Basic linear algebra background

Vectors and matrices

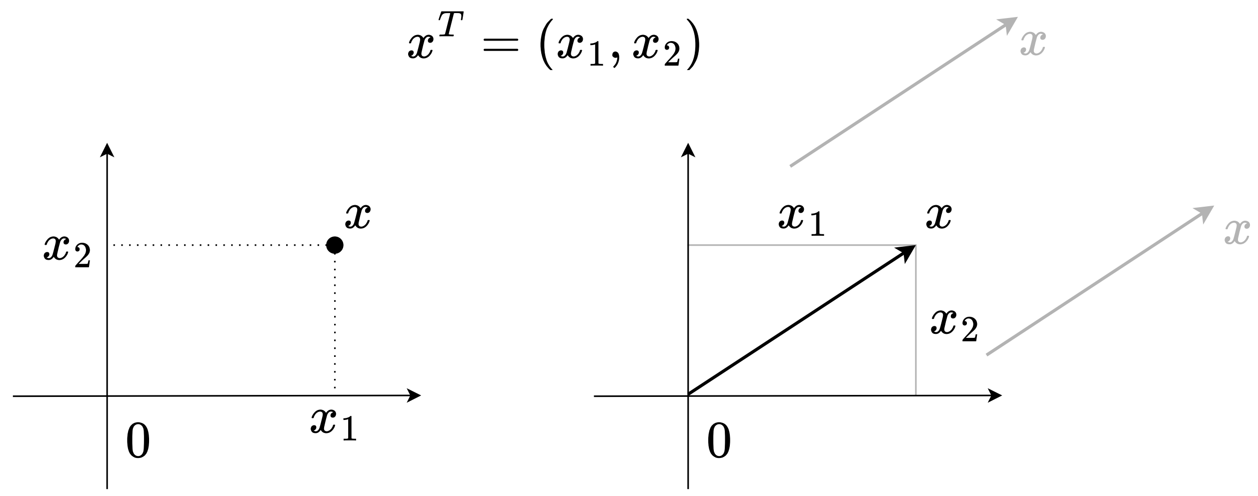
We will treat all vectors as column vectors by default. The space of real vectors of length n is denoted by $\mathbb{R}^n$, while the space of real-valued $m \times n$ matrices is denoted by $\mathbb{R}^{m \times n}$. That's it: [1]

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

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

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

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



A matrix is symmetric if $A = A^T$. It is denoted as $A \in \mathbb{S}^n$ (set of square symmetric matrices of dimension n). Note, that only square matrix could be symmetric by definition.

A matrix $A \in \mathbb{S}^n$ is called **positive (negative) definite** if for all $x \neq 0 : x^T A x > (<) 0$

. We denote this as $A \succ (\prec) 0$. The set of such matrices is denoted as $\mathbb{S}^n_{++} (\mathbb{S}^n_{--})$

A matrix $A \in \mathbb{S}^n$ is called **positive (negative) semidefinite** if for all $x : x^T Ax \geq (\leq) 0$. We denote this as $A \succeq (\preceq) 0$. The set of such matrices is denoted as $\mathbb{S}^n_{+} (\mathbb{S}^n_{-})$

🤔 **QUESTION**

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

Matrix and vector product

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.

🤔 **QUESTION**

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

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:

$$z = Ax$$

is given by:

$$z_i = \sum_{k=1}^n a_{ik} x_k$$

Remember, that:

- $C = AB \quad C^T = B^T A^T$
- $AB \neq BA$

- $e^A = \sum\limits_{k=0}^{\infty} \frac{1}{k!} A^k$
- $e^{A+B} \neq e^A e^B$ (but if A and B are commuting matrices, which means that $AB = BA$, $e^{A+B} = e^A e^B$)
- $\langle x, Ay \rangle = \langle A^T x, y \rangle$

Norms and scalar products

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

The norm should satisfy certain properties:

1. $\Vert \alpha x \Vert = \vert \alpha \vert \Vert x \Vert$, $\alpha \in \mathbb{R}$
2. $\Vert x + y \Vert \leq \Vert x \Vert + \Vert y \Vert$ (triangle inequality)
3. If $\Vert x \Vert = 0$ then $x = 0$

The distance between two vectors is then defined as

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

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

$$\Vert x \Vert_2 = \sqrt{\sum_{i=1}^n |x_i|^2},$$

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:

$$\Vert x \Vert_p = \Big(\sum_{i=1}^n |x_i|^p\Big)^{1/p}.$$

There are two very important special cases:

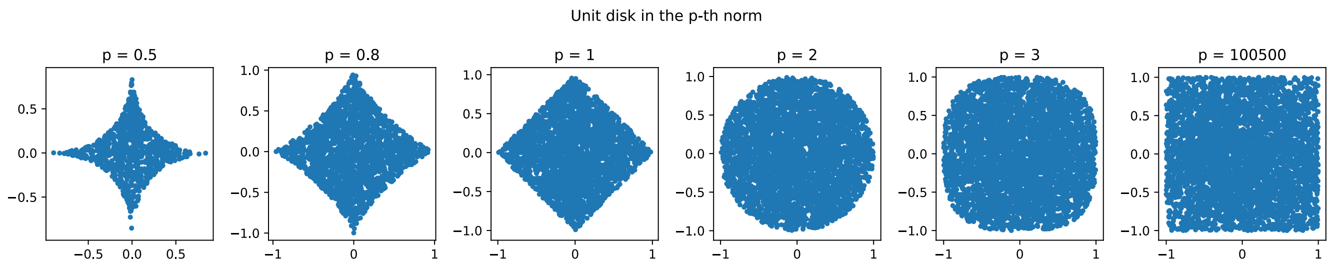
- Infinity norm, or Chebyshev norm is defined as the element of the maximal absolute value:

$$\Vert x \Vert_{\infty} = \max_i | x_i|$$

- L_1 norm (or **Manhattan distance**) which is defined as the sum of modules of the elements of x:

$$\|x\|_1 = \sum_i |x_i|$$

L_1 norm plays 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 picture below is available here: Open In Colab



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:

$$\|A\|_F = \left(\sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^2\right)^{1/2}$$

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.

🤔 **QUESTION**

Is it true, that all matrix norms satisfy submultiplicativity property: $\|AB\| \leq \|A\|\|B\|$? Hint: consider Chebyshev matrix norm $\|A\|_C = \max\limits_{i,j} |a_{ij}|$.

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.

🤔 **QUESTION**

Is there any connection between the norm $\| \cdot \|$ and scalar product $\langle \cdot, \cdot \rangle$?

🧑‍🏫 **EXAMPLE**

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

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

🧑‍🏫 **EXAMPLE**

Simplify the following expression:

$$\sum_{i=1}^{n} \langle S^{-1} a_i, a_i \rangle, \text{ where } S = \sum_{i=1}^{n} a_i a_i^T, a_i \in \mathbb{R}^n, \det(S) \neq 0$$

▼ Solution

Eigenvalues, eigenvectors, and the singular-value decomposition

Eigenvalues

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

$$Aq = \lambda q.$$

The 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.

🤓 **THEOREM**

$$A \succeq 0 \Leftrightarrow \text{all eigenvalues of } A \text{ are } \geq 0$$

$$A \succ 0 \Leftrightarrow \text{all eigenvalues of } A \text{ are } > 0$$

▼ Solution

We will just prove the first point here. The second one can be proved analogously.

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

$$Ax = \lambda x \rightarrow x^T Ax = \lambda x^T x < 0 \rightarrow A \nsucceq 0.$$

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 $x > in \mathbb{R}^n$.

$$x^T Ax = (\alpha_1 v_1 + \cdots + \alpha_n v_n)^T A(\alpha_1 v_1 + \cdots + \alpha_n v_n)$$

$$= \sum \alpha_i^2 v_i^T Av_i = \sum \alpha_i^2 \lambda_i v_i^T v_i \geq 0$$

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

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

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

where $Q \in \mathbb{R}^{n \times n}$ is orthogonal, i.e., satisfies $Q^T Q = I$, and $\Lambda = \operatorname{diag}(\lambda_1, ..., \lambda_n)$. 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]

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 ith largest eigenvalue of $A \in S$. We usually write the largest or maximum eigenvalue as $\lambda_1(A) = \lambda_{\max}(A)$, and the least or minimum eigenvalue as $\lambda_n(A) = \lambda_{\min}(A)$.

The largest and smallest eigenvalues satisfy

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

and consequently $\forall x \in \mathbb{R}^n$ (Rayleigh quotient):

$$\lambda_{\min}(A) x^T x \leq x^T A x \leq \lambda_{\max}(A) x^T x$$

The **condition number** of a nonsingular matrix is defined as

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

Suppose $A \in \mathbb{R}^{m \times n}$ with rank $A = r$. Then A can be factored as

$$A = U \Sigma V^T, \quad (A.12)$$

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 $\Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_r)$, such that

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

Singular value decomposition

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.

🧑‍🏫 **EXAMPLE**

Let $A \in \mathbb{R}^{m \times n}$, and let $q := \min m, n$. Show that

$$\sqrt{\|A\|_F} = \sum_{i=1}^{q} \sigma_i^2(A),$$

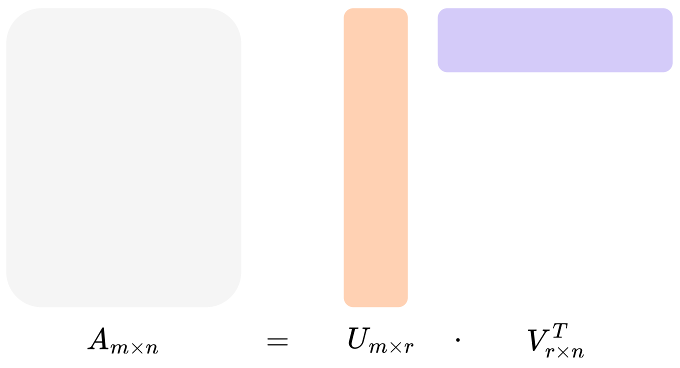
where $\sigma_1(A) \geq \ldots \geq \sigma_q(A) \geq 0$ are the singular values of matrix A.

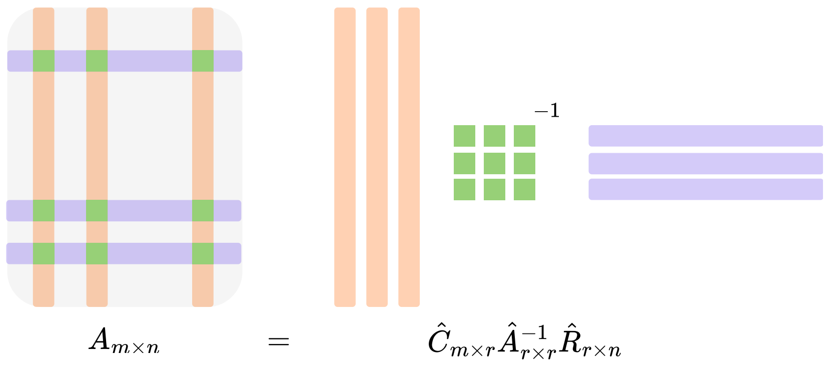
Skeleton decomposition

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 an ability to reconstruct the whole matrix exactly.





-1
$A_{m\times n}$
$=$
$\hat{C}_{m\times r}\hat{A}^{-1}_{r\times r}\hat{R}_{r\times n}$

🧑‍🏫 **EXAMPLE**

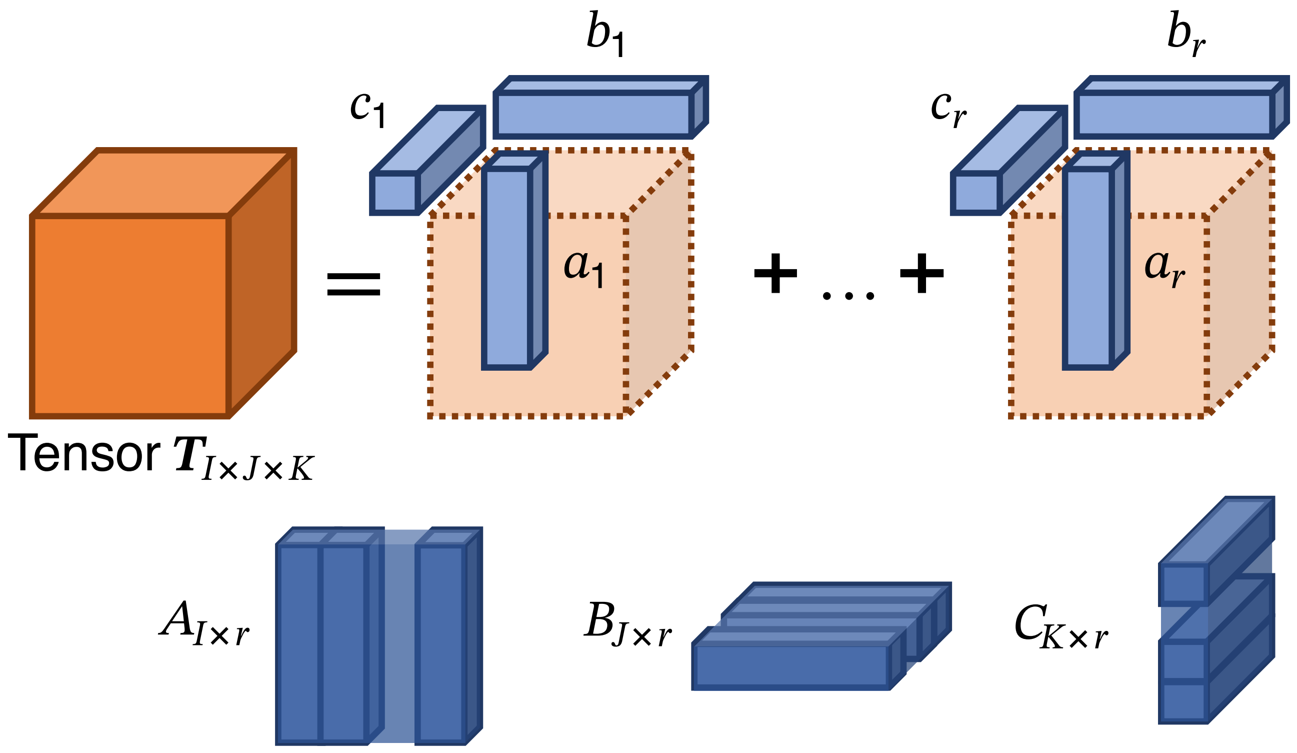
Simplify the following expression:

$$\sum_{i=1}^{n} \langle S^{-1}a_i, a_i \rangle, \text{ where } S = \sum_{i=1}^{n} a_i a_i^T, a_i \in \mathbb{R}^n, \det(S) \neq 0$$

▼ Solution

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 sum of r primitive tensors.



🧑‍🏫 **EXAMPLE**

Note, that there are many tensor decompositions: Canonical, Tucker, Tensor Train (TT), Tensor Ring (TR) and others. In tensor case we do not have the straightforward definition of *rank* for all type 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

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

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

- $\det A = 0$ if and only if A is singular;
- $\det AB = (\det A)(\det B)$;
- $\det A^{-1} = \frac{1}{\det A}$.

Don't forget about the cyclic property of a trace for a square matrices A, B, C, D:

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

Optimization bingo

Gradient

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

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

named gradient of $f(x)$. This vector indicates the direction of 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.

Hessian

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

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

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 $\left(H\left(f_1(x)\right), H\left(f_2(x)\right), \ldots, H\left(f_m(x)\right)\right)$.

Jacobian

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

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

Summary

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

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

Taylor approximations

Taylor approximations provide a way to approximate functions locally by polynomials. The idea is that for a smooth function, we can approximate it by its tangent (for first order) or by its parabola (for the second order) at a point.

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.
- $\nabla f(x_0)$ is the gradient of the function at the point x_0.

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.

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:

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

Where:

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

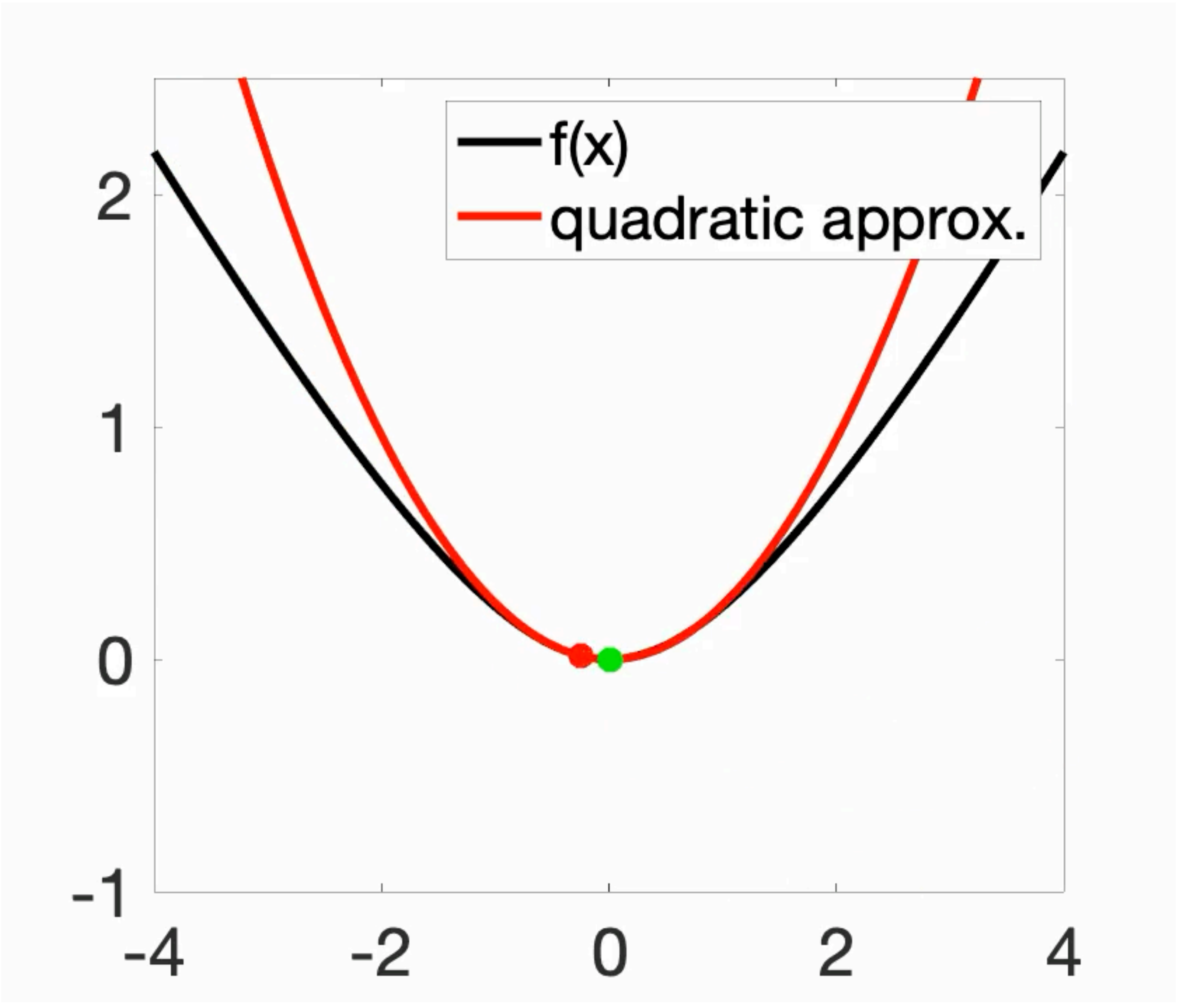
When using the linear approximation of the function not sufficient one can consider replacing the $f(x)$ with $f^{II}_{x_0}(x)$ near the point x_0. In general, Taylor approximations give us a way to locally approximate functions. The first order approximation is a plane tangent to the function at the 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.

🧑‍🏫 **EXAMPLE**

Calculate first and second order Taylor approximation of the function $f(x) = \frac{1}{2}x^T Ax - b^T x + c$

▼ Solution

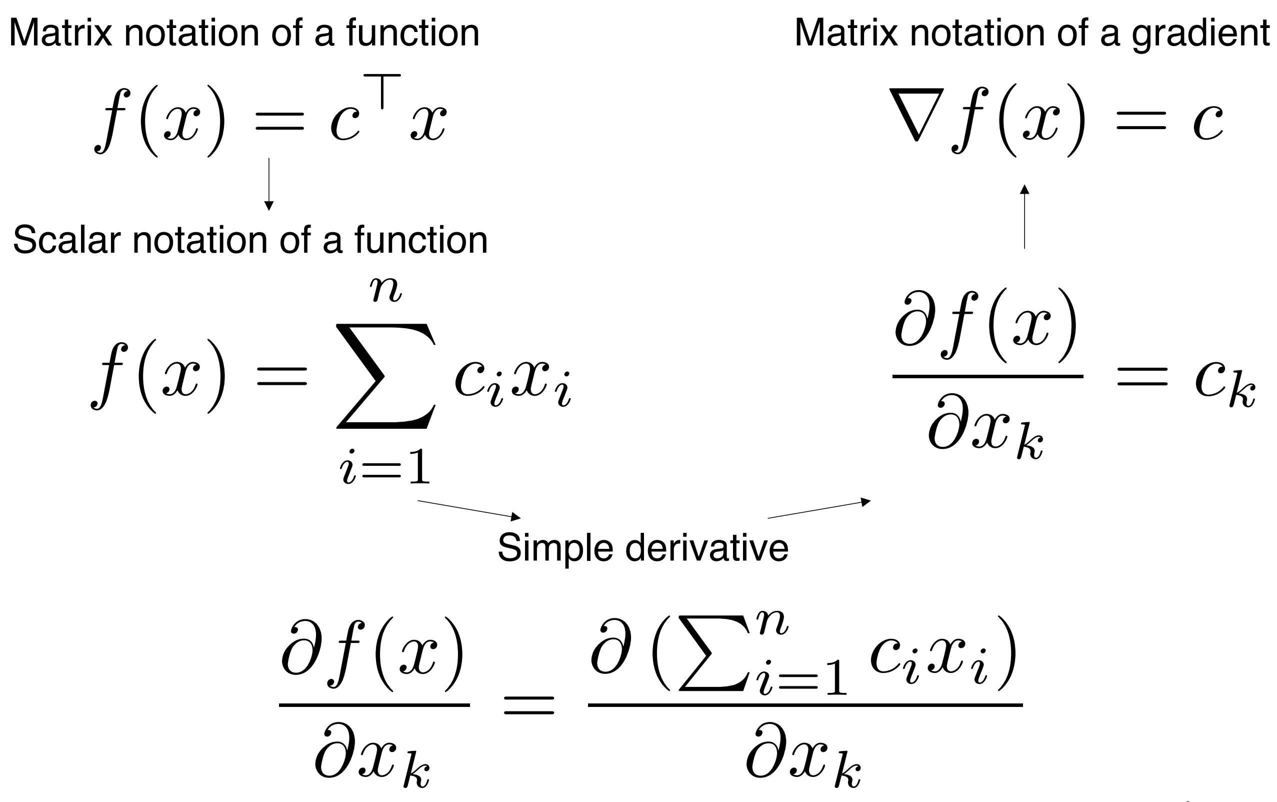
Note, that even the second order approximation could become inaccurate very quickly:



Derivatives

Naive approach

The basic idea of naive approach is to reduce matrix/vector derivatives to the well-known scalar derivatives.


Matrix notation of a function
$f(x) = c^\top x$
Scalar notation of a function
$f(x) = \sum_{i=1}^{n} c_i x_i$
Matrix notation of a gradient
$\nabla f(x) = c$
$\frac{\partial f(x)}{\partial x_k} = c_k$
Simple derivative
$\frac{\partial f(x)}{\partial x_k} = \frac{\partial \left(\sum_{i=1}^{n} c_i x_i\right)}{\partial x_k}$

One of the most important practical tricks here is to separate indices of sum (i) and partial derivatives (k). Ignoring this simple rule tends to produce mistakes.

Differential approach

The guru approach implies formulating a set of simple rules, which allows you to calculate derivatives just like in a scalar case. It might be convenient to use the differential notation here. [3]

Differentials

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

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

Then, if we have 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 $d(df) = d^2 f(x)$

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

Properties

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

- $dA = 0$

- $d(\alpha X) = \alpha(dX)$
- $d(AXB) = A(dX)B$
- $d(X+Y) = dX + dY$
- $d(X^T) = (dX)^T$
- $d(XY) = (dX)Y + X(dY)$
- $d\langle X, Y\rangle = \langle dX, Y\rangle + \langle X, dY\rangle$
- $d\left(\frac{X}{\phi}\right) = \frac{\phi dX - (d\phi)X}{\phi^2}$
- $d(\det X) = \det X \langle X^{-\top}, dX\rangle$
- $d(\text{tr } X) = \langle I, dX\rangle$
- $df(g(x)) = \frac{df}{dg} \cdot dg(x)$
- $H = (J(\nabla f))^T$
- $d(X^{-1}) = -X^{-1}(dX)X^{-1}$

🧑‍🏫 **EXAMPLE**

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

▼ Solution

1. Let's find the differential first:

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

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

🧑‍🏫 **EXAMPLE**

Find $df, \nabla f(X)$, if $f(X) = \|AX - B\|_F$.

▼ Solution

EXAMPLE

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

▼ Solution

EXAMPLE

Find the gradient $\nabla f(x)$ and hessian $\nabla^2 f(x)$, if $f(x) = \ln\left(1 + \exp\langle a, x\rangle\right)$

▼ Solution

References

- Convex Optimization book by S. Boyd and L. Vandenberghe - Appendix A. Mathematical background.
- Numerical Optimization by J. Nocedal and S. J. Wright. - Background Material.
- Matrix decompositions Cheat Sheet.
- Good introduction
- The Matrix Cookbook
- MSU seminars (Rus.)

- Online tool for analytic expression of a derivative.
- Determinant derivative
- Introduction to Applied Linear Algebra – Vectors, Matrices, and Least Squares - book by Stephen Boyd & Lieven Vandenberghe.
- Numerical Linear Algebra course at Skoltech

Footnotes

1. Full introduction to applied linear algebra could 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, useful refresher for linear algebra is in the appendix A of book Numerical Optimization by Jorge Nocedal Stephen J. Wright. ↩
2. Good cheatsheet with matrix decomposition is available at NLA course website. ↩
3. The most comprehensive and intuitive guide about the theory of taking matrix derivatives is presented in these notes by Dmitry Kropotov team ↩