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3. Matrix Analysis.

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Contents on this chapter

- Matrices: basic definitions.
- Norms in matrix spaces.
- Numerical condition of a problem.
- Numerical condition of the resolution of linear systems.

3.1. Basic notions on matrices.

Definition of a matrix

Definition

A matrix is a rectangular array of numbers. If a matrix has n rows and m columns, then the size of the matrix is said to be $n \times m$. If the matrix is $1 \times n$ or $n \times 1$, it is called a vector. If $m = n$, then it is called a square matrix of order n. Finally, the number that occurs in the i-th row and j-th column is called the (i, j)-th entry of the matrix. The space of matrices is denoted by $\mathbb{R}^{n \times m}$.

Throughout this course, unless stated otherwise, we consider column vectors belonging to $\mathbb{R}^{n \times 1}$. For simplification, this space is denoted as $\mathbb{R}^n$.

Remark

The criterion that the first number is used for the number of row is used by many computer programs, for instance Matlab, so it is important to learn it.

A practical way of stating matrices

For coherence with Matlab notation $A(i,j)$ denotes the element of the matrix that is in its i-th row and j-th column, $A(i,:)$ denotes the i-th row of A and $A(:,j)$ the j-th column of the matrix A. In general, we are also going to use the Matlab notation for submatrices: for instance, $A(1{:}m,:)$ means the submatrix with all the rows until the m-th (included). Similarly, for any vector v (row or column), its i-th element is denoted by $v(i)$.

Finally, when we are denoting a sequence of matrices, we shall do it as $A_1, A_2, A_3, \ldots$. Similarly, a sequence of vectors is denoted as v_1, v_2, v_3, ...

Adjoint of a matrix

Definition

Let $A \in \mathbb{R}^{n\times m}$ be a matrix. Then its **adjoint**, denoted as A', is the matrix belonging to $\mathbb{R}^{m\times n}$ which satisfies:

$$A'(i,j) = A(j,i), \quad \forall i = 1,\dots,m; \quad \forall j = 1,\dots n.$$

If $n = m$ and $A = A'$, then A is a symmetric matrix.

Example

Let $A = (a_{i,j}) = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$ be a matrix. Then:

- The order of A is 2×3.
- $A(1,1) = 1$, $A(1,2) = 2$, $A(1,3) = 3$, $A(2,1) = 4$, $A(2,2) = 5$, $A(2,3) = 6$.
- $A' = \begin{pmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{pmatrix}$.

Usual operations with matrices

Matrices can be added, or multiplied by a scalar. Also, there is the operation of matrix multiplication:

Definitions

Let $A \in \mathbb{R}^{n\times m}$, $B \in \mathbb{R}^{m\times \ell}$ and $v \in \mathbb{R}^m$. Then,

- The matrix product of A and v, is denoted by Av, belongs to $\mathbb{R}^n$-n and is given by:

$$(Av)(i) = \sum_{j=1}^{m} A(i,j)v(j).$$

- The matrix product of A and B, is denoted by AB, belongs to $\mathbb{R}^{n\times \ell}$ and is given by:

$$(AB)(i,j) = \sum_{k=1}^{m} A(i,k)B(k,j).$$

Properties of the addition and multiplication

Exercise

Define formally the addition of matrices and multiplication by a scalar in $\mathbb{R}^{n\times m}$. Show that it is a vector space.

Exercise

Let $n \geq 1$. Let us define the *identity matrix* $I \in \mathbb{R}^{n\times n}$ given by $I(i,i) = 1$ for all $i = 1, \dots n$, and $I(i,j) = 0$ if $i \neq j$. Then, show that,

- $AI = A$ for all $A \in \mathbb{R}^{m\times n}$.
- $IB = B$ for all $B \in \mathbb{R}^{n\times m}$.

Exercise

Show that the multiplication of matrices is associative, i.e., show that for all $A \in \mathbb{R}^{n\times m}$, $B \in \mathbb{R}^{m\times \ell}$ and $C \in \mathbb{R}^{\ell\times k}$:

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

Non-commutativity of the matrix product

Remember, in general it is not true that $AB = BA$. For instance, if

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix},$$

then:

$$AB = \begin{pmatrix} 1 & 2 \\ 6 & 8 \end{pmatrix}, \quad BA = \begin{pmatrix} 1 & 4 \\ 3 & 8 \end{pmatrix}.$$

Non-singular matrices

Definition

Let $A \in \mathbb{R}^{n \times n}$. Then A is *non-singular* or *invertible* if there is a matrix $B \in \mathbb{R}^{n \times n}$ such that $AB = BA = I$. In that case B is denoted as A^{-1}. Otherwise, it is called *singular* or *non-invertible*.

Proposition

A matrix $A \in \mathbb{R}^{n \times n}$ is non-singular if and only if $\det(A) \neq 0$.

Remark

The basic properties of the determinant were taught in the Linear Algebra course.

Inverse by cofactor

Proposition

Let $A \in \mathbb{R}^{n\times n}$ a non-singular matrix. Then A^{-1} is given by:

$$A^{-1}(i,j) = (\det A)^{-1}(-1)^{i+j}\det(A([1{:}j-1, j+1{:}n],[1{:}i-1, i+1{:}n])).$$

The term $A([1{:}j-1, j+1{:}n],[1{:}i-1, i+1{:}n])$ means the submatrix obtained after removing the j-th row and the i-th column.

The proof was shown in the Linear Algebra course.

Remark

This way of computing the inverse of a matrix is too expensive (when n is large). In the following chapters, we will see study efficient algorithms for computing it.

Permutation matrices

Let us define the following family of matrices:

Definition

A *permutation matrix* is any matrix $P \in \mathbb{R}^{n \times n}$ such that there is a bijection $\sigma : \{1, \dots, n\} \to \{1, \dots, n\}$ such that:

$$P(i,j) = \begin{cases} 1 & j = \sigma(i) \\ 0 & j \neq \sigma(i). \end{cases}$$

In that case we say that P is *induced* by σ.

Example

$P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$ is a permutation matrix.

Properties of the permutation matrices

Exercise

Show that following properties are satisfied:

1. The identity matrix I is a permutation matrix.
2. Let $P, Q \in \mathbb{R}^{n\times n}$ permutation matrices. Then $PQ \in \mathbb{R}^{n\times n}$ is a permutation matrix.
3. Let $P \in \mathbb{R}^{n\times n}$ permutation matrix. Then P' is a permutation matrix. Moreover, $PP' = P'P = I$; that is, P is invertible and $P' = P^{-1}$.

Lower and upper triangular matrices

Definition

A matrix $A \in \mathbb{R}^{n\times n}$ is *lower triangular* if $A(i,j)=0$ for all $j>i$, *upper triangular* if $A(i,j)=0$ for all $j<i$ and *diagonal* if $A(i,j)=0$ for all $j\neq 0$.

Example

$L=\begin{pmatrix}1 & 0 & 0\\ 2 & 3 & 0\\ -2 & 4 & 7\end{pmatrix}$ is lower triangular, $U=\begin{pmatrix}1 & 2 & 0\\ 0 & 4 & 5\\ 0 & 0 & 7\end{pmatrix}$ is upper triangular, and $D=\begin{pmatrix}1 & 0 & 0\\ 0 & 4 & 0\\ 0 & 0 & 7\end{pmatrix}$ is a diagonal matrix.

Properties of lower and upper triangular matrices

Exercise

Show that following properties are satisfied:

1. The identity matrix I is a diagonal matrix.
2. $D \in \mathbb{R}^{n \times n}$ is a diagonal matrix if and only if it is upper triangular and lower triangular.
3. If $L \in \mathbb{R}^{n \times n}$ is a lower triangular matrix, L' is an upper triangular matrix.
4. If $U \in \mathbb{R}^{n \times n}$ is an upper triangular matrix, U' is a lower triangular matrix.
5. If $L_1, L_2 \in \mathbb{R}^{n \times n}$ are lower triangular matrices, so are $L_1 + L_2$ and $L_1 L_2$.
6. If $U_1, U_2 \in \mathbb{R}^{n \times n}$ are upper triangular matrices, so are $U_1 + U_2$ and $U_1 U_2$.

3.2. Matrix norms.

Norms in vector space

Definition

Let V be a real vector space. A vector norm in V is a function $\|\cdot\|$, from V into $\mathbb{R}$, with the following properties:

- $\|v\| \geq 0$ for all $v \in V$.
- $\|v\| = 0$ if and only if $v = 0$.
- $\|\lambda v\| = |\lambda|\|v\|$ for all $\lambda \in \mathbb{R}, v \in V$.
- $\|v_1 + v_2\| \leq \|v_1\| + \|v_2\|$ for all $v_1, v_2 \in V$.

The last property is called the *triangular inequality* and the couple $(V, \|\cdot\|)$ is called the *normed space*.

Usual norms

The usual norms for $\mathbb{R}^n$ are the following ones:

- $\|v\|_1 = \sum_{i=1}^n |v(i)|$ (the *Manhattan norm*).
- $\|v\|_2 = \sqrt{\sum_{i=1}^n |v(i)|^2}$ (the *Euclidean norm*).
- $\|v\|_\infty = \sup_{i=1,\dots,n} |v(i)|$ (the *supremum norm*).

It is proved in the Calculus II course that these functions are a norm.

Important results in finite dimensional normed spaces

Theorem

Let $(V, \|\cdot\|)$ be a finite dimensional space normed space. Then, the unit sphere is compact.

Theorem

Let $(V_1, \|\cdot\|_a)$ and $(V_2, \|\cdot\|_b)$ be two finite dimensional normed space and let L a linear application from V_1 to V_2. Then, L is continuous and bounded. In particular, there is $C > 0$ such that:

$$\|Lv\|_b \leq C\|v\|_a \ \ \forall v \in V.$$

These results are proved in the Calculus II course.

Equivalence between norms

Proposition

Let V be a finite dimensional space, and let $\|\cdot\|_a$ and $\|\cdot\|_b$ any two norms defined on that space. Then there are $C_1, C_2 > 0$ such that:

$$C_1\|v\|_a \leq \|v\|_b \leq C_2\|v\|_a, \quad \forall v \in V.$$

This proposition is proved in the Calculus II course, and implies that the main results are not going to change depending on the norm that we are considering.

Scalar product

Definition

Let V a real finite dimensional vector spaces. Then a scalar product is any function $a : V \times V \to \mathbb{R}$ such that:

- $a(v, v) \geq 0$ for all $v \in V$.
- $a(v, v) = 0$ if and only if $v = 0$.
- $a(v_1, v_2) = a(v_2, v_1)$ for all $v_1, v_2 \in V$.
- $a(\lambda_1 v_1 + \lambda_2 v_2, v_3) = \lambda_1 a(v_1, v_3) + \lambda_2 a(v_2, v_3)$ for all $v_1, v_2, v_3 \in V$ and $\lambda_1, \lambda_2 \in \mathbb{R}$.

Example

In $\mathbb{R}^n$ we have the *canonical scalar product*:

$$v_1 \cdot v_2 = \sum_{i=1}^{n} v_1(i) v_2(i).$$

Scalar products and norms

Proposition

Let V a real finite dimensional vector spaces and a a scalar product. Then

$$\|v\|_a := \sqrt{a(v,v)} \ \ \forall v \in V$$

is a norm in that space. That norm is called the norm induced by the scalar product.

Example

In $\mathbb{R}^n$ the norm $\|\cdot\|_2$ is induced by the canonical scalar product.

Proposition (Cauchy-Schwarz inequality)

Let V a real finite dimensional vector spaces and a a scalar product. Then,

$$|a(v_1, v_2)| \leq \|v_1\|_a \|v_2\|_a \ \ \forall v_1, v_2 \in V,$$

and the equality is only satisfied if there is $\lambda \in \mathbb{R}$ such that $v_1 = \lambda v_2$.

Matrix norm

Definition

Let $n \in \mathbb{N}$ and $\| \cdot \|$ be a norm defined in $\mathbb{R}^{n\times n}$. Then, $\| \cdot \|$ is a *matrix norm* if:

$$\|AB\| \leq \|A\|\|B\|, \quad \forall A, B \in \mathbb{R}^{n\times n}.$$

That property is called the *multiplicative property*.

Remark

To show that an operator is a matrix norm, we must prove first it is a norm.

An example of a norm that is not a matrix norm

Let $\mathbb{R}^{2\times 2}$ and let us consider the norm defined by:

$$\|A\| = \max\left\{|a_{1,1}|, |a_{1,2}|, |a_{2,1}|, |a_{2,2}|\right\}.$$

$\|\cdot\|$ clearly is a norm, but it is not a matrix norm. Indeed, if

$$A = B = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},$$

then

$$\|A\| = \|B\| = 1, \quad \|AB\| = 2.$$

The Frobenius norm (i)

Proposition

Let us consider the space $\mathbb{R}^{n\times n}$. Then,

$$\|A\|_F := \sqrt{\sum_{i=1}^{n}\sum_{j=1}^{n}|A(i,j)|^2}$$

is a matrix norm. This norm is called the Frobenius norm.

The Frobenius norm is clearly induced by a scalar product in the matrix spaces, therefore it is a norm. Consequently, the only property that we need to prove is the multiplicative property.

The Frobenius norm (ii)

Let us show now that the Frobenius norm is multiplicative. If $A, B \in \mathbb{R}^{n\times n}$. Then,

$$\|AB\|_F^2 = \sum_{i=1}^{n}\sum_{j=1}^{n} |A(i,:)\cdot B(:,j)|^2.$$

Consequently, using Cauchy-Schwarz inequality:

$$\begin{aligned}
\|AB\|_F^2 &\leq \sum_{i=1}^{n}\sum_{j=1}^{n} \|A(i,:)\|_2^2\|B(:,j)\|_2^2 \\
&= \sum_{i=1}^{n} \|A(i,:)\|_2^2 \sum_{j=1}^{n} \|B(:,j)\|_2^2 \\
&= \left(\sum_{i=1}^{n}\sum_{j=1}^{n} |A(i,j)|^2\right)\left(\sum_{i=1}^{n}\sum_{j=1}^{n} |B(i,j)|^2\right) \\
&= \|A\|_F^2\|B\|_F^2.
\end{aligned}$$

Taking the square root at both sides, we conclude the proof.

Induced matrix norm (i)

To continue with, let us see a usual way of defining a matrix norm:

Theorem

Let $(\mathbb{R}^n, \|\cdot\|)$ *a normed vector space. Let us define*

$$F(A) = \sup_{v:\|v\|=1} \|Av\|.$$

Then, F is a matrix norm.

Remark

In the previous context, F is called the *matrix norm induced* by $\|\cdot\|$, and usually, with an abuse of notation is also denoted by $\|\cdot\|$.

Proof: *Step 1: well-defined.* Since $\|\cdot\|$ is positive, we have to show that $F(A) < +\infty$. As $v \mapsto Av$ is a linear function in a finite dimensional space, there is $C > 0$ such that $\|Av\| \leq C\|v\|$, and thus F is well-defined.

Induced matrix norm (ii)

Step 2: positivity. Clearly $F(A) \geq 0$, as the norm is positive.

Step 3: values in which F is null. Clearly $F(0) = 0$. Moreover, $F(A) = 0$ implies that $Av = 0$ for all v such that $\|v\| = 1$. By taking $v_i = \frac{e_i}{\|e_i\|}$ we obtain that:

$$Av_i = \frac{1}{\|e_i\|} A(:, i) = 0 \quad \forall i = 1, \dots, n.$$

Thus, $A = 0$. Consequently, $F(A) = 0$ if and only if $A = 0$.

Step 4: scalar multiplication. We have that:

$$F(\lambda A) = \sup_{v : \|v\| = 1} \|\lambda A v\| = \sup_{v : \|v\| = 1} |\lambda| \|Av\| = |\lambda| \sup_{v : \|v\| = 1} \|Av\| = |\lambda| F(A).$$

We have used that given any positive set S and $\lambda \geq 0$:

$$\sup\{\lambda s : s \in S\} = \lambda \sup S.$$

Induced matrix norm (iii)

Step 5: triangular inequality. Let $A, B \in \mathbb{R}^{n\times n}$. Then, for all $v \in \mathbb{R}^n$ such that $\|v\| = 1$:

$$\|(A+B)v\| \leq \|Av\| + \|Bv\| \leq F(A) + F(B).$$

Taking the supremum in the left-hand side, we obtain that:

$$F(A+B) \leq F(A) + F(B).$$

Step 6: multiplicative property. $A, B \in \mathbb{R}^{n\times n}$. Then, for all $v \in \mathbb{R}^n$ such that $\|v\| = 1$, if $w = \frac{Bv}{\|Bv\|}$:

$$\|ABv\| = \|Aw\|\|Bv\| \leq F(A)F(B).$$

Taking the supremum in the left-hand side, we obtain that:

$$F(AB) \leq F(A)F(B).\Box$$

Characterization of important matrix norms

Exercise

Let us consider $(\mathbb{R}^n, \|\cdot\|_1)$. Then, its induced matrix norm is given by:

$$F(A) = \max_{i=1,\dots,n} \|A(:,i)\|_1$$

Exercise

Let us consider $(\mathbb{R}^n, \|\cdot\|_\infty)$. Then, its induced matrix norm is given by:

$$F(A) = \max_{i=1,\dots,n} \|A(i,:)\|_1$$

3.3. Condition number and resolution of linear systems.

Condition number

In Numerical Analysis, the condition number of a function measures how much the output value of the function can change for a small change in the input argument. This is used to measure how sensitive a function is to changes or errors in the input, and how much error in the output results from an error in the input. Very frequently, one is solving the inverse problem: given $f(x) = y$, one is solving for x, and thus the condition number of the (local) inverse must be used.

The condition number is derived from the theory of propagation of uncertainty, and is formally defined as the value of the asymptotic worst-case relative change in output for a relative change in input. The "function" is the solution of a problem and the "arguments" are the data in the problem. The condition number is frequently applied to questions in linear algebra, in which case the derivative is straightforward but the error could be in many different directions, and is thus computed from the geometry of the matrix. More generally, condition numbers can be defined for non-linear functions in several variables.

A problem with a low condition number is said to be *well-conditioned*, while a problem with a high condition number is said to be *ill-conditioned*. In non-mathematical terms, an ill-conditioned problem is one where, for a small change in the inputs (the independent variables) there is a large change in the answer or dependent variable.

Absolute and relative error

Definition

Given a problem f and an algorithm $\tilde{f}$ with an input v and output $\tilde{f}(v)$, the *error* is $\delta f(v) := f(v) - \tilde{f}(v)$, the *absolute error* is $\|\delta f(v)\| = \|f(v) - \tilde{f}(v)\|$ and the *relative error* is $\frac{\|\delta f(v)\|}{\|f(v)\|} = \frac{\|f(v)-\tilde{f}(v)\|}{\|f(v)\|}$.

Example

The absolute error when we approximate 10^{-4} with 10^{-5} is 0.00009, but the relative error is 0.9.

Condition of a problem

Definition

Let us consider $(V, \|\cdot\|_V)$ and $(U, \|\cdot\|_U)$ two normed finite dimensional vector space. Let $f : V \to U$ a function. Then, the *absolute condition number* of f on v is:

$$\lim_{\varepsilon \to 0} \sup_{0 < \|\delta v\|_V \leq \varepsilon} \frac{\|f(v) - f(v + \delta v)\|_U}{\|\delta v\|_V}.$$

In addition, the *relative condition number* of f on v (for $v \neq 0$) is

$$\lim_{\varepsilon \to 0} \sup_{0 < \|\delta v\|_V \leq \varepsilon} \frac{\|f(v) - f(v + \delta v)\|_U / \|f(v)\|_U}{\|\delta v\|_V / \|v\|_V}.$$

Remark

What determines whether a numerical problem is well-posed it its relative condition number: it will be well-posed if and only if it is small.

A toy example (i)

Let us consider the problem of squaring:

$$f(x) = x^2.$$

Let us compute the absolute condition number (here $V = U = \mathbb{R}$ and $\|\cdot\|_U = \|\cdot\|_V = |\cdot|$) in a point $x \in \mathbb{R}$:

$$\begin{aligned}\lim_{h\to 0} \sup_{0<|h|\leq\varepsilon} \frac{\left|x^2 - (x+h)^2\right|}{|h|} &= \lim_{h\to 0} \sup_{0<|h|\leq\varepsilon} \frac{\left|2xh + h^2\right|}{|h|} \\ &= \lim_{h\to 0} \sup_{0<|h|\leq\varepsilon} |2x + h| = |2x|.\end{aligned}$$

We have used that $\sup_{0<|h|\leq\varepsilon} |2x+h| = \max\{|2x-h|, |2x+h|\}$. So, the absolute condition number depend on the point.

A toy example (ii)

Let us now compute the relative condition number:

$$\lim_{h\to 0} \sup_{0<|h|\leq\varepsilon} \frac{\left|x^2-(x+h)^2\right|/x^2}{|h|/|x|} = \lim_{h\to 0} \sup_{0<|h|\leq\varepsilon} \frac{\left|2xh+h^2\right|/x^2}{|h||x|}$$
$$= \lim_{h\to 0} \sup_{0<|h|\leq\varepsilon} \frac{|2x+h|}{|x|} = 2.$$

Consequently, the relative condition number is independent of the point. In addition, since it is a low number, square is a well-posed problem regardless of the point.

Resolution of a linear problem

Let us consider the linear problem

$$Ax = b \tag{$\dagger$}$$

Here b is in $(\mathbb{R}^n, \|\cdot\|)$, and A is in $(\mathbb{R}^{n\times n}, \|\cdot\|)$, where the norm of the space of matrices is the matrix norm induced by the norm of the vector space. We model the problem where the matrix A is known, and the vector b may contain imprecisions. As we know, if A is invertible, the solution of $(\dagger)$ is given by $f(b) = A^{-1}b$. In particular, the input and output of f are in $\mathbb{R}^n$.

Absolute condition number of resolution of a linear problem

Let us obtain a bound on the absolute condition number of the problem: As:

$$\frac{\|A^{-1}b - A^{-1}(b+\delta b)\|}{\|\delta b\|} = \frac{\|A^{-1}(\delta b)\|}{\|\delta b\|} \leq \frac{\|A^{-1}\|\|\delta b\|}{\|\delta b\|} = \|A^{-1}\|,$$

the absolute condition number is bounded by $\|A^{-1}\|$.

Absolute condition number of resolution of a linear problem

In a similar way, the relative condition number is bounded by

$$\frac{\|A^{-1}\|\|b\|}{\|A^{-1}b\|}.$$

Moreover, since:

$$\|b\| = \|A(A^{-1}b)\| \leq \|A\|\|A^{-1}b\|,$$

the relative condition number is bounded by:

$$\|A^{-1}\|\|A\|.$$

Important remarks about the condition number

- When computing the condition number it is usual to get an upper bound. Getting lower bounds is usually more difficult.
- The value obtained is independent of the numerical method that we are going to use to solve linear systems. Thus, if the condition number is high the probability of getting a precise answer is low.
- Even if the conditioning depends on the matrix norm, all norms are equivalent, so being ill-posed in one norm, usually implies being ill-posed in any norm.

Condition number of a matrix

Definition

Let $(\mathbb{R}^n, \|\cdot\|)$ a normed space and $\mathbb{R}^{n\times n}$ a normed space with the induced norm. Then, the *condition number* of any matrix $A \in \mathbb{R}^{n\times n}$ is given by:

$$\kappa(A) = \|A^{-1}\|\|A\|.$$

As shown before, the condition number of a matrix determines how well the problem $Ax = b$ can be solved when b is not known with whole precision.