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Hessian

In **mathematics**, the **Hessian matrix** or **Hessian** is a **square matrix** of second-order **partial derivatives** of a scalar-valued **function**, or **scalar field**. It describes the local curvature of a function of many

Suppose $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is a function taking as input a vector $\mathbf{x} \in \mathbb{R}^n$ and outputting a scalar $f(\mathbf{x}) \in \mathbb{R}$. If all second **partial derivatives** of f exist and are continuous over the domain of the function, then the Hessian matrix \mathbf{H} of f is a square $n \times n$ matrix, usually defined and arranged as follows:

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix},$$

or, by stating an equation for the coefficients using indices i and j ,

$$\mathbf{H}_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j}.$$

The Hessian matrix is a **symmetric matrix**, since the hypothesis of continuity of the second derivatives implies that the order of differentiation does not matter (**Schwarz's theorem**)

The **determinant** of the Hessian matrix is called the *Hessian determinant*.^[1]

The Hessian matrix of a function f is the **Jacobian matrix** of the **gradient** of the function: $\mathbf{H}(f(\mathbf{x})) = \mathbf{J}(\nabla f(\mathbf{x}))$.

Use in optimization [edit]

Hessian matrices are used in large-scale **optimization** problems within **Newton-type** methods because they are the coefficient of the quadratic term of a local **Taylor expansion** of a function. That is,

$$y = f(\mathbf{x} + \Delta \mathbf{x}) \approx f(\mathbf{x}) + \nabla f(\mathbf{x})^T \Delta \mathbf{x} + \frac{1}{2} \Delta \mathbf{x}^T \mathbf{H}(\mathbf{x}) \Delta \mathbf{x}$$

where ∇f is the **gradient** $(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n})$. Computing and storing the full Hessian matrix takes $\Theta(n^2)$ memory, which is infeasible for high-dimensional functions such as the **loss functions** of **neural nets**, **conditional random fields**, and other **statistical models** with large numbers of parameters. For such situations, **truncated-Newton** and **quasi-Newton** algorithms have been developed. The latter family of algorithms use approximations to the Hessian; one of the most popular quasi-Newton algorithms is **BFGS**.^[5]

Gradient

In **vector calculus**, the **gradient** of a **scalar-valued differentiable function** f of **several variables**, $f: \mathbf{R}^n \rightarrow \mathbf{R}$, is the **vector field**, or more simply a **vector-valued function**^[a] $\nabla f: \mathbf{R}^n \rightarrow \mathbf{R}^n$, whose value at a point p is the **vector**^[b] whose components are the **partial derivatives** of f at p .^{[1][2][3][4][5][6][7][8][9]}

$$\nabla f(p) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(p) \\ \vdots \\ \frac{\partial f}{\partial x_n}(p) \end{bmatrix}.$$

The gradient by Khan Academy 理解方向导数与梯度

Taylor expansion

In **mathematics**, the **Taylor series** of a **function** is an **infinite sum** of terms that are expressed in terms of the function's **derivatives** at a single point. For most common functions, the function and the sum of

The **partial sum** formed by the n first terms of a Taylor series is a **polynomial** of degree n that is called the n th **Taylor polynomial** of the function. Taylor polynomials are approximations of a function, which becomes generally better when n increases. **Taylor's theorem** gives quantitative estimates on the error introduced by the use of such approximations. If the Taylor series of a function is **convergent**, its sum is the **limit** of the **infinite sequence** of the Taylor polynomials. A

□

Definition [\[edit \]](#)

The Taylor series of a [real](#) or [complex-valued function](#) $f(x)$ that is [infinitely differentiable](#) at a [real](#) or [complex number](#) a is the [power series](#)

$$f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \cdots,$$

where $n!$ denotes the [factorial](#) of n . In the more compact [sigma notation](#), this can be written as

$$\sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!} (x-a)^n,$$

where $f^{(n)}(a)$ denotes the n th [derivative](#) of f evaluated at the point a . (The derivative of order zero of f is defined to be f itself and $(x-a)^0$ and $0!$ [are both defined to be 1](#).)

Field

In [mathematics](#), a **field** is a [set](#) on which [addition](#), [subtraction](#), [multiplication](#), and [division](#) are defined and behave as the corresponding operations on [rational](#) and [real numbers](#) do. A field is thus a fundamental [algebraic structure](#) which is widely used in [algebra](#), [number theory](#), and many other areas of mathematics.

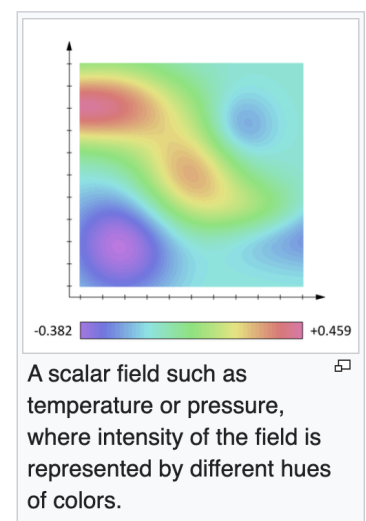
The best known fields are the field of [rational numbers](#), the field of [real numbers](#) and the field of [complex numbers](#). Many other fields, such as

Scalar Field

In [mathematics](#) and [physics](#), a **scalar field** associates a scalar value to every point in a [space](#) – possibly [physical space](#). The scalar may either be a ([dimensionless](#)) [mathematical number](#) or a [physical quantity](#). In a physical context, scalar fields are required to be independent of the choice of reference frame, meaning that any two observers using the same units will agree on the value of the scalar field at the same absolute point in space (or [spacetime](#)) regardless of their respective points of origin. Examples used in physics include the [temperature](#) distribution throughout space, the [pressure](#) distribution in a fluid, and spin-zero quantum fields, such as the [Higgs field](#). These fields are the subject of [scalar field theory](#).

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Scalar

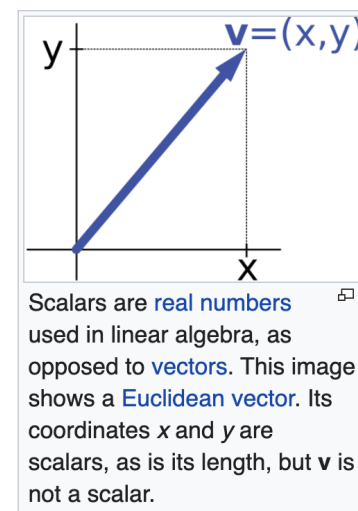
A **scalar** is an element of a **field** which is used to define a **vector space**. A quantity described by multiple scalars, such as having both direction and magnitude, is called a vector.^[1]

In **linear algebra**, real numbers or other elements of a field are called **scalars** and relate to vectors in a vector space through the operation of **scalar multiplication**, in which a vector can be multiplied by a number to produce another vector.^{[2][3][4]} More generally, a vector space may be defined by using any field instead of real numbers, such as **complex numbers**. Then the scalars of that vector space will be the elements of the associated field.

A **scalar product** operation – not to be confused with scalar multiplication – may be defined on a vector space, allowing two vectors to be multiplied to produce a scalar. A vector space equipped with a scalar product is called an **inner product space**.

The real component of a **quaternion** is also called its **scalar part**.

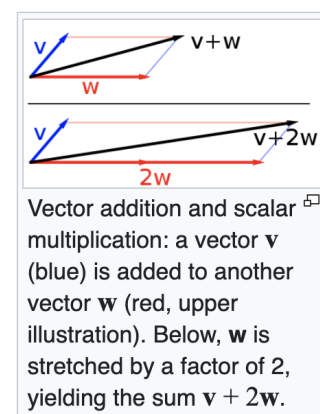
The term is also sometimes used informally to mean a vector, **matrix**, **tensor**, or other usually "compound" value that is actually reduced to a single component. Thus, for example, the product of a $1 \times n$ matrix and an $n \times 1$ matrix, which is formally a 1×1 matrix, is often said to be a **scalar**.



Vector space

A **vector space** (also called a **linear space**) is a collection of objects called **vectors**, which may be **added** together and **multiplied** ("scaled") by numbers, called **scalars**. Scalars are often taken to be **real numbers**, but there are also vector spaces with scalar multiplication by **complex numbers**, **rational numbers**, or generally any **field**. The operations of vector addition and scalar multiplication must satisfy certain requirements, called **axioms**, listed below, in § **Definition**. For specifying that the scalars are real or complex numbers, the terms **real vector space** and **complex vector space** are often used.

Euclidean vectors are an example of a vector space. They represent **physical quantities** such as **forces**: any two forces (of the same type) can be added to yield a third, and the multiplication of a **force vector** by a real multiplier is another force vector. In the same vein, but in a more **geometric** sense, vectors representing displacements in the plane or in **three-dimensional space** also form vector spaces. Vectors in vector spaces do not necessarily have to be arrow-like objects as they appear in the mentioned examples: vectors are regarded as abstract mathematical objects with particular properties, which in some cases can be visualized as arrows.



Jacobian

$$\mathbf{J} = \begin{bmatrix} \frac{\partial \mathbf{f}}{\partial x_1} & \cdots & \frac{\partial \mathbf{f}}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}.$$

Total derivative

In [mathematics](#), the **total derivative** of a function f at a point is the best [linear approximation](#) near this point of the function with respect to its arguments. Unlike [partial derivatives](#), the total derivative approximates the function with respect to all of its arguments, not just a single one. In many situations, this is the same as considering all partial derivatives simultaneously. The term "total derivative" is primarily used when f is a function of several variables, because when f is a function of a single variable, the total derivative is the same as the [derivative](#) of the function.^{[1]:198–203}

The total derivative as a differential form [\[edit \]](#)

When the function under consideration is real-valued, the total derivative can be recast using [differential forms](#). For example, suppose that $f: \mathbf{R}^n \rightarrow \mathbf{R}$ is a differentiable function of variables x_1, \dots, x_n . The total derivative of f at a may be written in terms of its Jacobian matrix, which in this instance is a row matrix (the [transpose](#) of the [gradient](#)):

$$df_a = \left(\frac{\partial f}{\partial x_1}, \quad \cdots \quad , \quad \frac{\partial f}{\partial x_n} \right).$$

The linear approximation property of the total derivative implies that if

$$\Delta x = (\Delta x_1, \quad \cdots \quad , \quad \Delta x_n)^T$$

is a small vector (where the T denotes transpose, so that this vector is a column vector), then

$$f(a + \Delta x) - f(a) \approx df_a \cdot \Delta x = \sum_{i=1}^n \frac{\partial f}{\partial x_i} \Delta x_i.$$

Heuristically, this suggests that if dx_1, \dots, dx_n are [infinitesimal](#) increments in the coordinate directions, then

$$df_a = \sum_{i=1}^n \frac{\partial f}{\partial x_i}(a) dx_i.$$

Some notes

梯度、散度、旋度、Jacobian、Hessian、Laplacian 的关系

by 王赞 Maigo

Products in Linear Algebra

Products between vectors

- dot product, also called as:
 - scalar product
 - inner product
 - projection product
- cross product (vector product)
- [exterior product](#) (wedge product)
- [outer product](#)
- Cartesian product (related to set theory)

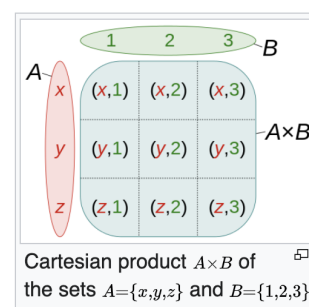
In [mathematics](#), specifically [set theory](#), the **Cartesian product** of two [sets](#) A and B , denoted $A \times B$, is the set of all [ordered pairs](#) (a, b) where a is in A and b is in B . In terms of [set-builder notation](#), that is

$$A \times B = \{ (a, b) \mid a \in A \text{ and } b \in B \}.$$
^[1]

A table can be created by taking the Cartesian product of a set of rows and a set of columns. If the Cartesian product $rows \times columns$ is taken, the cells of the table contain ordered pairs of the form (row value, column value).

One can similarly define the Cartesian product of n sets, also known as an **n -fold Cartesian product**, which can be represented by an n -dimensional array, where each element is an [\$n\$ -tuple](#). An ordered pair is a [2-tuple or couple](#). More generally still, one can define the

- Cartesian product of an [indexed family](#) of sets.



Products between matrices

- matrix product

In [mathematics](#), **matrix multiplication** is a [binary operation](#) that produces a [matrix](#) from two matrices. For matrix multiplication, the number of columns in the first matrix must be equal to the number of rows in the second matrix. The result matrix, known as the **matrix product**, has the number of rows of the first and the number of columns of the second matrix.

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Definition [\[edit \]](#)

If \mathbf{A} is an $m \times n$ matrix and \mathbf{B} is an $n \times p$ matrix,

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1p} \\ b_{21} & b_{22} & \cdots & b_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{np} \end{pmatrix}$$

the *matrix product* $\mathbf{C} = \mathbf{AB}$ (denoted without multiplication signs or dots) is defined to be the $m \times p$ matrix^{[4][5][6][7]}

$$\mathbf{C} = \begin{pmatrix} c_{11} & c_{12} & \cdots & c_{1p} \\ c_{21} & c_{22} & \cdots & c_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ c_{m1} & c_{m2} & \cdots & c_{mp} \end{pmatrix}$$

such that

$$c_{ij} = a_{i1}b_{1j} + a_{i2}b_{2j} + \cdots + a_{in}b_{nj} = \sum_{k=1}^n a_{ik}b_{kj},$$

for $i = 1, \dots, m$ and $j = 1, \dots, p$.

That is, the entry c_{ij} of the product is obtained by multiplying term-by-term the entries of the i th row of \mathbf{A} and the j th column of \mathbf{B} , and summing these n products. In other words, c_{ij} is the **dot product** of the i th row of \mathbf{A} and the j th column of \mathbf{B} .

Therefore, \mathbf{AB} can also be written as

$$\mathbf{C} = \begin{pmatrix} a_{11}b_{11} + \cdots + a_{1n}b_{n1} & a_{11}b_{12} + \cdots + a_{1n}b_{n2} & \cdots & a_{11}b_{1p} + \cdots + a_{1n}b_{np} \\ a_{21}b_{11} + \cdots + a_{2n}b_{n1} & a_{21}b_{12} + \cdots + a_{2n}b_{n2} & \cdots & a_{21}b_{1p} + \cdots + a_{2n}b_{np} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}b_{11} + \cdots + a_{mn}b_{n1} & a_{m1}b_{12} + \cdots + a_{mn}b_{n2} & \cdots & a_{m1}b_{1p} + \cdots + a_{mn}b_{np} \end{pmatrix}$$

Thus the product \mathbf{AB} is defined if and only if the number of columns in \mathbf{A} equals the number of rows in \mathbf{B} , in this case n .

Usually the entries are numbers, but they may be any kind of **mathematical objects** for which an addition and a multiplication are defined, that are **associative**, and such that the addition is **commutative**, and the multiplication is **distributive** with respect to the addition. In particular, the entries may be matrices themselves (see **block matrix**).

Illustration [\[edit \]](#)

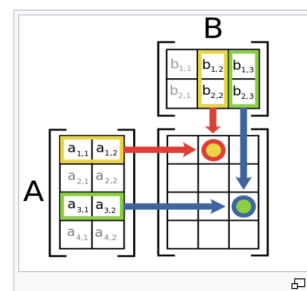
The figure to the right illustrates diagrammatically the product of two matrices \mathbf{A} and \mathbf{B} , showing how each intersection in the product matrix corresponds to a row of \mathbf{A} and a column of \mathbf{B} .

$$\begin{matrix} 4 \times 2 \text{ matrix} \\ \begin{bmatrix} a_{11} & a_{12} \\ \cdot & \cdot \\ a_{31} & a_{32} \\ \cdot & \cdot \end{bmatrix} \end{matrix} \begin{matrix} 2 \times 3 \text{ matrix} \\ \begin{bmatrix} \cdot & b_{12} & b_{13} \\ \cdot & b_{22} & b_{23} \end{bmatrix} \end{matrix} = \begin{matrix} 4 \times 3 \text{ matrix} \\ \begin{bmatrix} \cdot & c_{12} & c_{13} \\ \cdot & \cdot & \cdot \\ \cdot & c_{32} & c_{33} \\ \cdot & \cdot & \cdot \end{bmatrix} \end{matrix}$$

The values at the intersections marked with circles are:

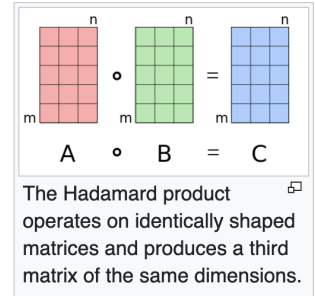
$$c_{12} = a_{11}b_{12} + a_{12}b_{22}$$

$$c_{33} = a_{31}b_{13} + a_{32}b_{23}$$



- Hadamard product

In [mathematics](#), the **Hadamard product** (also known as the **element-wise**, **entrywise**^{[1]:ch. 5} or **Schur**^[2] **product**) is a [binary operation](#) that takes two [matrices](#) of the same dimensions and produces another matrix of the same dimension as the operands where each element i, j is the product of elements i, j of the original two matrices. It should not be confused with the more common [matrix product](#). It is attributed to, and named after, either French mathematician [Jacques Hadamard](#) or German mathematician [Issai Schur](#).



- The Hadamard product is [associative](#) and [distributive](#). Unlike the matrix product, it is also [commutative](#).

Definition [\[edit \]](#)

For two matrices A and B of the same dimension $m \times n$, the Hadamard product $A \circ B$ (or $A \odot B$ ^{[3][4][5]}) is a matrix of the same dimension as the operands, with elements given by

$$(A \circ B)_{ij} = (A \odot B)_{ij} = (A)_{ij}(B)_{ij}.$$

For matrices of different dimensions ($m \times n$ and $p \times q$, where $m \neq p$ or $n \neq q$) the Hadamard product is undefined.

Example [\[edit \]](#)

For example, the Hadamard product for a 3×3 matrix \mathbf{A} with a 3×3 matrix \mathbf{B} is

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \circ \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} & a_{12}b_{12} & a_{13}b_{13} \\ a_{21}b_{21} & a_{22}b_{22} & a_{23}b_{23} \\ a_{31}b_{31} & a_{32}b_{32} & a_{33}b_{33} \end{bmatrix}.$$

Properties [\[edit \]](#)

- The Hadamard product is [commutative](#) (when working with a commutative ring), [associative](#) and [distributive](#) over addition.

That is, if \mathbf{A} , \mathbf{B} , and \mathbf{C} are matrices of the same size, and k is a scalar:

$$\begin{aligned} \mathbf{A} \circ \mathbf{B} &= \mathbf{B} \circ \mathbf{A}, \\ \mathbf{A} \circ (\mathbf{B} \circ \mathbf{C}) &= (\mathbf{A} \circ \mathbf{B}) \circ \mathbf{C}, \\ \mathbf{A} \circ (\mathbf{B} + \mathbf{C}) &= \mathbf{A} \circ \mathbf{B} + \mathbf{A} \circ \mathbf{C}, \\ (k\mathbf{A}) \circ \mathbf{B} &= \mathbf{A} \circ (k\mathbf{B}) = k(\mathbf{A} \circ \mathbf{B}), \\ \mathbf{A} \circ \mathbf{0} &= \mathbf{0} \circ \mathbf{A} = \mathbf{0}. \end{aligned}$$

- Kronecker product (generalization of cross product from vectors to matrices)

In [mathematics](#), the **Kronecker product**, sometimes denoted by \otimes , is an [operation](#) on two [matrices](#) of arbitrary size resulting in a [block matrix](#). It is a generalization of the [outer product](#) (which is denoted by the same symbol) from vectors to matrices, and gives the matrix of the [tensor product](#) with respect to a standard choice of [basis](#).

The Kronecker product should not be confused with the usual [matrix multiplication](#), which is an entirely different

- operation.

Definition [\[edit \]](#)

If \mathbf{A} is an $m \times n$ matrix and \mathbf{B} is a $p \times q$ matrix, then the Kronecker product $\mathbf{A} \otimes \mathbf{B}$ is the $pm \times qn$ block matrix:

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & \cdots & a_{mn}\mathbf{B} \end{bmatrix},$$

more explicitly:

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11}b_{11} & a_{11}b_{12} & \cdots & a_{11}b_{1q} & \cdots & \cdots & a_{1n}b_{11} & a_{1n}b_{12} & \cdots & a_{1n}b_{1q} \\ a_{11}b_{21} & a_{11}b_{22} & \cdots & a_{11}b_{2q} & \cdots & \cdots & a_{1n}b_{21} & a_{1n}b_{22} & \cdots & a_{1n}b_{2q} \\ \vdots & \vdots & \ddots & \vdots & & & \vdots & \vdots & \ddots & \vdots \\ a_{11}b_{p1} & a_{11}b_{p2} & \cdots & a_{11}b_{pq} & \cdots & \cdots & a_{1n}b_{p1} & a_{1n}b_{p2} & \cdots & a_{1n}b_{pq} \\ \vdots & \vdots & & \vdots & \ddots & & \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots & & \ddots & \vdots & \vdots & & \vdots \\ a_{m1}b_{11} & a_{m1}b_{12} & \cdots & a_{m1}b_{1q} & \cdots & \cdots & a_{mn}b_{11} & a_{mn}b_{12} & \cdots & a_{mn}b_{1q} \\ a_{m1}b_{21} & a_{m1}b_{22} & \cdots & a_{m1}b_{2q} & \cdots & \cdots & a_{mn}b_{21} & a_{mn}b_{22} & \cdots & a_{mn}b_{2q} \\ \vdots & \vdots & \ddots & \vdots & & & \vdots & \vdots & \ddots & \vdots \\ a_{m1}b_{p1} & a_{m1}b_{p2} & \cdots & a_{m1}b_{pq} & \cdots & \cdots & a_{mn}b_{p1} & a_{mn}b_{p2} & \cdots & a_{mn}b_{pq} \end{bmatrix}.$$

- Frobenius inner product (generalization of regular inner product from vectors to matrices)

In [mathematics](#), the **Frobenius inner product** is a binary operation that takes two [matrices](#) and returns a number. It is often denoted $\langle \mathbf{A}, \mathbf{B} \rangle_F$. The operation is a component-wise [inner product](#) of two matrices as though they are vectors. The two matrices must have the same dimension—same number of rows and columns—but are not

- restricted to be [square matrices](#).

Definition [\[edit \]](#)

Given two [complex number](#)-valued $n \times m$ matrices \mathbf{A} and \mathbf{B} , written explicitly as

$$\mathbf{A} = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1m} \\ A_{21} & A_{22} & \cdots & A_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \cdots & A_{nm} \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} B_{11} & B_{12} & \cdots & B_{1m} \\ B_{21} & B_{22} & \cdots & B_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ B_{n1} & B_{n2} & \cdots & B_{nm} \end{pmatrix}$$

the Frobenius inner product is defined by the following [summation](#) Σ of matrix elements,

$$\langle \mathbf{A}, \mathbf{B} \rangle_F = \sum_{i,j} \overline{A_{ij}} B_{ij} = \text{tr} \left(\overline{\mathbf{A}^T} \mathbf{B} \right)$$

where the overline denotes the [complex conjugate](#). Explicitly this sum is

$$\begin{aligned} \langle \mathbf{A}, \mathbf{B} \rangle_F &= \overline{A_{11}} B_{11} + \overline{A_{12}} B_{12} + \cdots + \overline{A_{1m}} B_{1m} \\ &\quad + \overline{A_{21}} B_{21} + \overline{A_{22}} B_{22} + \cdots + \overline{A_{2m}} B_{2m} \\ &\quad \vdots \\ &\quad + \overline{A_{n1}} B_{n1} + \overline{A_{n2}} B_{n2} + \cdots + \overline{A_{nm}} B_{nm} \end{aligned}$$

- The calculation is very similar to the [dot product](#), which in turn is an example of an inner product.