Univariate Functions

Let E and F be two non-empty subsets of IR.

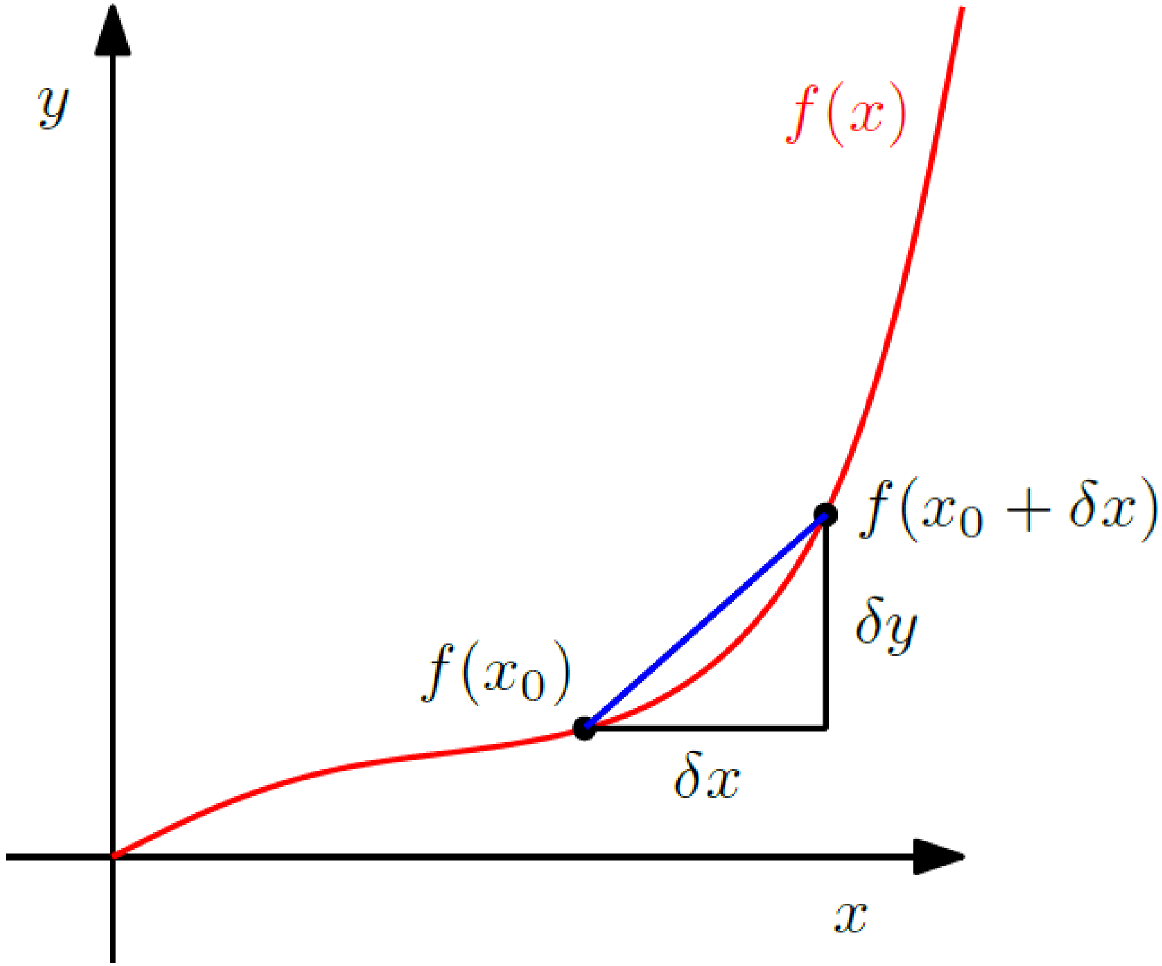
A function f is a collection of pairs of elements belonging to the cartesian product $E \times F$, such that for every element $x \in E$**, there is a single element** $y \in F$. This single element y is denoted by $f(x)$ and one writes

$$f : E \to F$$

The set E is called the **domain of *f***. One writes D_f.

The set $\{ y \in F : \exists x \in E \text{ so that } f(x) = y \}$ is called the **cotradomain of *f***.

Differentiation



(Difference Quotient). The *difference quotient*

$$\frac{\delta y}{\delta x} := \frac{f(x+\delta x) - f(x)}{\delta x}$$

computes the slope of the secant line through two points on the graph of f. In Figure these are the points with x-coordinates x_0 and $x_0 + \delta x$.

The difference quotient can also be considered the average slope of f between x and $x + \delta x$ if we assume f to be a linear function. In the limit for $\delta x \to 0$, we obtain the tangent of f at x, if f is differentiable. The tangent is then the derivative of f at x.

(Derivative). for $h > 0$ the *derivative* of f at x is defined as the limit

$$\frac{\mathrm{d}f}{\mathrm{d}x} := \lim_{h \to 0} \frac{f(x+h) - f(x)}{h},$$

and the secant in Figure becomes a tangent.

The derivative of f points in the direction of steepest ascent of f.

Differentiation Rules

In the following, we briefly state basic differentiation rules, where we denote the derivative of f by f'.

Product rule: $$(f(x)g(x))' = f'(x)g(x) + f(x)g'(x)$$

Quotient rule: $$\left(\frac{f(x)}{g(x)}\right)' = \frac{f'(x)g(x) - f(x)g'(x)}{(g(x))^2}$$

Sum rule: $$(f(x) + g(x))' = f'(x) + g'(x)$$

Chain rule: $$\big(g(f(x))\big)' = (g \circ f)'(x) = g'(f(x))f'(x)$$

Here, $g \circ f$ denotes function composition $x \mapsto f(x) \mapsto g(f(x))$.

Example (Chain Rule)

Let us compute the derivative of the function $h(x) = (2x+1)^4$ using the chain rule. With

$$h(x) = (2x+1)^4 = g(f(x))\,,$$
$$f(x) = 2x+1\,,$$
$$g(f) = f^4\,,$$

we obtain the derivatives of f and g as

$$f'(x) = 2\,,$$
$$g'(f) = 4f^3\,,$$

such that the derivative of h is given as

$$h'(x) = g'(f)f'(x) = (4f^3)\cdot 2 \;=\; 4(2x+1)^3\cdot 2 = 8(2x+1)^3\,,$$

where we used the chain rule and substituted the definition of f in $g'(f)$.

Taylor Series

The Taylor series is a representation of a function f as an infinite sum of terms. These terms are determined using derivatives of f evaluated at x_0.

(Taylor Polynomial). The *Taylor polynomial* of degree n of $f : \mathbb{R} \to \mathbb{R}$ at x_0 is defined as

$$T_n(x) := \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k \,, \tag{5.7}$$

where $f^{(k)}(x_0)$ is the kth derivative of f at x_0 (which we assume exists) and $\frac{f^{(k)}(x_0)}{k!}$ are the coefficients of the polynomial.

(Taylor Series). For a smooth function $f \in C^\infty$, $f : \mathbb{R} \to \mathbb{R}$, the *Taylor series* of f at x_0 is defined as

$$T_\infty(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k .$$

For $x_0 = 0$, we obtain the *Maclaurin series* as a special instance of the Taylor series. If $f(x) = T_\infty(x)$, then f is called *analytic*.

Remark. In general, a Taylor polynomial of degree n is an approximation of a function, which does not need to be a polynomial. The Taylor polynomial is similar to f in a neighborhood around x_0. However, a Taylor polynomial of degree n is an exact representation of a polynomial f of degree $k \leqslant n$ since all derivatives $f^{(i)}$, $i > k$ vanish.

Example (Taylor Polynomial)
We consider the polynomial

$$f(x) = x^4$$

and seek the Taylor polynomial T_6, evaluated at $x_0 = 1$. We start by computing the coefficients $f^{(k)}(1)$ for $k = 0, \ldots, 6$:

$$\begin{aligned} f(1) &= 1 \\ f'(1) &= 4 \\ f''(1) &= 12 \\ f^{(3)}(1) &= 24 \\ f^{(4)}(1) &= 24 \\ f^{(5)}(1) &= 0 \\ f^{(6)}(1) &= 0 \end{aligned}$$

Therefore, the desired Taylor polynomial is

$$\begin{aligned} T_6(x) &= \sum_{k=0}^{6} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k \\ &= 1 + 4(x-1) + 6(x-1)^2 + 4(x-1)^3 + (x-1)^4 + 0\,. \end{aligned}$$

Multiplying out and re-arranging yields

$$\begin{aligned} T_6(x) &= (1 - 4 + 6 - 4 + 1) + x(4 - 12 + 12 - 4) \\ &\quad + x^2(6 - 12 + 6) + x^3(4 - 4) + x^4 \\ &= x^4 = f(x)\,, \end{aligned}$$

i.e., we obtain an exact representation of the original function.

Example (Taylor Series)

Consider the function in Figure 5.4 given by

$$f(x) = \sin(x) + \cos(x) \in \mathcal{C}^\infty .$$

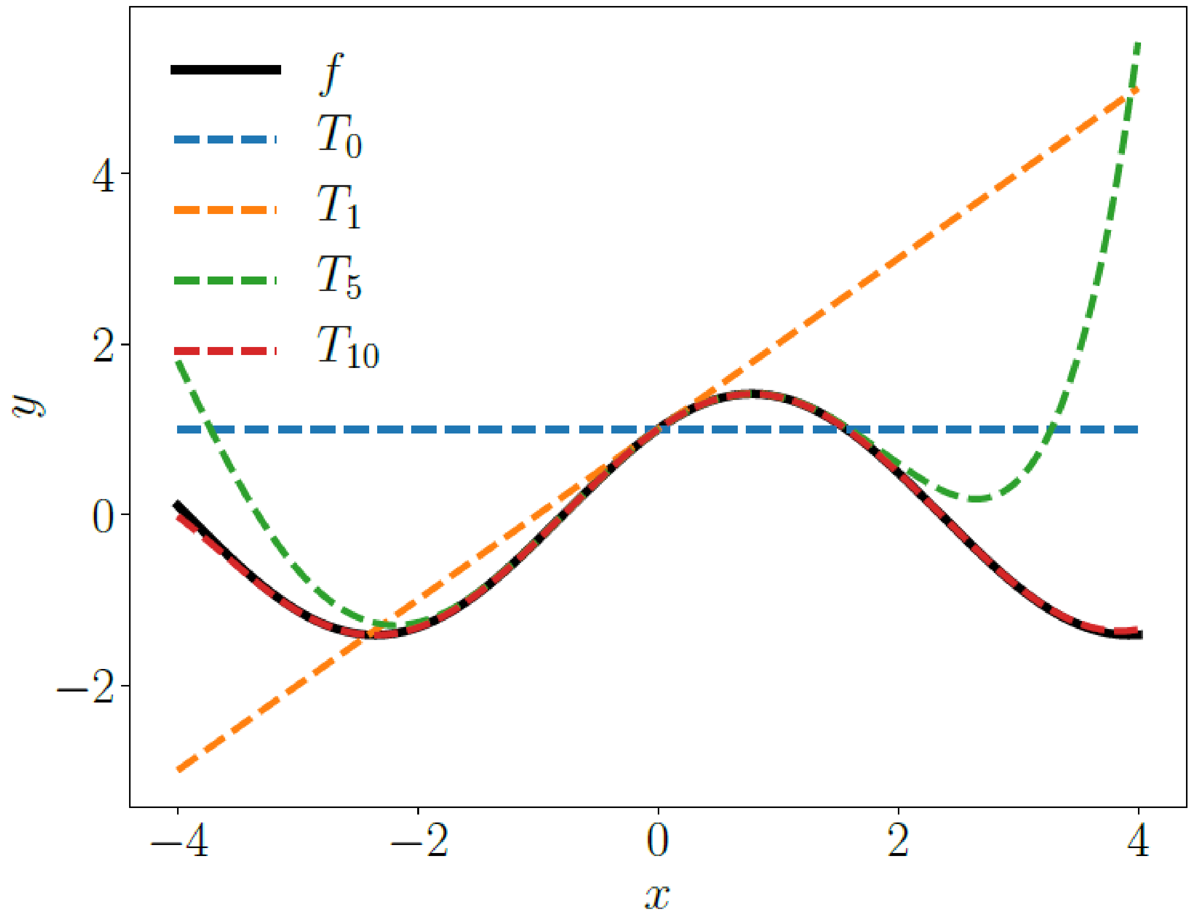
We seek a Taylor series expansion of f at $x_0 = 0$, which is the Maclaurin series expansion of f. We obtain the following derivatives:

$$\begin{aligned}
f(0) &= \sin(0) + \cos(0) = 1 \\
f'(0) &= \cos(0) - \sin(0) = 1 \\
f''(0) &= -\sin(0) - \cos(0) = -1 \\
f^{(3)}(0) &= -\cos(0) + \sin(0) = -1 \\
f^{(4)}(0) &= \sin(0) + \cos(0) = f(0) = 1 \\
&\vdots
\end{aligned}$$

We can see a pattern here: The coefficients in our Taylor series are only ± 1 (since $\sin(0) = 0$), each of which occurs twice before switching to the other one. Furthermore, $f^{(k+4)}(0) = f^{(k)}(0)$.

Therefore, the full Taylor series expansion of f at $x_0 = 0$ is given by

$$\begin{aligned}
T_\infty(x) &= \sum_{k=0}^{\infty} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k \\
&= 1 + x - \frac{1}{2!}x^2 - \frac{1}{3!}x^3 + \frac{1}{4!}x^4 + \frac{1}{5!}x^5 - \cdots \\
&= 1 - \frac{1}{2!}x^2 + \frac{1}{4!}x^4 \mp \cdots + x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 \mp \cdots \\
&= \sum_{k=0}^{\infty}(-1)^k \frac{1}{(2k)!}x^{2k} + \sum_{k=0}^{\infty}(-1)^k \frac{1}{(2k+1)!}x^{2k+1} \\
&= \cos(x) + \sin(x) ,
\end{aligned}$$



f
T_0
T_1
T_5
T_{10}
y
x
4
2
0
−2
−4

Multivariate functions

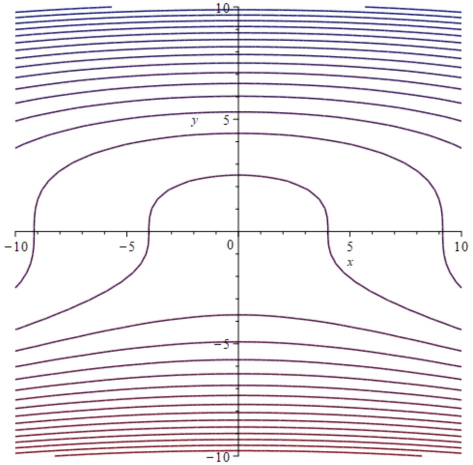
One writes, where D is an integer greater than one:

$$\begin{aligned} f : \mathbb{R}^D &\to \mathbb{R} \\ \boldsymbol{x} &\mapsto f(\boldsymbol{x}) \end{aligned}$$

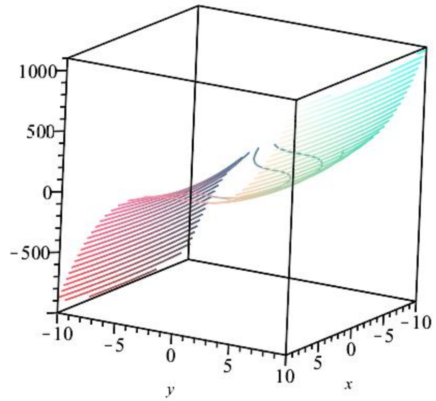
we will see some plots,

we will discuss how to compute gradients of functions,
which is often essential to facilitate learning in machine learning models
since the gradient points in the direction of steepest ascent.

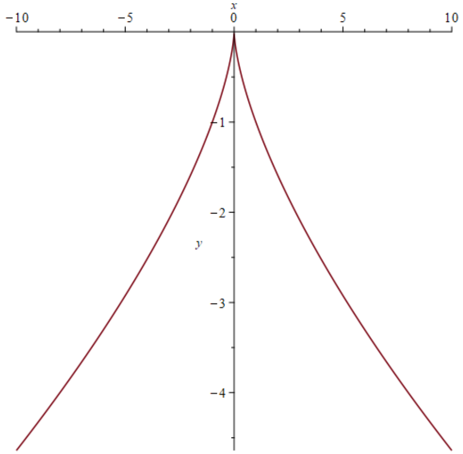
Example: $f(x, y) = x^2 + y^3$



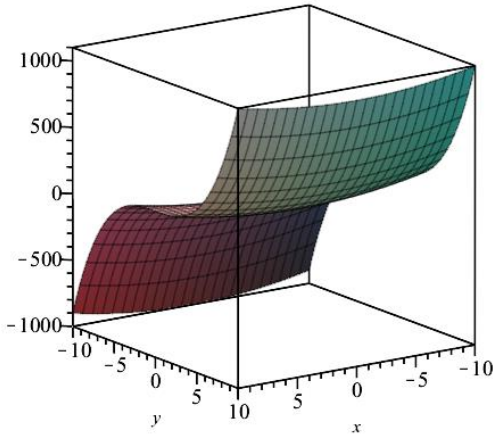
contourplot



contourplot3d



implicitplot



plot3d

Graphics. Graphs have the advantage of showing both the input space and the output space at once, but as a result, they are highly limited by dimension. For this reason, they are only really useful for single-variable functions and multi-variable functions with a two-dimensional input and a one-dimensional output.

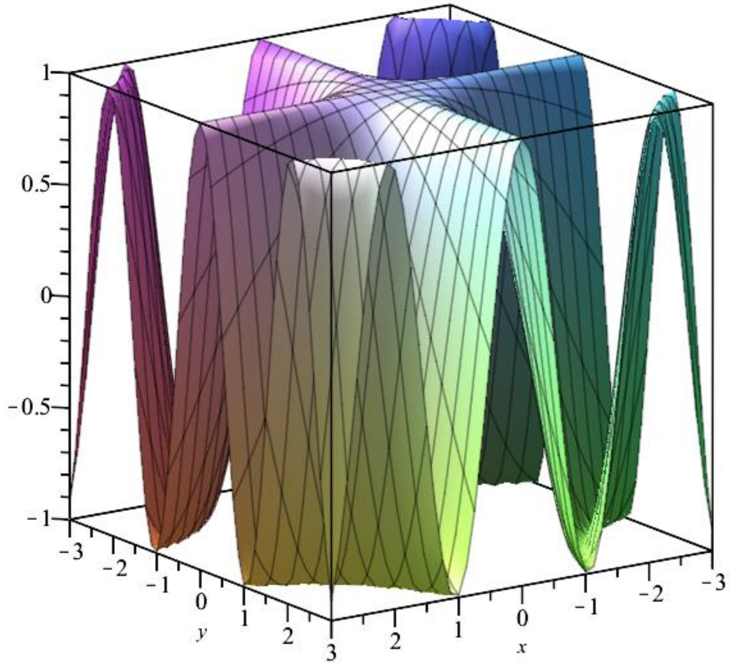
Contour maps. Contour maps show only the input space and are useful for functions with two-dimensional input and one-dimensional output.

Parameterized curves/surfaces. Parameterized curves and surfaces that show only the output space and are used for functions whose output space has more dimensions than the input space.

Vector fields. They apply to functions whose input and output spaces have the same number of dimensions. For example, functions with two-dimensional inputs and two-dimensional outputs, or three-dimensional inputs and three-dimensional outputs, can be used with vector fields.

Example: Three-dimensional plot

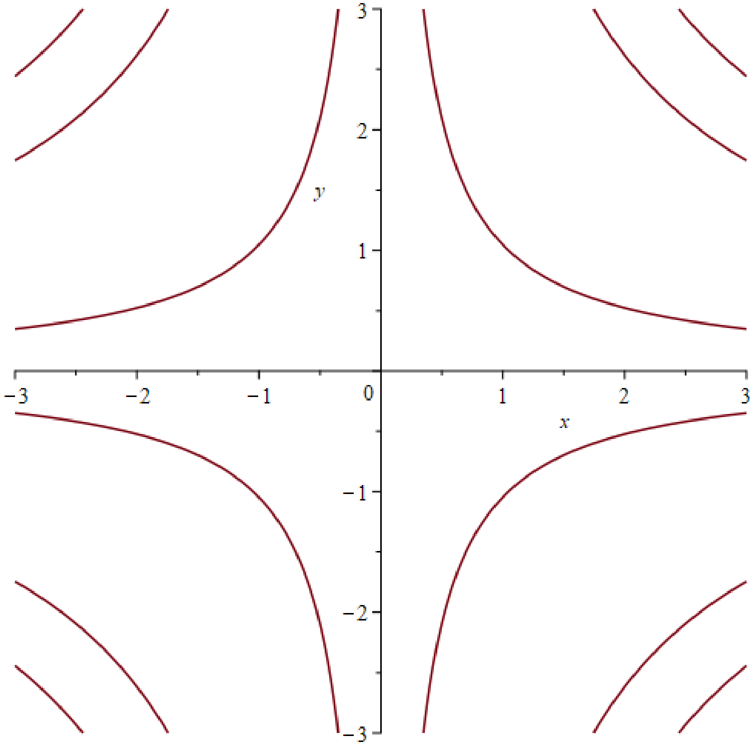
*f := (x, y) -> cos(y*x)*
plot3d(f(x,y),x=-3..3,y=-3..3)



Contour lines or level curves

A contour line of the function $z = f(x, y)$ is a two-dimensional curve with the equation $f(x, y) = k$, where k is a constant in the range of f. A contour line can be described as the intersection of the horizontal plane $z = k$ with the surface defined by f. Contour lines are also known as level curves.

with(plots)
contourplot(f(x,y), x = -3 .. 3, y = -3 .. 3)
implicitplot(f(x,y)=0.5, x = -3 .. 3, y = -3 .. 3)



Partial Differentiation and Gradients

The multivariable version of a derivative can mean something completely different for parametric functions, vector fields, or contour maps.

In the following, we consider the general case where the function f depends on one or more variables $\boldsymbol{x} \in \mathbb{R}^n$, e.g., $f(\boldsymbol{x}) = f(x_1, x_2)$. The generalization of the derivative to functions of several variables is the *gradient*.

We find the gradient of the function f with respect to $\boldsymbol{x}$ by *varying one variable at a time* and keeping the others constant. The gradient is then the collection of these *partial derivatives*.

Definition (Partial Derivative). For a function $f : \mathbb{R}^n \to \mathbb{R}$, $\boldsymbol{x} \mapsto f(\boldsymbol{x})$, $\boldsymbol{x} \in \mathbb{R}^n$ of n variables $x_1, \ldots, x_n$ we define the *partial derivatives* as

$$\frac{\partial f}{\partial x_1} = \lim_{h\to 0} \frac{f(x_1 + h, x_2, \ldots, x_n) - f(\boldsymbol{x})}{h}$$

$$\vdots$$

$$\frac{\partial f}{\partial x_n} = \lim_{h\to 0} \frac{f(x_1, \ldots, x_{n-1}, x_n + h) - f(\boldsymbol{x})}{h}$$

and collect them in the row vector

$$\nabla_{\boldsymbol{x}} f = \operatorname{grad} f = \frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \begin{bmatrix} \frac{\partial f(\boldsymbol{x})}{\partial x_1} & \frac{\partial f(\boldsymbol{x})}{\partial x_2} & \cdots & \frac{\partial f(\boldsymbol{x})}{\partial x_n} \end{bmatrix} \in \mathbb{R}^{1\times n},$$

where n is the number of variables and 1 is the dimension of the image/ range/codomain of f. Here, we defined the column vector $\boldsymbol{x} = [x_1, \ldots, x_n]^\top \in \mathbb{R}^n$. The row vector in is called the *gradient* of f or the *Jacobian* and is the generalization of the derivative

Example (Partial Derivatives Using the Chain Rule)

For $f(x,y) = (x+2y^3)^2$, we obtain the partial derivatives

$$\frac{\partial f(x,y)}{\partial x} = 2(x+2y^3)\frac{\partial}{\partial x}(x+2y^3) = 2(x+2y^3)\,,$$

$$\frac{\partial f(x,y)}{\partial y} = 2(x+2y^3)\frac{\partial}{\partial y}(x+2y^3) = 12(x+2y^3)y^2$$

Example (Gradient)

For $f(x_1, x_2) = x_1^2 x_2 + x_1 x_2^3 \in \mathbb{R}$, the partial derivatives (i.e., the derivatives of f with respect to x_1 and x_2) are

$$\frac{\partial f(x_1,x_2)}{\partial x_1} = 2x_1x_2 + x_2^3$$

$$\frac{\partial f(x_1,x_2)}{\partial x_2} = x_1^2 + 3x_1x_2^2$$

and the gradient is then

$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \begin{bmatrix}\frac{\partial f(x_1,x_2)}{\partial x_1} & \frac{\partial f(x_1,x_2)}{\partial x_2}\end{bmatrix} = \begin{bmatrix}2x_1x_2 + x_2^3 & x_1^2 + 3x_1x_2^2\end{bmatrix} \in \mathbb{R}^{1\times 2}\,.$$

Basic Rules of Partial Differentiation

In the multivariate case, where $\boldsymbol{x} \in \mathbb{R}^n$, the basic differentiation rules that we know still apply. However, when we compute derivatives with respect to vectors $\boldsymbol{x} \in \mathbb{R}^n$ we need to pay attention: Our gradients now involve vectors and matrices, and matrix multiplication is not commutative, i.e., the order matters.

Here are the general product rule, sum rule, and chain rule:

Product rule: $$\frac{\partial}{\partial \boldsymbol{x}}\big(f(\boldsymbol{x})g(\boldsymbol{x})\big) = \frac{\partial f}{\partial \boldsymbol{x}}g(\boldsymbol{x}) + f(\boldsymbol{x})\frac{\partial g}{\partial \boldsymbol{x}}$$

Sum rule: $$\frac{\partial}{\partial \boldsymbol{x}}\big(f(\boldsymbol{x}) + g(\boldsymbol{x})\big) = \frac{\partial f}{\partial \boldsymbol{x}} + \frac{\partial g}{\partial \boldsymbol{x}}$$

Chain rule: $$\frac{\partial}{\partial \boldsymbol{x}}(g \circ f)(\boldsymbol{x}) = \frac{\partial}{\partial \boldsymbol{x}}\big(g(f(\boldsymbol{x}))\big) = \frac{\partial g}{\partial f}\frac{\partial f}{\partial \boldsymbol{x}}$$

Chain Rule

Consider a function $f : \mathbb{R}^2 \to \mathbb{R}$ of two variables x_1, x_2. Furthermore, $x_1(t)$ and $x_2(t)$ are themselves functions of t. To compute the gradient of f with respect to t, we need to apply the chain rule for multivariate functions as

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1(t)}{\partial t} \\ \frac{\partial x_2(t)}{\partial t} \end{bmatrix} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t},$$

where d denotes the gradient and ∂ partial derivatives.

If $f(x_1, x_2)$ is a function of x_1 and x_2, where $x_1(s,t)$ and $x_2(s,t)$ are themselves functions of two variables s and t, the chain rule yields the partial derivatives

$$\frac{\partial f}{\partial s} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial s} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial s},$$
$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t},$$

Example

Consider $f(x_1, x_2) = x_1^2 + 2x_2$, where $x_1 = \sin t$ and $x_2 = \cos t$, then

$$\begin{aligned}
\frac{\mathrm{d}f}{\mathrm{d}t} &= \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t} \\
&= 2\sin t \frac{\partial \sin t}{\partial t} + 2\frac{\partial \cos t}{\partial t} \\
&= 2\sin t \cos t - 2\sin t = 2\sin t(\cos t - 1)
\end{aligned}$$

is the corresponding derivative of f with respect to t.

Gradients of Vector-Valued Functions

Thus far, we discussed partial derivatives and gradients of functions $f : \mathbb{R}^n \to \mathbb{R}$ mapping to the real numbers. In the following, we will generalize the concept of the gradient to vector-valued functions (vector fields) $\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^m$, where $n \geqslant 1$ and $m > 1$.

For a function $\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^m$ and a vector $\boldsymbol{x} = [x_1, \ldots, x_n]^\top \in \mathbb{R}^n$, the corresponding vector of function values is given as

$$\boldsymbol{f}(\boldsymbol{x}) = \begin{bmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_m(\boldsymbol{x}) \end{bmatrix} \in \mathbb{R}^m .$$

Writing the vector-valued function in this way allows us to view a vector-valued function $\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^m$ as a vector of functions $[f_1, \ldots, f_m]^\top$, $f_i : \mathbb{R}^n \to \mathbb{R}$ that map onto $\mathbb{R}$. The differentiation rules for every f_i are exactly the ones we discussed we know that the gradient of $\boldsymbol{f}$ with respect to a vector is the row vector of the partial derivatives, every partial derivative $\partial \boldsymbol{f} / \partial x_i$ is itself a column vector. Therefore, we obtain the gradient of $\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^m$ with respect to $\boldsymbol{x} \in \mathbb{R}^n$ by collecting these partial derivatives:

$$
\begin{aligned}
\frac{\mathrm{d}\boldsymbol{f}(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}} &= \left[\boxed{\frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_1}} \cdots \boxed{\frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_n}} \right] \\
&= \left[\boxed{\begin{matrix} \dfrac{\partial f_1(\boldsymbol{x})}{\partial x_1} \\ \vdots \\ \dfrac{\partial f_m(\boldsymbol{x})}{\partial x_1} \end{matrix}} \begin{matrix} \cdots \\ \\ \cdots \end{matrix} \boxed{\begin{matrix} \dfrac{\partial f_1(\boldsymbol{x})}{\partial x_n} \\ \vdots \\ \dfrac{\partial f_m(\boldsymbol{x})}{\partial x_n} \end{matrix}} \right] \in \mathbb{R}^{m \times n} .
\end{aligned}
$$

Definition (Jacobian). The collection of all first-order partial derivatives of a vector-valued function $\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^m$ is called the *Jacobian*. The Jacobian $\boldsymbol{J}$ is an $m \times n$ matrix, which we define and arrange as follows:

$$\boldsymbol{J} = \nabla_{\boldsymbol{x}} \boldsymbol{f} = \frac{\mathrm{d}\boldsymbol{f}(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}} = \begin{bmatrix} \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_n} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial f_1(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial f_1(\boldsymbol{x})}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_m(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial f_m(\boldsymbol{x})}{\partial x_n} \end{bmatrix},$$

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \quad J(i,j) = \frac{\partial f_i}{\partial x_j}.$$

Higher-Order Derivatives

we have discussed gradients, i.e., first-order derivatives. Sometimes, we are interested in derivatives of higher order, e.g., when we want to use Newton's Method for optimization, which requires second-order derivatives

we discussed the Taylor series to approximate functions using polynomials. In the multivariate case, we can do exactly the same.

- $\frac{\partial^2 f}{\partial x^2}$ is the second partial derivative of f with respect to x.
- $\frac{\partial^n f}{\partial x^n}$ is the nth partial derivative of f with respect to x.
- $\frac{\partial^2 f}{\partial y \partial x} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right)$ is the partial derivative obtained by first partial differentiating with respect to x and then with respect to y.
- $\frac{\partial^2 f}{\partial x \partial y}$ is the partial derivative obtained by first partial differentiating by y and then x.

The *Hessian* is the collection of all second-order partial derivatives.

If $f(x, y)$ is a twice (continuously) differentiable function, then

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x},$$

i.e., the order of differentiation does not matter, and the corresponding *Hessian matrix*

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix}$$

is symmetric. The Hessian is denoted as $\nabla^2_{x,y} f(x, y)$. Generally, for $\boldsymbol{x} \in \mathbb{R}^n$ and $f : \mathbb{R}^n \to \mathbb{R}$, the Hessian is an $n \times n$ matrix. The Hessian measures the curvature of the function locally around (x, y).

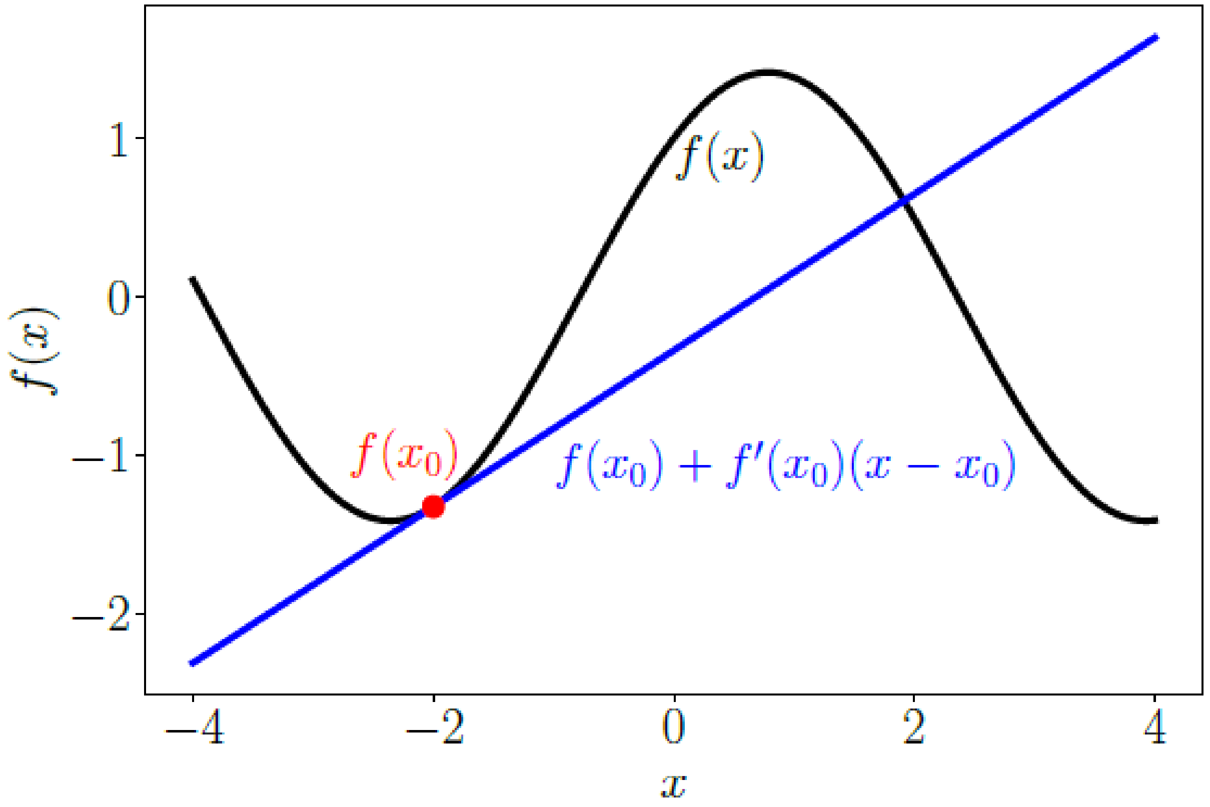
Remark (Hessian of a Vector Field). If $f : \mathbb{R}^n \to \mathbb{R}^m$ is a vector field, the Hessian is an $(m \times n \times n)$-tensor.

Linearization and Multivariate Taylor Series

The gradient ∇f of a function f is often used for a locally linear approximation of f around $\boldsymbol{x}_0$:

$$f(\boldsymbol{x}) \approx f(\boldsymbol{x}_0) + (\nabla_{\boldsymbol{x}} f)(\boldsymbol{x}_0)(\boldsymbol{x} - \boldsymbol{x}_0)\,.$$

Here $(\nabla_{\boldsymbol{x}} f)(\boldsymbol{x}_0)$ is the gradient of f with respect to $\boldsymbol{x}$, evaluated at $\boldsymbol{x}_0$. Figure illustrates the linear approximation of a function f at an input x_0. The original function is approximated by a straight line. This approximation is locally accurate, but the farther we move away from x_0 the worse the approximation gets. Equation is a special case of a multivariate Taylor series expansion of f at $\boldsymbol{x}_0$, where we consider only the first two terms. We discuss the more general case in the following, which will allow for better approximations.



Linear approximation of a function. The original function f is linearized at $x_0 = -2$ using a first-order Taylor series expansion.

Definition (Multivariate Taylor Series). We consider a function

$$\begin{aligned} f : \mathbb{R}^D &\to \mathbb{R} \\ \boldsymbol{x} &\mapsto f(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^D, \end{aligned}$$

that is smooth at $\boldsymbol{x}_0$. When we define the difference vector $\boldsymbol{\delta} := \boldsymbol{x} - \boldsymbol{x}_0$, the *multivariate Taylor series* of f at $(\boldsymbol{x}_0)$ is defined as

$$f(\boldsymbol{x}) = \sum_{k=0}^{\infty} \frac{D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)}{k!} \boldsymbol{\delta}^k,$$

where $D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)$ is the k-th (total) derivative of f with respect to $\boldsymbol{x}$, evaluated at $\boldsymbol{x}_0$.

Definition (Taylor Polynomial). The *Taylor polynomial* of degree n of f at $\boldsymbol{x}_0$ contains the first $n+1$ components of the series

$$T_n(\boldsymbol{x}) = \sum_{k=0}^{n} \frac{D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)}{k!} \boldsymbol{\delta}^k.$$

Example (Taylor Series Expansion of a Function with Two Variables)

Consider the function

$$f(x, y) = x^2 + 2xy + y^3 \,.$$

We want to compute the Taylor series expansion of f at $(x_0, y_0) = (1, 2)$. Before we start, let us discuss what to expect: The function is a polynomial of degree 3. We are looking for a Taylor series expansion, which itself is a linear combination of polynomials. Therefore, we do not expect the Taylor series expansion to contain terms of fourth or higher order to express a third-order polynomial. This means that it should be sufficient to determine the first four terms for an exact alternative representation

To determine the Taylor series expansion, we start with the constant term and the first-order derivatives, which are given by

$$f(1, 2) = 13$$

$$\frac{\partial f}{\partial x} = 2x + 2y \implies \frac{\partial f}{\partial x}(1,2) = 6$$
$$\frac{\partial f}{\partial y} = 2x + 3y^2 \implies \frac{\partial f}{\partial y}(1,2) = 14\,.$$

Therefore, we obtain

$$D^1_{x,y} f(1,2) = \nabla_{x,y} f(1,2) = \begin{bmatrix} \frac{\partial f}{\partial x}(1,2) & \frac{\partial f}{\partial y}(1,2) \end{bmatrix} = \begin{bmatrix} 6 & 14 \end{bmatrix} \in \mathbb{R}^{1\times 2}$$

such that

$$\frac{D^1_{x,y} f(1,2)}{1!}\boldsymbol{\delta} = \begin{bmatrix} 6 & 14 \end{bmatrix} \begin{bmatrix} x-1 \\ y-2 \end{bmatrix} = 6(x-1) + 14(y-2)\,.$$

Note that $D^1_{x,y} f(1,2)\boldsymbol{\delta}$ contains only linear terms, i.e., first-order polynomials.

The second-order partial derivatives are given by

$$\frac{\partial^2 f}{\partial x^2} = 2 \implies \frac{\partial^2 f}{\partial x^2}(1,2) = 2$$
$$\frac{\partial^2 f}{\partial y^2} = 6y \implies \frac{\partial^2 f}{\partial y^2}(1,2) = 12$$
$$\frac{\partial^2 f}{\partial y \partial x} = 2 \implies \frac{\partial^2 f}{\partial y \partial x}(1,2) = 2$$
$$\frac{\partial^2 f}{\partial x \partial y} = 2 \implies \frac{\partial^2 f}{\partial x \partial y}(1,2) = 2\,.$$

When we collect the second-order partial derivatives, we obtain the Hessian

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 6y \end{bmatrix},$$

such that

$$\boldsymbol{H}(1,2) = \begin{bmatrix} 2 & 2 \\ 2 & 12 \end{bmatrix} \in \mathbb{R}^{2\times 2}.$$

Therefore, the next term of the Taylor-series expansion is given by

$$\begin{aligned} \frac{D^2_{x,y} f(1,2)}{2!} \boldsymbol{\delta}^2 &= \frac{1}{2} \boldsymbol{\delta}^\top \boldsymbol{H}(1,2) \boldsymbol{\delta} \\ &= \frac{1}{2} \begin{bmatrix} x-1 & y-2 \end{bmatrix} \begin{bmatrix} 2 & 2 \\ 2 & 12 \end{bmatrix} \begin{bmatrix} x-1 \\ y-2 \end{bmatrix} \\ &= (x-1)^2 + 2(x-1)(y-2) + 6(y-2)^2 . \end{aligned}$$

Here, $D^2_{x,y} f(1,2)\boldsymbol{\delta}^2$ contains only quadratic terms, i.e., second-order polynomials.

The third-order derivatives are obtained as

$$D^3_{x,y}f = \begin{bmatrix} \frac{\partial \boldsymbol{H}}{\partial x} & \frac{\partial \boldsymbol{H}}{\partial y} \end{bmatrix} \in \mathbb{R}^{2\times 2\times 2}\,,$$

$$D^3_{x,y}f[:,:,1] = \frac{\partial \boldsymbol{H}}{\partial x} = \begin{bmatrix} \frac{\partial^3 f}{\partial x^3} & \frac{\partial^3 f}{\partial x^2 \partial y} \\ \frac{\partial^3 f}{\partial x \partial y \partial x} & \frac{\partial^3 f}{\partial x \partial y^2} \end{bmatrix}\,,$$

$$D^3_{x,y}f[:,:,2] = \frac{\partial \boldsymbol{H}}{\partial y} = \begin{bmatrix} \frac{\partial^3 f}{\partial y \partial x^2} & \frac{\partial^3 f}{\partial y \partial x \partial y} \\ \frac{\partial^3 f}{\partial y^2 \partial x} & \frac{\partial^3 f}{\partial y^3} \end{bmatrix}\,.$$

Since most second-order partial derivatives in the Hessian are constant, the only nonzero third-order partial derivative is

$$\frac{\partial^3 f}{\partial y^3} = 6 \implies \frac{\partial^3 f}{\partial y^3}(1,2) = 6\,.$$

Higher-order derivatives and the mixed derivatives of degree 3 (e.g., $\frac{\partial f^3}{\partial x^2 \partial y}$) vanish, such that

$$D^3_{x,y}f[:,:,1] = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}\,, \quad D^3_{x,y}f[:,:,2] = \begin{bmatrix} 0 & 0 \\ 0 & 6 \end{bmatrix}$$

and

$$\frac{D^3_{x,y}f(1,2)}{3!}\boldsymbol{\delta}^3 = (y-2)^3\,,$$

which collects all cubic terms of the Taylor series. Overall, the (exact) Taylor series expansion of f at $(x_0, y_0) = (1, 2)$ is

$$f(x) = f(1,2) + D^1_{x,y} f(1,2)\boldsymbol{\delta} + \frac{D^2_{x,y} f(1,2)}{2!}\boldsymbol{\delta}^2 + \frac{D^3_{x,y} f(1,2)}{3!}\boldsymbol{\delta}^3$$

$$\begin{aligned}
&= f(1,2) + \frac{\partial f(1,2)}{\partial x}(x-1) + \frac{\partial f(1,2)}{\partial y}(y-2) \\
&\quad + \frac{1}{2!}\left(\frac{\partial^2 f(1,2)}{\partial x^2}(x-1)^2 + \frac{\partial^2 f(1,2)}{\partial y^2}(y-2)^2 \right. \\
&\quad \left. + 2\frac{\partial^2 f(1,2)}{\partial x \partial y}(x-1)(y-2)\right) + \frac{1}{6}\frac{\partial^3 f(1,2)}{\partial y^3}(y-2)^3 \\
&= 13 + 6(x-1) + 14(y-2) \\
&\quad + (x-1)^2 + 6(y-2)^2 + 2(x-1)(y-2) + (y-2)^3 .
\end{aligned}$$

the polynomial is identical to the original polynomial. In this particular example, this result is not sur-
prising since the original function was a third-order polynomial, which we expressed through a linear combination of constant terms, first-order, second-order, and third-order polynomials