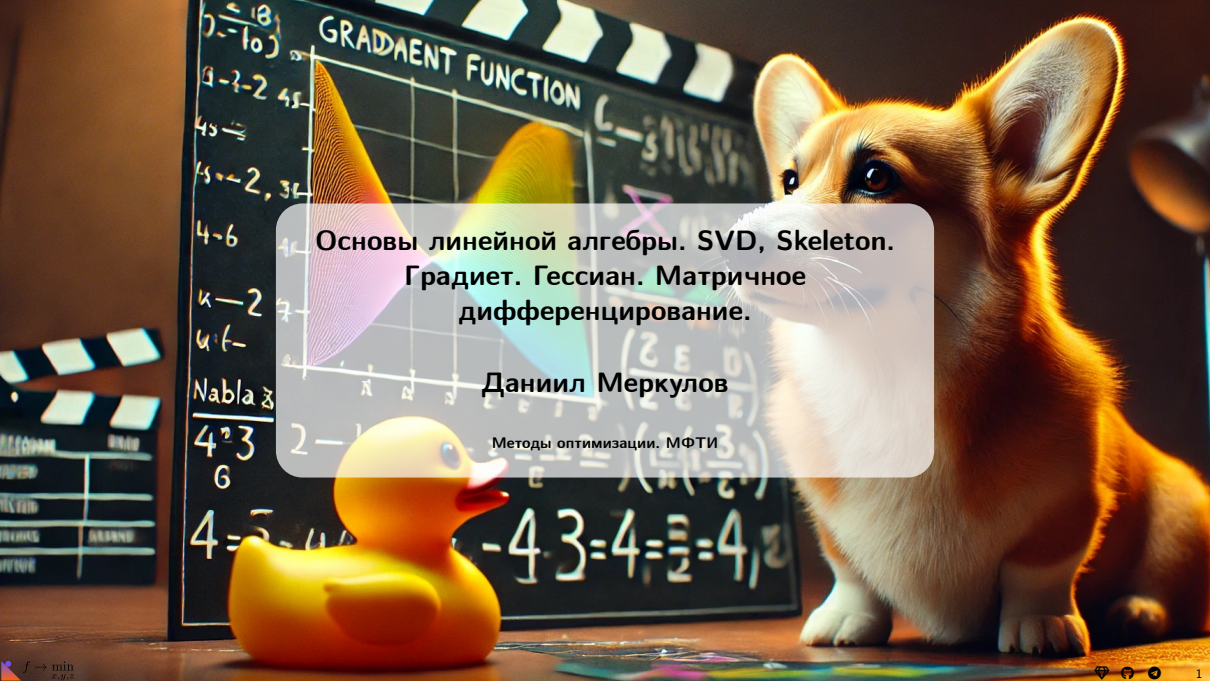

Основы линейной алгебры. SVD, Skeleton. Градиет. Гессиан. Матричное дифференцирование.

Даниил Меркулов

Методы оптимизации. МФТИ

Основы линейной алгебры

Векторы и матрицы

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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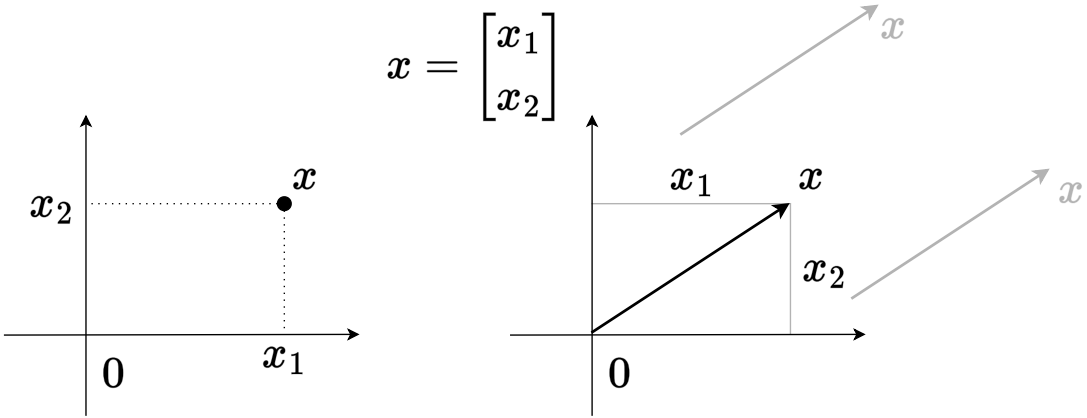

Рис. 1: Equivivalent representations of a vector

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

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Матричное умножение (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:

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

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

Умножение матрицы на вектор (matvec)

Let A be a matrix of shape $m \times n$, and x be $n \times 1$ vector, then the i-th component of the product:

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

Пример. Простой, но важный сюжет про матричное умножение

Suppose, you have the following expression

$$b = A_1 A_2 A_3 x,$$

where the $A_1, A_2, A_3 \in \mathbb{R}^{3\times 3}$ - random square dense matrices and $x \in \mathbb{R}^n$ - vector. You need to compute b.

Which one way is the best to do it?

1. $A_1 A_2 A_3 x$ (from left to right)

Check the simple code snippet after all.

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4. The results of the first two options will not be the same.

Check the simple code snippet after all.

Нормы

Norm is a **qualitative measure of the smallness of a vector** and is typically denoted as $\|x\|$.

The norm should satisfy certain properties:

1. $\|\alpha x\| = |\alpha|\|x\|$, $\alpha \in \mathbb{R}$

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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-норма вектора

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.

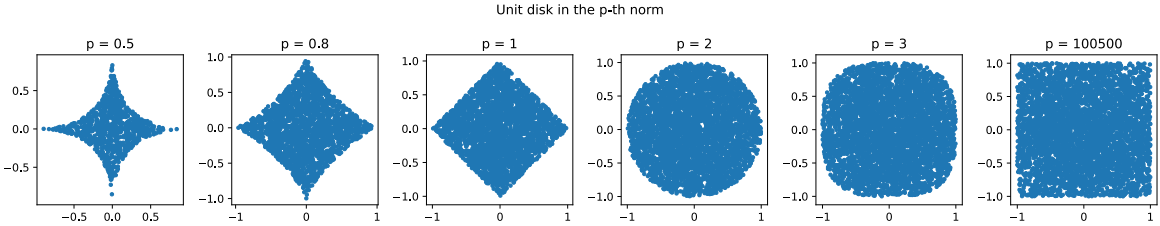

Рис. 2: Balls in different norms on a plane

Матричные нормы

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.

Скалярное произведение

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 $\langle x, yB \rangle = \langle xB^T, y \rangle$

Скалярное произведение матриц

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 $\langle \cdot, \cdot \rangle$?

Собственные числа и собственные вектора

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.

Собственные числа и собственные вектора

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

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which contradicts the condition of $A \succeq 0$.

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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 $i \neq j$.

Спектральное разложение матрицы

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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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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Ещё о собственных значениях

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

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where $U \in \mathbb{R}^{m \times r}$ satisfies $U^T U = I$, $V \in \mathbb{R}^{n \times r}$ satisfies $V^T V = I$, and Σ is a diagonal matrix with $\Sigma = \text{diag}(\sigma_1, ..., \sigma_r)$, such that

$$\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_r > 0.$$

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.

Сингулярное разложение

Question

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

Сингулярное разложение

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

Question

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

Ранговое разложение (Skeleton)

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

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

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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.

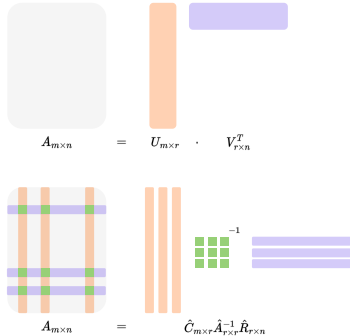

Рис. 3: Illustration of Skeleton decomposition

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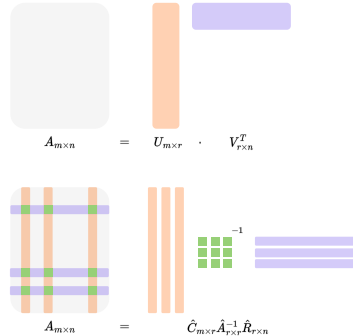

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- Model reduction, data compression, and speedup of computations in numerical analysis: given rank-r matrix with $r \ll n, m$ one needs to store $\mathcal{O}((n+m)r) \ll nm$ elements.
- Feature extraction in machine learning, where it is also known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

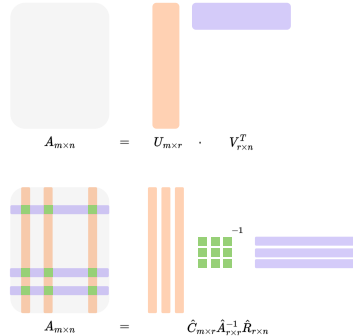

Рис. 3: Illustration of Skeleton decomposition

Каноническое тензорное разложение

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.

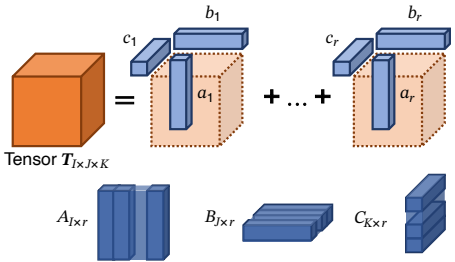

Рис. 4: Illustration of Canonical Polyadic decomposition

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.

Определитель и след матрицы

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

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

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

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

Question

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

Аппроксимация Тейлора первого порядка

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:

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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.

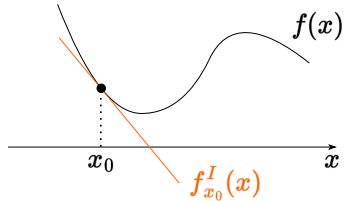

Рис. 5: First order Taylor approximation near the point x_0

Аппроксимация Тейлора второго порядка

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:

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

Where $\nabla^2 f(x_0)$ is the Hessian matrix of f at the point 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.

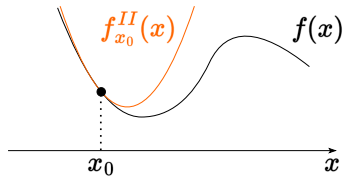

Рис. 6: Second order Taylor approximation near the point x_0

Матричное дифференцирование

Градиент

Let $f(x) : \mathbb{R}^n \to \mathbb{R}$, then vector, which contains all first-order partial derivatives:

$$\nabla f(x) = \frac{df}{dx} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

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named gradient of $f(x)$. This vector indicates the direction of the steepest ascent. Thus, vector $-\nabla f(x)$ means the direction of the steepest descent of the function in the point. Moreover, the gradient vector is always orthogonal to the contour line in the point.

Example

For the function $f(x, y) = x^2 + y^2$, the gradient is:

$$\nabla f(x, y) = \begin{bmatrix} 2x \\ 2y \end{bmatrix}$$

This gradient points in the direction of the steepest ascent of the function.

Question

How does the magnitude of the gradient relate to the steepness of the function?

Гессиан

Let $f(x) : \mathbb{R}^n \to \mathbb{R}$, then matrix, containing all the second order partial derivatives:

$$f''(x) = \nabla^2 f(x) = \frac{\partial^2 f}{\partial x_i \partial x_j} = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{pmatrix}$$

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In fact, Hessian could be a tensor in such a way: $(f(x) : \mathbb{R}^n \to \mathbb{R}^m)$ is just 3d tensor, every slice is just hessian of corresponding scalar function $(\nabla^2 f_1(x), \dots, \nabla^2 f_m(x))$.

Example

For the function $f(x, y) = x^2 + y^2$, the Hessian is:

$$H_f(x, y) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

This matrix provides information about the curvature of the function in different directions.

Question

How can the Hessian matrix be used to determine the concavity or convexity of a function?

Теорема Шварца

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a function. If the mixed partial derivatives $\frac{\partial^2 f}{\partial x_i \partial x_j}$ and $\frac{\partial^2 f}{\partial x_j \partial x_i}$ are both continuous on an open set containing a point a, then they are equal at the point a. That is,

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Given the Schwartz theorem, if the mixed partials are continuous on an open set, the Hessian matrix is symmetric. That means the entries above the main diagonal mirror those below the main diagonal:

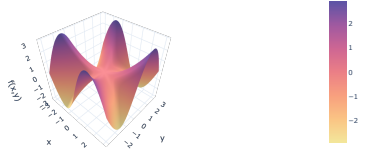
$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i} \quad \nabla^2 f(x) = (\nabla^2 f(x))^T$$

This symmetry simplifies computations and analysis involving the Hessian matrix in various applications, particularly in optimization.

Контрпример Шварца

$$f(x,y) = \begin{cases} \frac{xy(x^2-y^2)}{x^2+y^2} & \text{for } (x,\, y) \neq (0,\, 0), \\ 0 & \text{for } (x,y) = (0,0). \end{cases}$$

Counterexample ♣



One can verify, that $\frac{\partial^2 f}{\partial x \partial y}(0,0) \neq \frac{\partial^2 f}{\partial y \partial x}(0,0)$, although the mixed partial derivatives do exist, and at every other point the symmetry does hold.

Якобиан

The extension of the gradient of multidimensional $f(x) : \mathbb{R}^n \to \mathbb{R}^m$ is the following matrix:

$$J_f = f'(x) = \frac{df}{dx^T} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_2}{\partial x_1} & \dots & \frac{\partial f_m}{\partial x_1} \\ \frac{\partial f_1}{\partial x_2} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_m}{\partial x_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_1}{\partial x_n} & \frac{\partial f_2}{\partial x_n} & \dots & \frac{\partial f_m}{\partial x_n} \end{pmatrix}$$

This matrix provides information about the rate of change of the function with respect to its inputs.

Question

Can we somehow connect those three definitions above (gradient, jacobian, and hessian) using a single correct statement?

Example

For the function

$$f(x, y) = \begin{bmatrix} x + y \\ x - y \end{bmatrix},$$

the Jacobian is:

$$J_f(x, y) = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Question

How does the Jacobian matrix relate to the gradient for scalar-valued functions?

Резюме

$$f(x) : X \to Y; \qquad \frac{\partial f(x)}{\partial x} \in G$$

X	Y	G	Name
$\mathbb{R}$	$\mathbb{R}$	$\mathbb{R}$	$f'(x)$ (derivative)
$\mathbb{R}^n$	$\mathbb{R}$	$\mathbb{R}^n$	$\frac{\partial f}{\partial x_i}$ (gradient)
$\mathbb{R}^n$	$\mathbb{R}^m$	$\mathbb{R}^{n \times m}$	$\frac{\partial f_i}{\partial x_j}$ (jacobian)
$\mathbb{R}^{m \times n}$	$\mathbb{R}$	$\mathbb{R}^{m \times n}$	$\frac{\partial f}{\partial x_{ij}}$

Дифференциалы

Theorem

Let $x \in S$ be an interior point of the set S, and let $D : U \to V$ be a linear operator. We say that the function f is differentiable at the point x with derivative D if for all sufficiently small $h \in U$ the following decomposition holds:

$$f(x + h) = f(x) + D[h] + o(\|h\|)$$

If for any linear operator $D : U \to V$ the function f is not differentiable at the point x with derivative D, then we say that f is not differentiable at the point x.

Дифференциалы

After obtaining the differential notation of df we can retrieve the gradient using the following formula:

$$df(x) = \langle \nabla f(x), dx \rangle$$

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Then, if we have a differential of the above form and we need to calculate the second derivative of the matrix/vector function, we treat ``old'' dx as the constant dx_1, then calculate $d(df) = d^2 f(x)$

$$d^2 f(x) = \langle \nabla^2 f(x) dx_1, dx \rangle = \langle H_f(x) dx_1, dx \rangle$$

Свойства дифференциалов

Let A and B be the constant matrices, while X and Y are the variables (or matrix functions).

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- $d\langle X, Y\rangle = \langle dX, Y\rangle + \langle X, dY\rangle$

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- $d\langle X, Y\rangle = \langle dX, Y\rangle + \langle X, dY\rangle$
- $d\left(\dfrac{X}{\phi}\right) = \dfrac{\phi dX - (d\phi)X}{\phi^2}$

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- $d\left(\dfrac{X}{\phi}\right) = \dfrac{\phi dX - (d\phi)X}{\phi^2}$
- $d\left(\det X\right) = \det X \langle X^{-T}, dX\rangle$

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Let A and B be the constant matrices, while X and Y are the variables (or matrix functions).

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- $d(\alpha X) = \alpha(dX)$
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- $d(X + Y) = dX + dY$
- $d(X^T) = (dX)^T$
- $d(XY) = (dX)Y + X(dY)$
- $d\langle X, Y\rangle = \langle dX, Y\rangle + \langle X, dY\rangle$
- $d\left(\dfrac{X}{\phi}\right) = \dfrac{\phi dX - (d\phi)X}{\phi^2}$
- $d\left(\det X\right) = \det X \langle X^{-T}, dX\rangle$
- $d\left(\mathsf{tr}\ X\right) = \langle I, dX\rangle$

Свойства дифференциалов

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Матричное дифференцирование. Пример 1

Example

Find $df, \nabla f(x)$, if $f(x) = \langle x, Ax \rangle - b^T x + c$.

Матричное дифференцирование. Пример 2

Example

Find $df, \nabla f(x)$, if $f(x) = \ln\langle x, Ax\rangle$.

1. It is essential for A to be positive definite, because it is a logarithm argument. So, $A \in \mathbb{S}^n_{++}$Let's find the differential first:

$$df = d\left(\ln\langle x, Ax\rangle\right) = \frac{d\left(\langle x, Ax\rangle\right)}{\langle x, Ax\rangle} = \frac{\langle dx, Ax\rangle + \langle x, d(Ax)\rangle}{\langle x, Ax\rangle} =$$

$$= \frac{\langle Ax, dx\rangle + \langle x, Adx\rangle}{\langle x, Ax\rangle} = \frac{\langle Ax, dx\rangle + \langle A^T x, dx\rangle}{\langle x, Ax\rangle} = \frac{\langle (A + A^T)x, dx\rangle}{\langle x, Ax\rangle}$$

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2. Note, that our main goal is to derive the form $df = \langle \cdot, dx\rangle$

$$df = \left\langle \frac{2Ax}{\langle x, Ax\rangle}, dx \right\rangle$$

Hence, the gradient is $\nabla f(x) = \dfrac{2Ax}{\langle x, Ax\rangle}$

Матричное дифференцирование. Пример 3

Example

Find $df, \nabla f(X)$, if $f(X) = \langle S, X \rangle - \log \det X$.