Numerical Analysis
Introduction

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Széchenyi István University

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Motivation: ill-conditioned systems

Consider the system of equations:

$$1000x + 999y = 1$$

$$999x + 998y = 1$$

Solution: $x = 1,\ y = -1.$

$$1000x + 999y = 1$$

$$999x + 998y = 0.999$$

Solution: $x = 0.001,\ y = 0.$

Ill-conditioned systems of equations

Condition number of a self-adjoint matrix

$$\text{cond}(A) := \frac{|\lambda|_{\max}}{|\lambda|_{\min}}$$

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Motivation: computation of a determinant

Let $A \in \mathbf{M}_{200\times 200}$ be an arbitrary matrix. What is the computational cost of the calculation of $\det(A)$ by definition (i.e. performing an expansion by minors)?

$c_N :=$ number of multiplications.

$$c_N = N \cdot c_{N-1}$$

$$c_{200} = 200 \cdot c_{199} = 200 \cdot 199 \cdot c_{198} = \ldots = 200!$$

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Vectors and matrices

$\mathbf{R}^N$: the set of ordered N-tuples of real numbers.

$\mathbf{R}^N$ is a vector space (with respect to the componentwise operations).

$\mathbf{M}_{N\times M}$: the set of N-by-M matrices.

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Matrices

Matrix multiplication

If $A \in \mathbf{M}_{N\times M}$, $B \in \mathbf{M}_{M\times K}$, then AB is defined by

$$(AB)_{kj} = \sum_{i=1}^{M} A_{ki} B_{ij} \qquad (k = 1, ..., N, \quad j = 1, ..., K)$$

$AB \in \mathbf{M}_{N\times K}$. The multiplication is not commutative but associative.

- Unit matrix: I, diagonal elements $= 1$, off-diagonal elements $= 0$
- For arbitrary $A \in \mathbf{M}_{N\times N}$: $\quad AI = IA = A$
- Inverse matrix of A: $\quad A^{-1}A = I$

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- Regular or invertible matrix: which has an inverse
- Adjoint matrix of A: $A^*_{kj} = A_{jk}$
- The matrix is called self-adjoint, if $A^* = A$

Eigenvalue equation: $As = \lambda s$ (λ: eigenvalue, s: eigenvector)

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Self-adjoint matrices

The self-adjoint matrix $A \in \mathbf{M}_{N\times N}$ is called

- *positive definite*, if $x^*Ax > 0$ for every vector $x \neq \mathbf{0}$;
- *positive semidefinite*, if $x^*Ax \geq 0$ for every vector x;
- *negative definite*, if $x^*Ax < 0$ for every vector $x \neq \mathbf{0}$;
- *negative semidefinite*, if $x^*Ax \leq 0$ for every vector x;
- *indefinite*, if x^*Ax takes both positive and negative values.

Self-adjoint matrices

The self-adjoint matrix $A \in \mathbf{M}_{N\times N}$ is

- positive definite, if all eigenvalues of A are positive;
- positive semidefinite, if all eigenvalues of A are nonnegative;
- negative definite, if all eigenvalues of A are negative;
- negative semidefinite, if all eigenvalues of A are nonpositive;
- indefinite, if A has both positive and negative eigenvalues.

Vector norms

How to define a vector $(x_1, x_2, ..., x_N)$ from $\mathbf{R}^N$ to be 'great' or 'small'?

Let $x := (x_1, x_2, ..., x_N) \in \mathbf{R}^N$ be an N-dimensional vector. Then the 'greatness' of x can be characterized in several ways:

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Maximum norm

$$||x||_{\max} := \max_{1 \le k \le N} |x_k|$$

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Sum norm

$$||x||_1 := \sum_{k=1}^{N} |x_k|$$

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Euclidean norm

$$||x||_2 := ||x|| := \sqrt{\sum_{k=1}^{N} |x_k|^2}$$

Properties of the vector norms

For any vector norm:

$||x|| \geq 0,$ and $||x|| = 0$ if and only if $x = (0, 0, ..., 0)$

$||\alpha \cdot x|| = |\alpha| \cdot ||x||$ for arbitrary $\alpha \in \mathbf{R}$

$||x + y|| \leq ||x|| + ||y||$ (triangle inequality)

For the Euclidean norm: this is a consequence of the *Cauchy inequality* (see later).

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Distance of vectors

How to measure that two vectors are 'near' or 'far'?

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Limit of a vector sequence

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The sequence of vectors $x^{(1)}$, $x^{(2)}$, $x^{(3)}$, ... is called to be **convergent**, and to tend to the vector x, if the distances of the vectors $x^{(n)}$ and x converges to 0, i.e.:

$$||x^{(n)} - x|| \to 0 \qquad (n \to +\infty),$$

where $||.||$ is a given vector norm.

If the sequence of vectors $x^{(n)}$ from $\mathbf{R}^N$ is convergent with respect to a vector norm, then the convergence remains valid with respect to any other vector norm.

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Inner product of vectors

Inner product

Let $x = (x_1, x_2, ..., x_N)$, $y = (y_1, y_2, ..., y_N) \in \mathbf{R}^N$ be N-dimensional vectors. The following number is called their **inner product** (scalar product):

$$\langle x, y \rangle := \sum_{k=1}^{N} x_k \cdot y_k$$

The inner product generates the Euclidean norm in the following sense:

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Properties of the inner product

Let $x, y, z \in \mathbf{R}^N$ be N-dimensional vectors, and let $\alpha \in \mathbf{R}$ be an arbitrary number. Then:

$\langle x, x \rangle \geq 0$, and $\langle x, x \rangle = 0$ if and only if $x = (0, 0, ..., 0)$

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Properties of the inner product

Useful equalities:

$$||x+y||^2 = ||x||^2 + 2\langle x,y\rangle + ||y||^2$$

$$||x-y||^2 = ||x||^2 - 2\langle x,y\rangle + ||y||^2$$

$$\langle Ax,y\rangle = \langle x,A^*y\rangle$$

Cauchy inequality

$|\langle x,y\rangle| \leq ||x|| \cdot ||y||$

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Properties of the inner product

Proof of the Cauchy inequality: For arbitrary scalar $\alpha \in \mathbf{R}$, obviously $||x - \alpha y||^2 \geq 0$, therefore:

$$||x||^2 - 2\alpha\langle x, y\rangle + \alpha^2||y||^2 \geq 0$$

Define α by $\alpha := \frac{||x||}{||y||}$, then:

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whence

$$\langle x, y\rangle \leq ||x|| \cdot ||y||$$

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Proof of the triangle inequality:
Let $x, y \in \mathbf{R}^N$ be arbitrary vectors, then:

$$||x+y||^2 = \langle x+y, x+y\rangle = \langle x,x\rangle + \langle x,y\rangle + \langle y,x\rangle + \langle y,y\rangle$$

$$= ||x||^2 + 2\langle x,y\rangle + ||y||^2$$

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Orthogonality

Let $x, y \in \mathbf{R}^N$ be N-dimensional vectors.

Ortogonality

The N-dimensional vectors $x, y \in \mathbf{R}^N$ are said to be **orthogonal**, if $\langle x, y \rangle = 0$.

Pythagoras's theorem

Let $x^{(1)}, x^{(2)}, ..., x^{(m)} \in \mathbf{R}^N$ be pairwise orthogonal vectors, then:

$$||\sum_{j=1}^{m} x^{(j)}||^2 = \sum_{j=1}^{m} ||x^{(j)}||^2.$$

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The Gram-Schmidt orthogonalization

Let $a^{(1)}, a^{(2)}, ..., a^{(N)} \in \mathbf{R}^N$ be linearly independent vectors. Define $\tilde{e}^{(1)} := a^{(1)}$, $e^{(1)} := \frac{\tilde{e}^{(1)}}{||\tilde{e}^{(1)}||}$, and for $k = 2, 3, ..., N$:

$$\tilde{e}^{(k)} := a^{(k)} - \sum_{j=1}^{k-1} \langle a^{(k)}, e^{(j)} \rangle \cdot e^{(j)}, \qquad e^{(k)} := \frac{\tilde{e}^{(k)}}{||\tilde{e}^{(k)}||}$$

Gram-Schmidt orthogonalization

The vectors $e^{(1)}, e^{(2)}, ..., e^{(N)}$ form an **orthonormal vector system** (i.e. $\langle e^{(k)}, e^{(j)} \rangle = 0$, if $k \neq j$, and $||e^{(k)}|| = 1$), and the vector systems $a^{(1)}, a^{(2)}, ..., a^{(k)}$ and $e^{(1)}, e^{(2)}, ..., e^{(k)}$ generate the same subspace of $\mathbf{R}^N$ for all $k = 1, 2, ..., N$.

The Gram-Schmidt orthogonalization

Let $a^{(1)}, a^{(2)}, ..., a^{(N)} \in \mathbf{R}^N$ be linearly independent vectors. Define $\tilde{e}^{(1)} := a^{(1)}$, $e^{(1)} := \frac{\tilde{e}^{(1)}}{||\tilde{e}^{(1)}||}$, and for $k = 2, 3, ..., N$:

$$\tilde{e}^{(k)} := a^{(k)} - \sum_{j=1}^{k-1} \langle a^{(k)}, e^{(j)} \rangle \cdot e^{(j)}, \qquad e^{(k)} := \frac{\tilde{e}^{(k)}}{||\tilde{e}^{(k)}||}$$

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Orthogonal projection

Let $X_0 \subset \mathbf{R}^N$ be a subspace spanned by the orthonormal system $e^{(1)}, e^{(2)}, ..., e^{(M)}$. For arbitrary vector $x \in \mathbf{R}^N$:

$$x^{(0)} := \sum_{j=1}^{M} \langle x, e^{(j)} \rangle \cdot e^{(j)}$$

is the *orthogonal projection of x to X_0*, i.e. $(x - x_0)$ is orthogonal to X_0.

Proof: Complete the orthonormal system by the vectors $e^{(M+1)}, ..., e^{(N)}$ to an orthonormal basis. Then $x = \sum_{j=1}^{N} \langle x, e^{(j)} \rangle \cdot e^{(j)}$, therefore for each

$k = 1, 2, ..., M$: $\langle x - x^{(0)}, e^{(k)} \rangle = \sum_{j=M+1}^{N} \langle x, e^{(j)} \rangle \cdot \langle e^{(j)}, e^{(k)} \rangle = 0.$

Orthogonal projection

Numerical Analysis

by Csaba Gáspár

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Motivations
Vectors and matrices
Norm and distance in $\mathbf{R}^N$
Inner product
Orthogonality
Matrix norms
Linear systems

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The matrix $A \in \mathbf{M}_{N\times N}$ is called **orthogonal**, if its column vectors form an orthonormal system in $\mathbf{R}^N$.

Example: The 2-by-2 matrix $A := \begin{pmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{pmatrix}$ is an orthogonal matrix.

The inverse of orthogonal matrices can be computed in an extremely simple way:

If the matrix $A \in \mathbf{M}_{N\times N}$ is orthogonal, then $A^{-1} = A^*$

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The matrix $A \in \mathbf{M}_{N\times N}$ is called **normal**, if it is interchangeable with its adjoint, i.e. $AA^* = A^*A$.

Examples:
1) All self-adjoint matrices are normal.
2) All orthogonal matrices are normal.

Theorem

If the matrix $A \in \mathbf{M}_{N\times N}$ is normal, then A has a system of eigenvectors which form an orthonormal system. In this basis, A has a diagonal form.

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How to measure that a matrix is 'great' or 'small'?

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$$||A|| := \max\{|A_{kj}| : \ 1 \le k \le N, \ 1 \le j \le M\}$$

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$$||A|| := \sqrt{\sum_{k=1}^{N}\sum_{j=1}^{M} |A_{kj}|^2}$$

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These norms similar to the vector norms are rarely used. The use of the **matrix norm induced by a vector norm** is much more important.

Matrix norms induced by vector norms

Denote by $||.||$ a vector norm in $\mathbf{R}^N$, and $||.||$ a vector norm in $\mathbf{R}^M$ (possibly of another type). The matrix norm of $A \in \mathbf{M}_{N\times M}$ **induced by the above vector norms** is defined as follows:

$$||A|| := \max\{||Ax|| : \quad x \in \mathbf{R}^M, \ ||x|| \leq 1\}$$

Induced matrix norms, basic features

For every $x \in \mathbf{R}^M$: $||Ax|| \leq ||A|| \cdot ||x||$.

For arbitrary vector $\mathbf{0} \neq x \in \mathbf{R}^M$, the norm of the vector $\frac{x}{||x||}$ equals to 1, therefore:

$$||Ax|| = ||A\frac{x}{||x||}|| \cdot ||x|| \leq ||A|| \cdot ||x||.$$

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If the number $C \geq 0$ is such that for any vector $x \in \mathbf{R}^M$, the following estimation holds: $||Ax|| \leq C \cdot ||x||$, then $||A|| \leq C$, i.e. $||A||$ is the least number with this property.

In particular, for any vector x, for which $||x|| \leq 1$:
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We know already that $||A|| \leq C$. Moreover, forn the above vector x:

$$C \cdot ||x|| = ||Ax|| \leq ||A|| \cdot ||x||,$$

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The norm of the zero matrix is always 0, while the norm of the unit matrix is always 1 (with respect to arbitrary vector norm).

Consequently, if $N > 1$, then in $\mathbf{M}_{N\times N}$, neither the maximum norm nor the sum norm nor the Frobenius norm can be induced by any vector norm.

$||A|| \geq 0$, and $||A|| = 0$ if and only if $A = 0$

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Induced matrix norms, examples

Row norm

Suppose that both in $\mathbf{R}^N$ and in $\mathbf{R}^M$, the maximum norm is defined. Then

$$||A|| = \max_{1 \le k \le N} \sum_{j=1}^{M} |A_{kj}|$$

Column norm

Suppose that both in $\mathbf{R}^N$ and in $\mathbf{R}^M$, the sum norm is given. Then

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Suppose that in $\mathbf{R}^N$, the Euclidean norm is given. Then for every **self-adjoint** matrix $A \in \mathbf{M}_{N\times N}$:

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where $\lambda_1,\ldots,\lambda_N$ are the eigenvalues of A.

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Let the eigenvalues of the matrix $A \in \mathbf{M}_{N\times N}$ be the following (gerenally complex) numbers: $\lambda_1,\ldots,\lambda_N$. The **spectral radius** of the matrix A is defined by:

$$\rho(A) := \max_{1\le k\le N} |\lambda_k|$$

The spectral radius is not greater than any matrix norm induced by some vector norm:

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Moreover, if A is **self-adjoint**, then $\rho(A) = ||A||$, where $||A||$ denotes the matrix norm of A induced by the Euclidean norm.

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The **condition number** of a regular matrix $A \in \mathbf{M}_{N\times N}$ is defined by:

$$\text{cond}(A) := ||A|| \cdot ||A^{-1}||$$

Obviously: $\text{cond}(A) \geq 1$, and $\text{cond}(I) = 1$.

If $A \in \mathbf{M}_{N\times N}$ is self-adjoint, then the condition number can be computed from the extremal eigenvalues:

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Linear systems of equations

Let $A = [a_{kj}] \in \mathbf{M}_{N\times N}$ be a given matrix, and let $b \in \mathbf{R}^N$ be a given vector. Consider the equation

$$Ax = b$$

This is equivalent to the following system of linear equations with N unknowns:

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \ldots + a_{1N}x_N &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \ldots + a_{2N}x_N &= b_2 \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ a_{N1}x_1 + a_{N2}x_2 + \ldots + a_{NN}x_N &= b_N \end{aligned}$$

The system is **homogeneous**, if $b = \mathbf{0}$. In this case, $x = \mathbf{0}$ is always a solution (**trivial solution**). The solution x is said to be a **nontrivial solution**, if at least one component of x differs from zero.

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Solvability of linear systems

The matrix $A \in \mathbf{M}_{N\times N}$ is regular if and only if the equation $Ax = b$ has a solution for every right-hand side. In this case, the solution is unique, namely: $x = A^{-1}b$.

The matrix $A \in \mathbf{M}_{N\times N}$ is regular if and only if the corresponding homogeneous equation $Ax = \mathbf{0}$ has the trivial solution only , i.e. the matrix A is singular if and only if the corresponding homogeneous equation has a nontrivial solution (in this case, infinitely many nontrivial solutions exist).

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Perturbed linear systems

Consider the system of linear equations $Ax = b$ and the perturbed system as well: $A(x + \Delta x) = b + \Delta b$.

Hence $A\Delta x = \Delta b$, therefore $\boxed{||\Delta x|| \leq ||A^{-1}|| \cdot ||\Delta b||}$.

On the other hand: $||b|| = ||Ax|| \leq ||A|| \cdot ||x||$, therefore $\boxed{\frac{1}{||x||} \cdot \frac{1}{||A||} \leq \frac{1}{||b||}}$.

This implies:

Perturbation lemma

$$\frac{||\Delta x||}{||x||} \leq \text{cond}(A) \cdot \frac{||\Delta b||}{||b||}$$

The condition number characterizes how sensitive the solution of the system is to the changes in the right-hand side.

Perturbed linear systems

Consider the system of linear equations $Ax = b$ and the perturbed system as well: $A(x + \Delta x) = b + \Delta b$.

Hence $A\Delta x = \Delta b$, therefore $\boxed{||\Delta x|| \le ||A^{-1}|| \cdot ||\Delta b||}$.

On the other hand: $||b|| = ||Ax|| \le ||A|| \cdot ||x||$, therefore $\boxed{\frac{1}{||x||} \cdot \frac{1}{||A||} \le \frac{1}{||b||}}$.

This implies:

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