Basic linear algebra recap. Convergence rates

Daniil Merkulov

Optimization for ML. Faculty of Computer Science. HSE University

Basic linear algebra background

Vectors and matrices

We will treat all vectors as column vectors by default. The space of real vectors of length n is denoted by $\mathbb{R}^n$, while the space of real-valued $m \times n$ matrices is denoted by $\mathbb{R}^{m \times n}$. That's it: [1]

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad x^T = \begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix} \quad x \in \mathbb{R}^n, x_i \in \mathbb{R} \tag{1}$$

[1] A full introduction to applied linear algebra can be found in Introduction to Applied Linear Algebra -- Vectors, Matrices, and Least Squares - book by Stephen Boyd & Lieven Vandenberghe, which is indicated in the source. Also, a useful refresher for linear algebra is in Appendix A of the book Numerical Optimization by Jorge Nocedal Stephen J. Wright.

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Similarly, if $A \in \mathbb{R}^{m \times n}$ we denote transposition as $A^T \in \mathbb{R}^{n \times m}$:

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix} \quad A^T = \begin{bmatrix} a_{11} & a_{21} & \dots & a_{m1} \\ a_{12} & a_{22} & \dots & a_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1n} & a_{2n} & \dots & a_{mn} \end{bmatrix} \quad A \in \mathbb{R}^{m \times n}, a_{ij} \in \mathbb{R}$$

We will write $x \geq 0$ and $x \neq 0$ to indicate componentwise relationships

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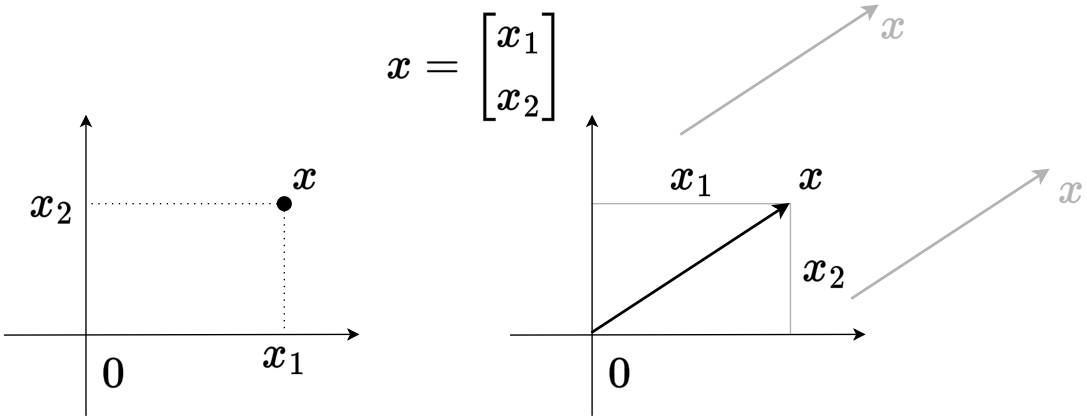

Рис. 1: Equivivalent representations of a vector

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> Is it correct, that a positive definite matrix has all positive entries?

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Matrix product (matmul)

Let A be a matrix of size $m \times n$, and B be a matrix of size $n \times p$, and let the product AB be:

$$C = AB$$

then C is a $m \times p$ matrix, with element (i, j) given by:

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

This operation in a naive form requires $\mathcal{O}(n^3)$ arithmetical operations, where n is usually assumed as the largest dimension of matrices.

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> Is it possible to multiply two matrices faster, than $\mathcal{O}(n^3)$? How about $\mathcal{O}(n^2)$, $\mathcal{O}(n)$?

Matrix by vector product (matvec)

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- $\langle x, Ay \rangle = \langle A^T x, y \rangle$

Norms

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The distance between two vectors is then defined as

$$d(x, y) = \|x - y\|.$$

The most well-known and widely used norm is **Euclidean norm**:

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

which corresponds to the distance in our real life. If the vectors have complex elements, we use their modulus. Euclidean norm, or 2-norm, is a subclass of an important class of p-norms:

$$\|x\|_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}.$$

p-norm of a vector

There are two very important special cases. The infinity norm, or Chebyshev norm is defined as the element of the maximal absolute value:

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L_1 norm plays a very important role: it all relates to the **compressed sensing** methods that emerged in the mid-00s as one of the most popular research topics. The code for the picture below is available here:. Check also this video.

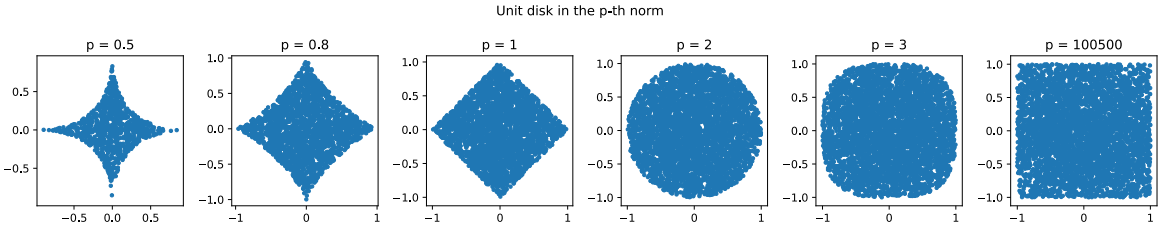

Рис. 2: Balls in different norms on a plane

Matrix norms

In some sense there is no big difference between matrices and vectors (you can vectorize the matrix), and here comes the simplest matrix norm **Frobenius** norm:

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Spectral norm, $\|A\|_2$ is one of the most used matrix norms (along with the Frobenius norm).

$$\|A\|_2 = \sup_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2},$$

It can not be computed directly from the entries using a simple formula, like the Frobenius norm, however, there are efficient algorithms to compute it. It is directly related to the **singular value decomposition** (SVD) of the matrix. It holds

$$\|A\|_2 = \sigma_1(A) = \sqrt{\lambda_{\max}(A^T A)}$$

where $\sigma_1(A)$ is the largest singular value of the matrix A.

Scalar product

The standard **scalar (inner) product** between vectors x and y from $\mathbb{R}^n$ is given by

$$\langle x, y \rangle = x^T y = \sum_{i=1}^{n} x_i y_i = y^T x = \langle y, x \rangle$$

Here x_i and y_i are the scalar i-th components of corresponding vectors.

> Example
>
> Prove, that you can switch the position of a matrix inside a scalar product with transposition: $\langle x, Ay \rangle = \langle A^T x, y \rangle$ and $\langle x, yB \rangle = \langle xB^T, y \rangle$

Matrix scalar product

The standard **scalar (inner) product** between matrices X and Y from $\mathbb{R}^{m \times n}$ is given by

$$\langle X, Y \rangle = \text{tr}(X^T Y) = \sum_{i=1}^{m} \sum_{j=1}^{n} X_{ij} Y_{ij} = \text{tr}(Y^T X) = \langle Y, X \rangle$$

> **Question**
>
> Is there any connection between the Frobenious norm $\|\cdot\|_F$ and scalar product between matrices $\langle \cdot, \cdot \rangle$?

Eigenvectors and eigenvalues

A scalar value λ is an eigenvalue of the $n \times n$ matrix A if there is a nonzero vector q such that

$$Aq = \lambda q.$$

he vector q is called an eigenvector of A. The matrix A is nonsingular if none of its eigenvalues are zero. The eigenvalues of symmetric matrices are all real numbers, while nonsymmetric matrices may have imaginary eigenvalues. If the matrix is positive definite as well as symmetric, its eigenvalues are all positive real numbers.

Eigenvectors and eigenvalues

Theorem

$$A \succeq (\succ) 0 \Leftrightarrow \text{all eigenvalues of } A \text{ are } \geq (>) 0$$

Proof

1. $\rightarrow$ Suppose some eigenvalue λ is negative and let x denote its corresponding eigenvector. Then

$$Ax = \lambda x \rightarrow x^T Ax = \lambda x^T x < 0$$

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   which contradicts the condition of $A \succeq 0$.
2. $\leftarrow$ For any symmetric matrix, we can pick a set of eigenvectors $v_1, \ldots, v_n$ that form an orthogonal basis of $\mathbb{R}^n$. Pick any $x \in \mathbb{R}^n$.

$$\begin{aligned} x^T Ax &= (\alpha_1 v_1 + \ldots + \alpha_n v_n)^T A(\alpha_1 v_1 + \ldots + \alpha_n v_n) \\ &= \sum \alpha_i^2 v_i^T A v_i = \sum \alpha_i^2 \lambda_i v_i^T v_i \geq 0 \end{aligned}$$

   here we have used the fact that $v_i^T v_j = 0$, for $i \neq j$.

Eigendecomposition (spectral decomposition)

Suppose $A \in S_n$, i.e., A is a real symmetric $n \times n$ matrix. Then A can be factorized as

$$A = Q\Lambda Q^T,$$

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where $Q \in \mathbb{R}^{n \times n}$ is orthogonal, i.e., satisfies $Q^T Q = I$, and $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. The (real) numbers λ_i are the eigenvalues of A and are the roots of the characteristic polynomial $\det(A - \lambda I)$. The columns of Q form an orthonormal set of eigenvectors of A. The factorization is called the spectral decomposition or (symmetric) eigenvalue decomposition of A. [2]

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We usually order the eigenvalues as $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. We use the notation $\lambda_i(A)$ to refer to the i-th largest eigenvalue of $A \in S$. We usually write the largest or maximum eigenvalue as $\lambda_1(A) = \lambda_{\mathsf{max}}(A)$, and the least or minimum eigenvalue as $\lambda_n(A) = \lambda_{\mathsf{min}}(A)$.

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Eigenvalues

The largest and smallest eigenvalues satisfy

$$\lambda_{\mathsf{min}}(A) = \inf_{x \neq 0} \frac{x^T A x}{x^T x}, \qquad \lambda_{\mathsf{max}}(A) = \sup_{x \neq 0} \frac{x^T A x}{x^T x}$$

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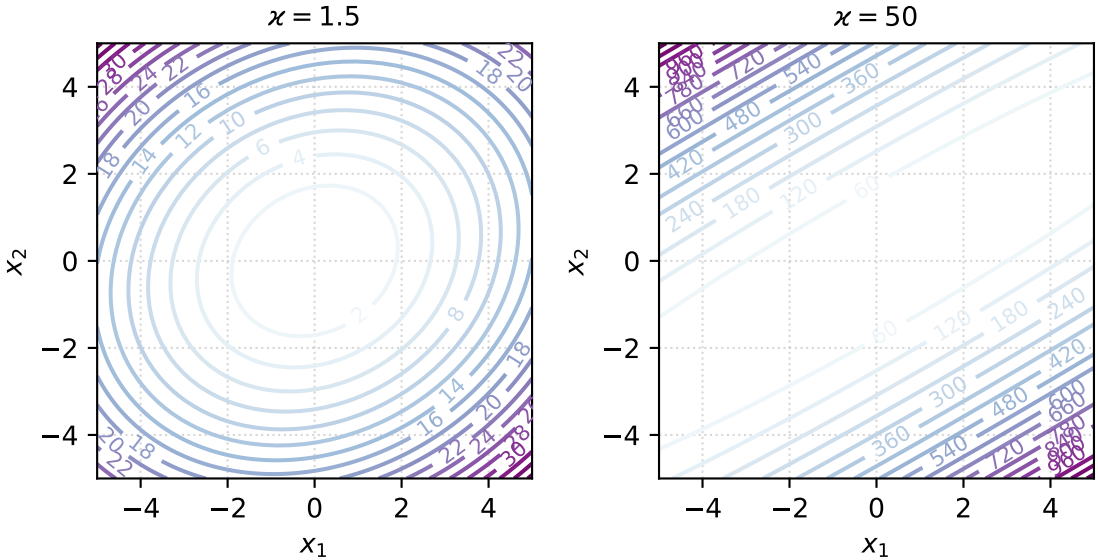
If we use spectral matrix norm, we can get:

$$\kappa(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}$$

If, moreover, $A \in \mathbb{S}^n_{++}$: $\kappa(A) = \dfrac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$

Condition number



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This factorization is called the **singular value decomposition (SVD)** of A. The columns of U are called left singular vectors of A, the columns of V are right singular vectors, and the numbers σ_i are the singular values. The singular value decomposition can be written as

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

where $u_i \in \mathbb{R}^m$ are the left singular vectors, and $v_i \in \mathbb{R}^n$ are the right singular vectors.

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Question

Suppose, matrix $A \in \mathbb{S}^n_{++}$. What can we say about the connection between its eigenvalues and singular values?

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Question

How do the singular values of a matrix relate to its eigenvalues, especially for a symmetric matrix?

Skeleton decomposition

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Use cases for Skeleton decomposition are:

- Model reduction, data compression, and speedup of computations in numerical analysis: given rank-r matrix with $r \ll n, m$ one needs to store $\mathcal{O}((n+m)r) \ll nm$ elements.

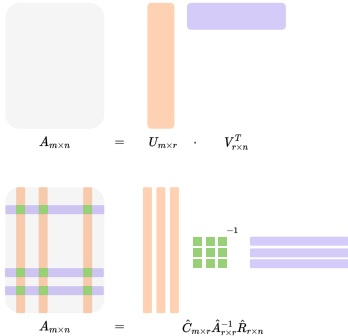

Рис. 3: Illustration of Skeleton decomposition

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- Feature extraction in machine learning, where it is also known as matrix factorization

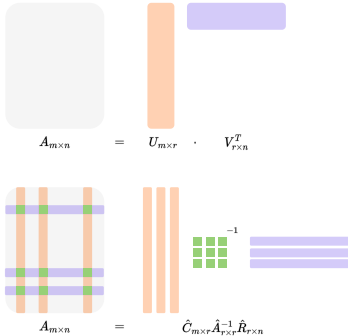

Рис. 3: Illustration of Skeleton decomposition

Skeleton decomposition

Simple, yet very interesting decomposition is Skeleton decomposition, which can be written in two forms:

$$A = UV^T \quad A = \hat{C}\hat{A}^{-1}\hat{R}$$

The latter expression refers to the fun fact: you can randomly choose r linearly independent columns of a matrix and any r linearly independent rows of a matrix and store only them with the ability to reconstruct the whole matrix exactly.
Use cases for Skeleton decomposition are:

- Model reduction, data compression, and speedup of computations in numerical analysis: given rank-r matrix with $r \ll n, m$ one needs to store $\mathcal{O}((n+m)r) \ll nm$ elements.
- Feature extraction in machine learning, where it is also known as matrix factorization
- All applications where SVD applies, since Skeleton decomposition can be transformed into truncated SVD form.

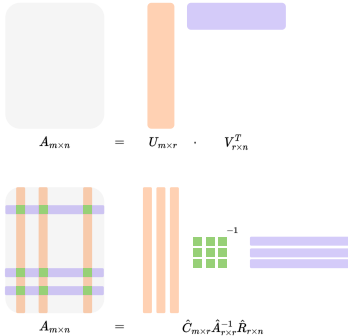

Рис. 3: Illustration of Skeleton decomposition

Canonical tensor decomposition

One can consider the generalization of Skeleton decomposition to the higher order data structure, like tensors, which implies representing the tensor as a sum of r primitive tensors.

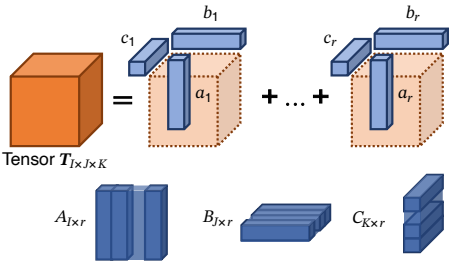

Рис. 4: Illustration of Canonical Polyadic decomposition

Example

Note, that there are many tensor decompositions: Canonical, Tucker, Tensor Train (TT), Tensor Ring (TR), and others. In the tensor case, we do not have a straightforward definition of rank for all types of decompositions. For example, for TT decomposition rank is not a scalar, but a vector.

Determinant and trace

The determinant and trace can be expressed in terms of the eigenvalues

$$\det A = \prod_{i=1}^{n} \lambda_i, \qquad \mathrm{tr} A = \sum_{i=1}^{n} \lambda_i$$

The determinant has several appealing (and revealing) properties. For instance,

- $\det A = 0$ if and only if A is singular;

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Don't forget about the cyclic property of a trace for arbitrary matrices A, B, C, D (assuming, that all dimensions are consistent):

$$\operatorname{tr}(ABCD) = \operatorname{tr}(DABC) = \operatorname{tr}(CDAB) = \operatorname{tr}(BCDA)$$

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Question

How does the determinant of a matrix relate to its invertibility?

First-order Taylor approximation

The first-order Taylor approximation, also known as the linear approximation, is centered around some point x_0. If $f : \mathbb{R}^n \to \mathbb{R}$ is a differentiable function, then its first-order Taylor approximation is given by:

$$f^I_{x_0}(x) = f(x_0) + \nabla f(x_0)^T (x - x_0)$$

Where:

- $f(x_0)$ is the value of the function at the point x_0.

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It is very usual to replace the $f(x)$ with $f^I_{x_0}(x)$ near the point x_0 for simple analysis of some approaches.

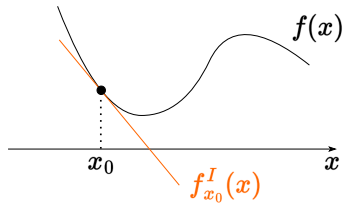

Рис. 5: First order Taylor approximation near the point x_0

Second-order Taylor approximation

The second-order Taylor approximation, also known as the quadratic approximation, includes the curvature of the function. For a twice-differentiable function $f : \mathbb{R}^n \to \mathbb{R}$, its second-order Taylor approximation centered at some point x_0 is:

$$f_{x_0}^{II}(x) = f(x_0) + \nabla f(x_0)^T (x - x_0) + \frac{1}{2}(x - x_0)^T \nabla^2 f(x_0)(x - x_0)$$

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Where $\nabla^2 f(x_0)$ is the Hessian matrix of f at the point x_0.
When using the linear approximation of the function is not sufficient one can consider replacing the $f(x)$ with $f_{x_0}^{II}(x)$ near the point x_0. In general, Taylor approximations give us a way to locally approximate functions. The first-order approximation is a plane tangent to the function at the point x_0, while the second-order approximation includes the curvature and is represented by a parabola. These approximations are especially useful in optimization and numerical methods because they provide a tractable way to work with complex functions.

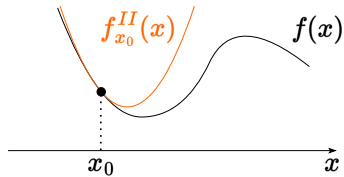

Рис. 6: Second order Taylor approximation near the point x_0

Convergence rates

Convergence rate

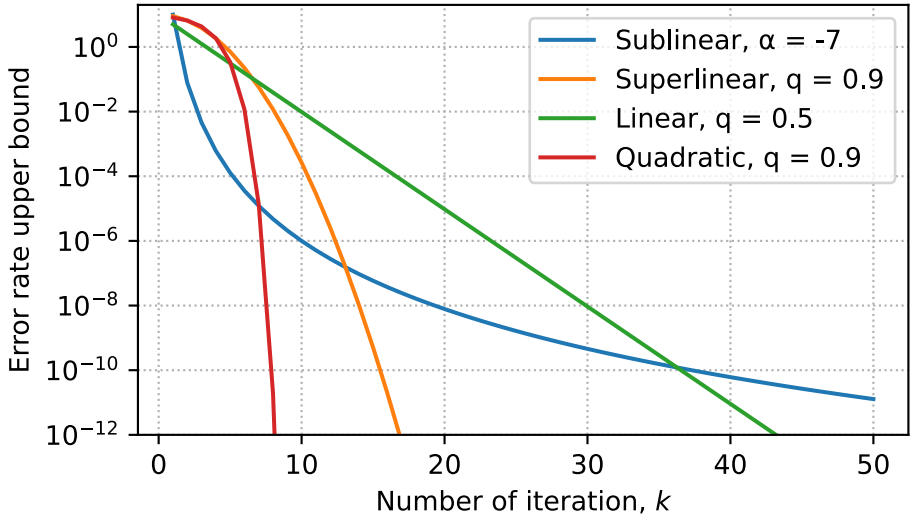

Рис. 7: Difference between the convergence speed

Linear convergence

To compare the performance of algorithms, we must define the terminology for different types of convergence. Let r_k be a sequence of non-negative real numbers that converges to zero. Typically, we have an iterative method producing a sequence of iterates x_k approaching the optimal solution x^*, and $r_k = \|x_k - x^*\|_2$.

The **linear convergence** of r_k is defined as follows:

A sequence $\{r_k\}_{k=m}^{\infty}$ converges linearly with a parameter $0 < q < 1$ if there exists a constant $C > 0$ such that:

$$r_k \leq Cq^k, \quad \text{for all } k \geq m.$$

If such a q exists, the sequence is said to have linear convergence. The **exact lower bound** of all q satisfying the inequality is called the **rate of linear convergence** of the sequence.

> **Question**
>
> Suppose, you have two sequences with linear convergence rates $q_1 = 0.1$ and $q_2 = 0.7$, which one is faster?

Linear convergence

Example

Let us have the following sequence:

$$r_k = \frac{1}{2^k}$$

One can immediately conclude, that we have a linear convergence with parameters $q = \frac{1}{2}$ and $C = 0$.

Question

Determine the convergence of the following sequence

$$r_k = \frac{3}{2^k}$$

Sublinear convergence

If the sequence r_k converges to zero, but does not have linear convergence, the convergence is said to be sublinear. Sometimes we can consider the following class of sublinear convergence:

$$\|x_{k+1} - x^*\|_2 \leq Ck^q,$$

where $q < 0$ and $0 < C < \infty$. Informally, sublinear convergence means the sequence converges slower than any geometric progression.

Superlinear convergence

A sequence $\{r_k\}_{k=m}^{\infty}$ is said to have **superlinear convergence** if it converges to zero faster than any linearly convergent sequence. Verify, that a sequence $\{r_k\}_{k=m}^{\infty}$ is superlinear if it converges linearly with the rate $q = 0$.

For $p > 1$, a sequence has **superlinear convergence of order** p if there exists $C > 0$ and $0 < q < 1$ such that:

$$r_k \leq C q^{p^k}, \quad \text{for all } k \geq m.$$

When $p = 2$, this is called **quadratic convergence**.

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Illustrative Example

Suppose $x^* = 1.23456789$ (the true solution), and the iterative sequence starts with an error $r_k = 10^{-3}$, corresponding to 3 correct significant digits (1.234).

1. After the first iteration:

$$r_{k+1} \approx r_k^2 = (10^{-3})^2 = 10^{-6}.$$

Now the error is 10^{-6}, and we have 6 correct digits (1.23456).

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Now the error is 10^{-6}, and we have 6 correct digits (1.23456).
2. After the second iteration:
$$r_{k+2} \approx r_{k+1}^2 = (10^{-6})^2 = 10^{-12}.$$
Now the error is 10^{-12}, and we have 12 correct digits (1.234567890123).

Convergence rates practical observations:

- $\|x_{k+1} - x^*\|_2 \leq \frac{1}{k^{\frac{1}{p}}}\|x_0 - x^*\|_2$ implies sublinear convergence rate

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- $\|x_{k+1} - x^*\|_2 \leq q\|x_k - x^*\|_2$ implies linear convergence rate, where $q < 1$
- $\|x_{k+1} - x^*\|_2 \leq q\|x_k - x^*\|_2^2$ implies quadratic convergence rate, where $q\|x_0 - x^*\| < 1$

Root test

Theorem

Let $(r_k)_{k=m}^{\infty}$ be a sequence of non-negative numbers converging to zero, and let $\alpha := \limsup_{k\to\infty} r_k^{1/k}$. (Note that $\alpha \geq 0$.)

(a) If $0 \leq \alpha < 1$, then $(r_k)_{k=m}^{\infty}$ converges linearly with constant α.

Proof.

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Proof.

1. let us show that if $(r_k)_{k=m}^{\infty}$ converges linearly with constant $0 \leq \beta < 1$, then necessarily $\alpha \leq \beta$. Indeed, by the definition of the constant of linear convergence, for any $\varepsilon > 0$ satisfying $\beta + \varepsilon < 1$, there exists $C > 0$ such that $r_k \leq C(\beta+\varepsilon)^k$ for all $k \geq m$. From this, $r_k^{1/k} \leq C^{1/k}(\beta+\varepsilon)$ for all $k \geq m$. Passing to the limit as $k \to \infty$ and using $C^{1/k} \to 1$, we obtain $\alpha \leq \beta + \varepsilon$. Given the arbitrariness of ε, it follows that $\alpha \leq \beta$.

Root test

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2. Thus, in the case $\alpha = 1$, the sequence $(r_k)_{k=m}^{\infty}$ cannot have linear convergence according to the above result (proven by contradiction). Since, nevertheless, $(r_k)_{k=m}^{\infty}$ converges to zero, it must converge sublinearly.

Root test

Theorem

1. Now consider the case $0 \leq \alpha < 1$. Let $\varepsilon > 0$ be an arbitrary number such that $\alpha + \varepsilon < 1$. According to the properties of the limsup, there exists $N \geq m$ such that $r_k^{1/k} \leq \alpha + \varepsilon$ for all $k \geq N$. Hence, $r_k \leq (\alpha + \varepsilon)^k$ for all $k \geq N$. Therefore, $(r_k)_{k=m}^{\infty}$ converges linearly with parameter $\alpha + \varepsilon$ (it does not matter that the inequality is only valid from the number N). Due to the arbitrariness of ε, this means that the constant of linear convergence of $(r_k)_{k=m}^{\infty}$ does not exceed α. Since, as shown above, the constant of linear convergence cannot be less than α, this means that the constant of linear convergence of $(r_k)_{k=m}^{\infty}$ is exactly α.

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2. Finally, let's show that the case $\alpha > 1$ is impossible. Indeed, suppose $\alpha > 1$. Then from the definition of limsup, it follows that for any $N \geq m$, there exists $k \geq N$ such that $r_k^{1/k} \geq 1$, and, in particular, $r_k \geq 1$. But this means that r_k has a subsequence that is bounded away from zero. Hence, $(r_k)_{k=m}^{\infty}$ cannot converge to zero, which contradicts the condition.

Ratio test

Let $\{r_k\}_{k=m}^{\infty}$ be a sequence of strictly positive numbers converging to zero. Let

$$q = \lim_{k \to \infty} \frac{r_{k+1}}{r_k}$$

- If there exists q and $0 \leq q < 1$, then $\{r_k\}_{k=m}^{\infty}$ has linear convergence with constant q.

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- If q does not exist, but $q = \lim\limits_{k \to \infty} \sup_k \dfrac{r_{k+1}}{r_k} < 1$, then $\{r_k\}_{k=m}^{\infty}$ has linear convergence with a constant not exceeding q.

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- If $\lim\limits_{k \to \infty} \inf_k \dfrac{r_{k+1}}{r_k} = 1$, then $\{r_k\}_{k=m}^{\infty}$ has sublinear convergence.

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- The case $\lim\limits_{k\to\infty} \inf_k \dfrac{r_{k+1}}{r_k} > 1$ is impossible.
- In all other cases (i.e., when $\lim\limits_{k\to\infty} \inf_k \dfrac{r_{k+1}}{r_k} < 1 \leq \lim\limits_{k\to\infty} \sup_k \dfrac{r_{k+1}}{r_k}$) we cannot claim anything concrete about the convergence rate $\{r_k\}_{k=m}^{\infty}$.

Ratio test lemma

Theorem

Let $(r_k)_{k=m}^{\infty}$ be a sequence of strictly positive numbers. (The strict positivity is necessary to ensure that the ratios $\frac{r_{k+1}}{r_k}$, which appear below, are well-defined.) Then

$$\liminf_{k\to\infty} \frac{r_{k+1}}{r_k} \le \liminf_{k\to\infty} r_k^{1/k} \le \limsup_{k\to\infty} r_k^{1/k} \le \limsup_{k\to\infty} \frac{r_{k+1}}{r_k}.$$

Proof.

1. The middle inequality follows from the fact that the liminf of any sequence is always less than or equal to its limsup. Let's prove the last inequality; the first one is proved analogously.

Ratio test lemma

Theorem

Let $(r_k)_{k=m}^{\infty}$ be a sequence of strictly positive numbers. (The strict positivity is necessary to ensure that the ratios $\frac{r_{k+1}}{r_k}$, which appear below, are well-defined.) Then

$$\liminf_{k\to\infty} \frac{r_{k+1}}{r_k} \le \liminf_{k\to\infty} r_k^{1/k} \le \limsup_{k\to\infty} r_k^{1/k} \le \limsup_{k\to\infty} \frac{r_{k+1}}{r_k}.$$

Proof.

1. The middle inequality follows from the fact that the liminf of any sequence is always less than or equal to its limsup. Let's prove the last inequality; the first one is proved analogously.
2. Denote $L := \limsup_{k\to\infty} \frac{r_{k+1}}{r_k}$. If $L = +\infty$, then the inequality is obviously true, so let's assume L is finite. Note that $L \ge 0$, since the ratio $\frac{r_{k+1}}{r_k}$ is positive for all $k \ge m$. Let $\varepsilon > 0$ be an arbitrary number. According to the properties of limsup, there exists $N \ge m$ such that $\frac{r_{k+1}}{r_k} \le L + \varepsilon$ for all $k \ge N$. From here, $r_{k+1} \le (L+\varepsilon) r_k$ for all $k \ge N$. Applying induction, we get $r_k \le (L+\varepsilon)^{k-N} r_N$ for all $k \ge N$. Let $C := (L+\varepsilon)^{-N} r_N$. Then $r_k \le C(L+\varepsilon)^k$ for all $k \ge N$, from which $r_k^{1/k} \le C^{1/k}(L+\varepsilon)$. Taking the limsup as $k \to \infty$ and using $C^{1/k} \to 1$, we get $\limsup_{k\to\infty} r_k^{1/k} \le L + \varepsilon$. Given the arbitrariness of ε, it follows that $\limsup_{k\to\infty} r_k^{1/k} \le L$.

Summary

Summary

Определения

1. Положительно определённая матрица.
2. Евклидова норма вектора.
3. Неравенство треугольника для нормы.
4. p-норма вектора.
5. Как выглядит единичный шар в p - норме на плоскости для $p = 1, 2, \infty$?
6. Норма Фробениуса для матрицы.
7. Спектральная норма матрицы.
8. Скалярное произведение двух векторов.
9. Скалярное произведение двух матриц, согласованное с нормой Фробениуса.
10. Собственные значения матрицы. Спектр матрицы.
11. Связь спектра матрицы и её определенности.
12. Спектральное разложение матрицы.
13. Сингулярное разложение матрицы.
14. Связь определителя и собственных чисел для квадратной матрицы.
15. Связь следа и собственных чисел для квадратной матрицы.
16. Линейная сходимость последовательности.
17. Сублинейная сходимость последовательности.
18. Сверхлинейная сходимость последовательности.
19. Квадратичная сходимость последовательности.
20. Тест корней для определения скорости сходимости последовательности.
21. Тест отношений для определения скорости сходимости последовательности.

Теоремы

1. Критерий положительной определенности матрицы через знаки собственных значений матрицы.
2. Тест корней
3. Тест отношений