisfied and there exists a unique solution, which is $x = A^{-1}b$;
- \cdot the set of solutions (4) is a linear variety, as represented in figure.



A useful property

In the following we will use the following property.

Property

For any $A \in \mathbb{R}^{m \times n}$:

$$\operatorname{rank}(A) = \operatorname{rank}(A^{\top}A) = \operatorname{rank}(AA^{\top}).$$

Proof.

We first prove the first equality. Let $x \in \ker(A^\top A)$. Then $(A^\top A)x = 0$ and multiplying by x^\top to the left we get $x^\top A^\top Ax = 0$ which implies that $\|Ax\| = 0$, thus $x \in \ker(A)$. We have proven that $x \in \ker(A^\top A) \implies x \in \ker(A)$. The opposite implication is obvious, thus

$$x \in \ker(A^{\top}A) \iff x \in \ker(A).$$

In other words, A and $A^{\top}A$ have the same nullspace. Since they have the same number of columns n, by the rank-nullity theorem, the dimension of their columnspaces must be the same. The second equality follows by the fact that $\operatorname{rank} M = \operatorname{rank} M^{\top}$.

Least-squares (approximate) solution to overdetermined systems

When trying to fit a model with real, noisy, data, overdetermined systems of equations are frequently encountered.

We want to solve Ax = b for x, but $b \notin \operatorname{im} A$. In that case the system admits no solution, but still one may want to find the x such that Ax is the closest possible to b. If we measure the distance using the Euclidean norm we can state the problem:

$$\min_{x} \|Ax - b\|_2^2.$$

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Least-squares (approximate) solution to overdetermined systems (cont.)

In the frequent case when rank A = n (full column rank), the problem admits a unique solution. Indeed:

$$||Ax - b||_2^2 = (Ax - b)^{\top} (Ax - b) = (x^{\top} A^{\top} - b^{\top}) (Ax - b) = x^{\top} A^{\top} Ax - 2x^{\top} A^{\top} b + b^{\top} b.$$

By taking the gradient with respect to x and equating to zero, we get

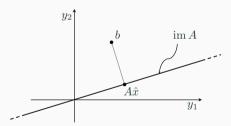
$$2A^{\top}Ax - 2A^{\top}b = 0$$
 or $A^{\top}Ax = A^{\top}b$.

Notice that $A^{\top}A \in \mathbb{R}^{n \times n}$ and its rank is n. Thus it is invertible, and, as a consequence, the unique solution is

$$\hat{x} = (A^{\top}A)^{-1}A^{\top}b. \tag{5}$$

Least-squares (approximate) solution to overdetermined systems (cont.)

The least-squares approximate solution admits a geometric interpretation. Indeed, $A\hat{x}$ is (by definition) the point in $\operatorname{im} A$ that is closest to b, i.e. is the projection of b onto $\operatorname{im} A$.



Minimum-norm solution to underdetermined systems

Another situation that may occur is that of an *underdetermined* system (more variables than independent equations), typically having the form

Assuming that m > n and rank A = m (full row rank) infinite solutions exist.

It can be useful to find the *minimum norm solution*, i.e. solve the problem:

$$\begin{aligned} \min \left\| x \right\|_2 \\ \text{subject to} \quad Ax = b \end{aligned}$$

The minimum norm solution \hat{x} can be shown to be:

$$\hat{x} = A^{\top} (AA^{\top})^{-1} b.$$

Minimum-norm solution to underdetermined systems (cont.)

Indeed, the minimization problem can be stated as:

$$\begin{array}{l} \min x^\top x \\ \text{subject to} \quad Ax = b \end{array}.$$

By introducing the Lagrange multipliers vector $\lambda \in \mathbb{R}^m$, we get the Lagrangian

$$\mathcal{L}(x,\lambda) = x^{\top}x + \lambda^{\top}(Ax - b).$$

The stationarity conditions are

$$\nabla_x \mathcal{L}(x,\lambda) = 2x + A^{\top} \lambda = 0$$
 and $\nabla_{\lambda} \mathcal{L}(x,\lambda) = Ax - b = 0$.

From the first we get $x = -A^{\top}\lambda/2$ thus, from the second, we have $\lambda = -2(AA^{\top})^{-1}b$. Notice that $AA^{\top} \in \mathbb{R}^{m \times m}$ is certainly invertible, being rank m. Finally, by substituting in the first we get

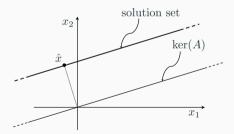
$$\hat{x} = A^{\top} (AA^{\top})^{-1} b. \tag{6}$$

Minimum-norm solution to underdetermined systems (cont.)

The minimum norm solution is orthogonal to ker A, indeed, for any $y \in \ker A$ we have Ay = 0 and also $y^{\top}A^{\top} = 0$. Thus

$$y^{\top} \hat{x} = y^{\top} A^{\top} (A A^{\top})^{-1} b = 0.$$

The minimum norm solution admits a geometric interpretation. Indeed, \hat{x} is the projection of the origin of \mathbb{R}^n onto the solution set of Ax = b.





Singular value decomposition

Any matrix $A \in \mathbb{R}^{m \times n}$ can be seen as a linear map from \mathbb{R}^n to \mathbb{R}^m (it associates $Ax \in \mathbb{R}^m$ to $x \in \mathbb{R}^n$).

The singular value decomposition of A reveals a lot about this map.

Theorem (Singular Value Decomposition)

Any matrix $A \in \mathbb{R}^{m \times n}$ can be written as

$$A = U \Sigma V^{\top},$$

where $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ are orthogonal matrices and $\Sigma \in \mathbb{R}^{m \times n}$ has the form:

$$oldsymbol{\Sigma} = \left[egin{array}{ccc} oldsymbol{\Sigma}_1 & 0 & & & & & \\ oldsymbol{\Sigma}_1 & 0 & oldsymbol{\Sigma}_1 & & & & \\ oldsymbol{0} & \sigma_2 & 0 & \dots & \\ & \vdots & \vdots & \ddots & \\ & 0 & \dots & 0 & \sigma_p \end{array}
ight] \in \mathbb{R}^{p imes p}$$

where $\sigma_1 \geq \sigma_2 \geq \dots \sigma_p \geq 0$, and $p = \min\{m, n\}$.

Definition

The real values $\sigma_1, \sigma_2, \dots, \sigma_p$ are called the *singular values* of A.

Definition

The columns u_1, u_2, \ldots, u_m of U are called the *left singular vectors* of A.

The columns v_1, v_2, \ldots, v_n of V are called the right singular vectors of A.

Observe that, for 1 < i < p:

$$Av_{i} = U\Sigma V^{\top} v_{i} = U\Sigma \begin{bmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \end{bmatrix} = U \begin{bmatrix} 0 \\ \vdots \\ \sigma_{i} \\ 0 \\ \vdots \end{bmatrix} = \sigma_{i} u_{i}. \tag{7}$$

Similarly, we get

$$A^{\top} u_i = \sigma_i v_i. \tag{8}$$

Multiplying (7) to the left by A^{\top} and substituting (8) we get:

$$(A^{\top}A)v_i = \sigma_i^2 u_i, \quad i = 1, \dots, p,$$

thus (v_i, σ_i^2) is an eigenpair of $A^{\top}A$. Similarly we obtain:

$$(AA^{\top})u_i = \sigma_i^2 v_i, \quad i = 1, \dots, p,$$

thus (u_i, σ_i^2) is an eigenpair of AA^{\top} .

Indeed, the following property holds true.

Property

Let $A \in \mathbb{R}^{m \times n}$.

If $n \geq m$, the singular values of A are the square root of the eigenvalues of AA^{\top} .

If $m \geq n$, the singular values of A are the square root of the eigenvalues of $A^{\top}A$.

Property

The rank of A equals the number of non-zero singular values of A.

Proof.

It is sufficient to observe that, since U and V^{\top} are nonsingular:

$$rank(A) = rank(U\Sigma V^{\top}) = rank(\Sigma).$$

The singular value decomposition provides bases for im A and ker A, as shown by the next proposition.

Proposition

If $A = U \Sigma V^{\top}$ is a singular value decomposition of A, and rank(A) = r, then:

- the first r columns of U are a basis for im A:
- the last n-r columns of V are a basis for ker A.

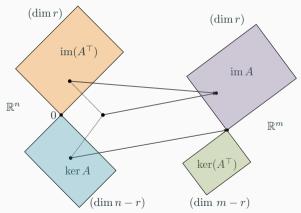
Moreover, the Frobenius norm and the 2-norm of A can be characterized in terms of singular value decomposition:

$$||A||_F^2 = \sigma_1^2 + \sigma_2^2 + \dots + \sigma_p^2$$

 $||A||_2 = \sigma_1.$

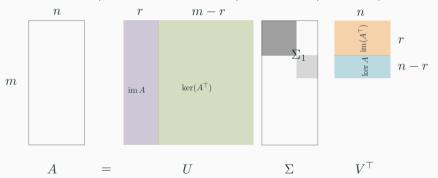
Four subspaces

The diagram below shows the four subspaces associated to A (sometimes called the four fundamental subspaces) and their relationship to the linear map y=Ax.



Four subspaces (cont.)

The singular value decomposition provides orthogonal bases for the four subspaces, as represented in the figure below. The colors of the partitions of U and V correspond to the subspaces of the previous slide.

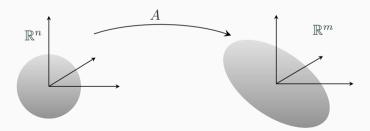


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Geometrical interpretation

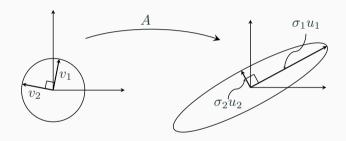
The singular values admit the following geometrical interpretation.

The singular values of $A \in \mathbb{R}^{m \times n}$ represent the length of the semiaxes of the hyperellipse in \mathbb{R}^m obtained by applying the linear map A to the unit hypersphere of \mathbb{R}^n (centered in the origin).



Geometrical interpretation (cont.)

As an example, consider the case $\mathbb{R}^2 \longrightarrow \mathbb{R}^2$:



We have

$$||Av_1|| = ||\sigma_1 u_1|| = \sigma_1 ||u_1|| = \sigma_1$$

 $||Av_2|| = ||\sigma_2 u_2|| = \sigma_2 ||u_2|| = \sigma_2$

Singular values and eigenvalues

The singular values are different from the eigenvalues. In particular:

- the singular values are defined for any matrix, while the eigenvalues exist only for square matrices;
- the singular values are always real:
- the singular values are always non negative:
- if A is square, then the singular values can be computed by taking the square root of the eigenvalues of either $A^{\top}A$ or AA^{\top} :

$$\sigma_i = \sqrt{\lambda_i(A^\top A)} = \sqrt{\lambda_i(AA^\top)}.$$

Example

Let

$$A = \left[\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 2 & 0 \end{array} \right],$$

thus the map is from \mathbb{R}^3 to \mathbb{R}^2 . We can compute the singular values as $\sqrt{\lambda_i(AA^\top)}$:

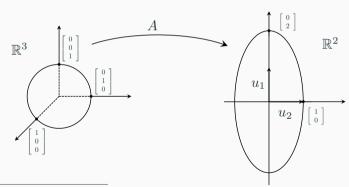
$$AA^{\top} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 2 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 4 \end{bmatrix} \implies \lambda_1 = 4, \lambda_2 = 1$$

thus $\sigma_1 = 2$, $\sigma_2 = 1$.

Example (cont.)

It can be easily checked that a singular value decomposition is³

$$A = \left[\begin{array}{cc|c} 0 & 1 \\ 1 & 0 \end{array} \right] \left[\begin{array}{cc|c} 2 & 0 & 0 \\ 0 & 1 & 0 \end{array} \right] \left[\begin{array}{cc|c} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{array} \right]$$



 $^{^3}$ the singular value decomposition is not unique: for instance one can change the sign of both u_i and v_i and get a different SVD, but this is not the only source of ambiguity.

Compact SVD and dyadic expansion

Proposition (Compact SVD)

Let $A \in \mathbb{R}^{m \times n}$ and let $\operatorname{rank}(A) = r$. If $A = U \Sigma V^{\top}$ is the singular value decomposition of A, it can be shown that:

$$A = U_r \mathbf{\Sigma}_r V_r^{\top}, \tag{9}$$

where $U_r = [u_1 \ u_2 \ \dots u_r], V_r = [v_1 \ v_2 \ \dots v_r], \text{ and } \Sigma_r = \mathsf{diag}\{\sigma_1, \sigma_2, \dots, \sigma_r\}.$

Moreover, A admits the following dyadic expansion:

$$A = \sum_{i=1}^r \sigma_i u_i v_i^ op = \sum_{i=1}^r \sigma_i Z_i,$$
 (where, clearly, $Z_i \in \mathbb{R}^{m imes n}$ and $\mathsf{rank}(Z_i) = 1$)

For instance, the matrix of the previous example has the following compact SVD and dyadic expansion:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} = 2 \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}}_{\eta_0 \eta^\top} + 1 \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\eta_0 \eta^\top}$$

Low rank approximation

Theorem

Let $k < r = \operatorname{rank}(A)$ and $A_{(k)} = \sum_{i=1}^k \sigma_i u_i v_i^{\top}$. Then:

$$\min_{\text{rank}(B) \le k} \|A - B\|_2 = \|A - A_{(k)}\|_2 = \sigma_{k+1}.$$

In other words, $A_{(k)}$ is the best approximation of rank $\leq k$ of A, with respect to the 2-norm.

Theorem

Let $k < r = \operatorname{rank}(A)$ and $A_{(k)} = \sum_{i=1}^k \sigma_i u_i v_i^{\top}$. Then:

$$\min_{\operatorname{rank}(B) \leq k} \|A - B\|_F = \left\|A - A_{(k)}\right\|_F = \sum_{i=k+1}^r \sigma_i.$$

In other words, $A_{(k)}$ is the best approximation of rank $\leq k$ of A, with respect to the Frobenius norm.

Notice that $A_{(k)}$ can be written as:

$$A_{(k)} = U_k \mathbf{\Sigma}_k V_k^{\top}$$

where $U_k = [u_1 \ u_2 \ \dots u_k], V_k = [v_1 \ v_2 \ \dots v_k], \text{ and } \Sigma_r = \text{diag}\{\sigma_1, \sigma_2, \dots, \sigma_k\}.$

Non-trivial approximate solutions to homogeneous systems

Consider the homogeneous system Ax=0, where $A\in\mathbb{R}^{m\times n}$. If A is full column rank, the only solution is x=0. Otherwise, the system admits non-trivial solutions (in other words, A has non-trivial nullspace).

When trying to fit a model with real, noisy, data, it may well happen that A is full column rank due to noise or measurement errors, although from a theoretical point of view it should not. Still, one may be interested in non-trivial approximate solutions. In particular, an approximate solution can be found by solving:

$$\min_{\|x\|=1} \|Ax\|^2 \,, \tag{10}$$

where we state the constraint ||x|| = 1 to exclude the trivial solution x = 0 (the choice of the value 1 is arbitrary, basically because we are interested in the direction of x).

The solution of (10) is easily proven to be the right singular vector associated to the smallest singular value.

Non-trivial approximate solutions to homogeneous systems (cont.)

Theorem

Let $A \in \mathbb{R}^{m \times n}$ and let $A = U \Sigma V^{\top}$ be its singular value decomposition. The solution of the following constrained minimization problem:

$$\min_{\|x\|=1} \|Ax\|^2,$$

is $x = v_n$, where v_n is the nth column of V, i.e. the right singular vector associated to the smallest singular value.

Proof.

Recalling that U and V are orthogonal, we have:

$$\min_{\|x\|=1} \|Ax\|^2 = \min_{\|x\|=1} \left\| U \Sigma V^\top x \right\|^2 = \min_{\|x\|=1} \left\| \Sigma V^\top x \right\|^2 = \min_{\|y\|=1} \|\Sigma y\|^2 = \min_{\|y\|=1} \sum_i \sigma_i^2 y_i.$$

Since the singular values appear in Σ in decreasing order, the minimum is achieved for $y = [0 \dots 0 \ 1]^{\top}$, thus the solution is $x = v_n$.

Orthogonal Procrustes problem

The Orthogonal Procrustes⁴ problem amounts to finding the orthogonal transformation W that renders the transformed matrix WB as close as possible to A (in Frobenius norm). Its solution can be expressed in terms of an SVD.

Theorem (Orthogonal Procrustes problem)

Given two matrices A and B, the solution to the problem

$$\min_{W^\top W=I} \|A - WB\|_F^2$$

is $W = VU^{\top}$, where $BA^{\top} = U\Sigma V^{\top}$ is the singular value decomposition of BA^{\top} .

An important special case, frequently encountered in Computer Vision and in Robotics, is B = I, when the aim is to find the orthogonal matrix W which is closest to a given A:

$$\min_{W^{\top}W = I} ||A - W||_F^2$$
.

The solution corresponds to substituting Σ with the identity matrix in the SVD of A.

⁴"He killed Damastes, surnamed Procrustes, by compelling him to make his own body fit his bed, as he had been wont to do with those of strangers." (Plutarch, Life of Theseus).

SVD and PCA

We have seen that the PCA of matrix X amounts to performing an eigenvalue decomposition of the (symmetric and positive semidefinite) matrix XX^{\top} :

$$XX^{\top} = T \Lambda T^{\top}. \tag{11}$$

Now, considering the SVD of X:

$$X = U \Sigma V^{\top},$$

we can express the matrix XX^{\top} as follows:

$$XX^{\top} = \left(U\Sigma V^{\top}\right) \left(U\Sigma V^{\top}\right)^{\top} = U\Sigma \underbrace{V^{\top} V}_{I} \Sigma U^{\top} = U\Sigma^{2} U^{\top}$$
(12)

Since Σ^2 is diagonal, (12) is an eigenvalue decomposition as well as (11) is, and the columns u_i of U are eigenvectors of XX^{\top} associated to the eigenvalues σ_i^2 .

Thus PCA reduces to computing the SVD of X (without forming XX^{\top}) and, denoting by U_k the matrix containing the first k columns of U, the vector of the first k principal components of x is $U_k^{\top}x$.

PCA, dimensionality reduction and SVD

Suppose we are given n points in \mathbb{R}^m

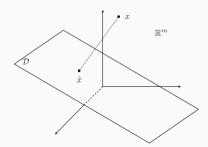
$$X = \left[\begin{array}{ccc} x_1 & x_2 & \dots & x_n \end{array} \right] \in R^{m \times n}$$

Let

$$D = \left[\begin{array}{ccc} d_1 & d_2 & \dots & d_k \end{array} \right] \in R^{m \times k}$$

where k < m be an orthonormal basis for a subspace $\mathcal D$ of $\mathbb R^m$. The projection onto $\mathcal D$ of a vector $x \in \mathbb R^m$ is

$$\hat{x} = DD^{\top} x.$$



PCA, dimensionality reduction and SVD (cont.)

We can reduce the dimensionality of the set $\{x_1,\ldots,x_n\}$ by encoding each x_i as the vector $z_i \in \mathbb{R}^k$ of the components of \hat{x}_i along the basis $\{d_1, \ldots, d_k\}$:

$$z_i = D^{\top} x_i.$$

For a given k < m (i.e for a given target dimensionality) what is a reasonable criterion for the choice of D? From $z_i \in \mathbb{R}^k$ we can reconstruct $\hat{x}_i = Dz_i \in \mathbb{R}^m$; thus, a reasonable criterion is the minimization of the sum of the squared reconstruction errors, i.e.

$$D_{\text{opt}} = \underset{D^{\top}D=I}{\operatorname{argmin}} \sum_{i=1}^{n} \left\| x_i - \underbrace{DD^{\top}x_i}_{\hat{x}_i} \right\|_{2}^{2}, \tag{13}$$

where the constraint guarantees that the columns of D form an orthonormal basis. Recalling the Frobenius matrix norm. Eq. (13) can be written in compact form as

$$D_{\text{opt}} = \underset{D^{\top}D = I}{\operatorname{argmin}} \quad \left\| X - \underbrace{DD^{\top}X}_{F} \right\|_{F}^{2}. \tag{14}$$

PCA, dimensionality reduction and SVD (cont.)

Now observe that:

• since D is rank k we have:

$$\mathsf{rank}\, B \leq k$$

• hence, problem (14) can be seen as a constrained low-rank approximation problem (it is constrained because B must be of the form $DD^{\top}X$ where D has orthogonal, unit norm columns).

If $X = U \Sigma V^{\top}$ is the SVD of X, the solution of the unconstrained problem is well-known to be

$$B = U_k \mathbf{\Sigma}_k V_k^{\top},$$

where $U_k = [u_1 \ u_2 \ \dots u_k], \ V_k = [v_1 \ v_2 \ \dots v_k], \ \text{and} \ \Sigma_k = \text{diag}\{\sigma_1, \sigma_2, \dots, \sigma_k\}$ (see the second theorem of slide 80).

We now show that the unconstrained solution satisfies the constraint and, as a consequence, is the solution of the constrained problem. More precisely, we show that the unconstrained solution has the form $DD^{\top}X$ with $D=U_k$.

PCA, dimensionality reduction and SVD (cont.)

Indeed we have:

$$\begin{split} U_k U_k^\top X &= U_k U_k^\top U \Sigma V^\top \\ &= U_k \left[\begin{array}{cc} I_k & 0 \end{array} \right] \left[\begin{array}{cc} \Sigma_k & 0 \\ 0 & \star \end{array} \right] \left[\begin{array}{cc} V_k^\top \\ \star \end{array} \right] \\ &= U_k \left[\begin{array}{cc} \Sigma_k & 0 \end{array} \right] \left[\begin{array}{cc} V_k^\top \\ \star \end{array} \right] \\ &= U_k \Sigma_k V_k^\top \end{split}$$

where * denotes a submatrix that does not affect the result.

References

Kolter, Z. (2019). Linear Algebra Review and Reference. Accessed: October 13, 2019.

Meyer, C. D. (2000). Matrix analysis and applied linear algebra. SIAM.

Strang, G. (2016). Introduction to Linear Algebra, 5th Edition. Wellesley - Cambridge Press.

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