where the $g_i(\cdot)$ are elementary functions and $x_{\mathrm{Pa}(x_i)}$ are the parent nodes of the variable x_i in the graph. Given a function defined in this way, we can use the chain rule to compute the derivative of the function in a step-by-step fashion. Recall that by definition $f = x_D$ and hence

$$\frac{\partial f}{\partial x_D} = 1\,. \tag{5.144}$$

For other variables x_i, we apply the chain rule

$$\frac{\partial f}{\partial x_i} = \sum_{x_j : x_i \in \mathrm{Pa}(x_j)} \frac{\partial f}{\partial x_j}\frac{\partial x_j}{\partial x_i} = \sum_{x_j : x_i \in \mathrm{Pa}(x_j)} \frac{\partial f}{\partial x_j}\frac{\partial g_j}{\partial x_i}\,, \tag{5.145}$$

where $\mathrm{Pa}(x_j)$ is the set of parent nodes of x_j in the computation graph. Equation (5.143) is the forward propagation of a function, whereas (5.145) is the backpropagation of the gradient through the computation graph. For neural network training, we backpropagate the error of the prediction with respect to the label.

Auto-differentiation in reverse mode requires a parse tree.

The automatic differentiation approach above works whenever we have a function that can be expressed as a computation graph, where the elementary functions are differentiable. In fact, the function may not even be a mathematical function but a computer program. However, not all computer programs can be automatically differentiated, e.g., if we cannot find differential elementary functions. Programming structures, such as `for` loops and `if` statements, require more care as well.

5.7 Higher-Order Derivatives

So far, 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 (Nocedal and Wright, 2006). In Section 5.1.1, we discussed the Taylor series to approximate functions using polynomials. In the multivariate case, we can do exactly the same. In the following, we will do exactly this. But let us start with some notation.

Consider a function $f : \mathbb{R}^2 \to \mathbb{R}$ of two variables x, y. We use the following notation for higher-order partial derivatives (and for gradients):

- $\frac{\partial^2 f}{\partial x^2}$ 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.

Hessian

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

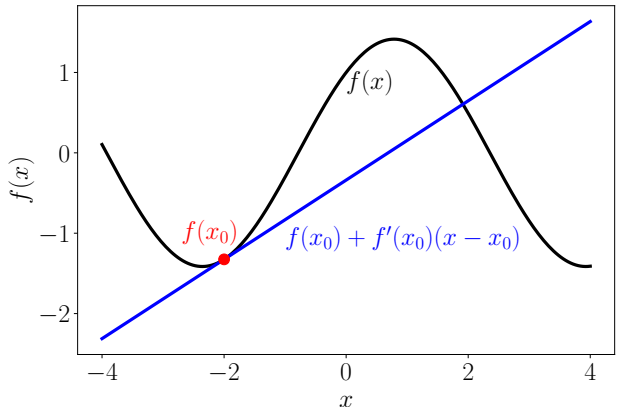


Figure 5.12 Linear approximation of a function. The original function f is linearized at $x_0 = -2$ using a first-order Taylor series expansion.

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

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x}, \tag{5.146}$$

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

Hessian matrix

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} \tag{5.147}$$

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).

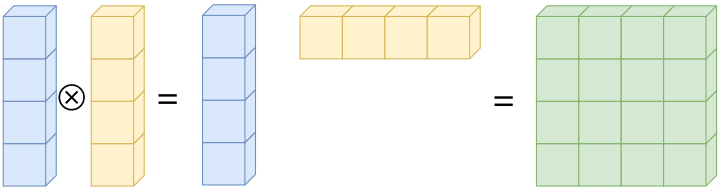
Remark (Hessian of a Vector Field). If $f : \mathbb{R}^n \to \mathbb{R}^m$ is a vector field, the Hessian is an $(m \times n \times n)$-tensor. ♢

5.8 Linearization and Multivariate Taylor Series

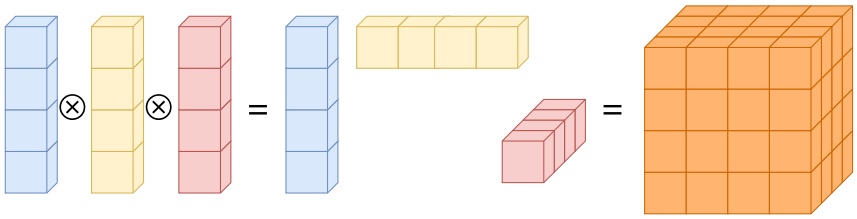
The gradient ∇f of a function f is often used for a locally linear approximation of f around $\boldsymbol{x}_0$:

$$f(\boldsymbol{x}) \approx f(\boldsymbol{x}_0) + (\nabla_{\boldsymbol{x}} f)(\boldsymbol{x}_0)(\boldsymbol{x} - \boldsymbol{x}_0). \tag{5.148}$$

Here $(\nabla_{\boldsymbol{x}} f)(\boldsymbol{x}_0)$ is the gradient of f with respect to $\boldsymbol{x}$, evaluated at $\boldsymbol{x}_0$. Figure 5.12 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 (5.148) 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.



(a) Given a vector $\boldsymbol{\delta} \in \mathbb{R}^4$, we obtain the outer product $\boldsymbol{\delta}^2 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} = \boldsymbol{\delta}\boldsymbol{\delta}^\top \in \mathbb{R}^{4\times 4}$ as a matrix.



(b) An outer product $\boldsymbol{\delta}^3 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} \otimes \boldsymbol{\delta} \in \mathbb{R}^{4\times 4\times 4}$ results in a third-order tensor ("three-dimensional matrix"), i.e., an array with three indexes.

Figure 5.13 Visualizing outer products. Outer products of vectors increase the dimensionality of the array by 1 per term. (a) The outer product of two vectors results in a matrix; (b) the outer product of three vectors yields a third-order tensor.

Definition 5.7 (Multivariate Taylor Series)**.** We consider a function

$$f : \mathbb{R}^D \to \mathbb{R} \tag{5.149}$$

$$\boldsymbol{x} \mapsto f(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^D, \tag{5.150}$$

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

multivariate Taylor series

$$f(\boldsymbol{x}) = \sum_{k=0}^{\infty} \frac{D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)}{k!} \boldsymbol{\delta}^k, \tag{5.151}$$

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

Taylor polynomial

Definition 5.8 (Taylor Polynomial)**.** The *Taylor polynomial* of degree n of f at $\boldsymbol{x}_0$ contains the first $n+1$ components of the series in (5.151) and is defined as

$$T_n(\boldsymbol{x}) = \sum_{k=0}^{n} \frac{D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)}{k!} \boldsymbol{\delta}^k. \tag{5.152}$$

In (5.151) and (5.152), we used the slightly sloppy notation of $\boldsymbol{\delta}^k$, which is not defined for vectors $\boldsymbol{x} \in \mathbb{R}^D$, $D > 1$, and $k > 1$. Note that both $D_{\boldsymbol{x}}^k f$ and $\boldsymbol{\delta}^k$ are k-th order tensors, i.e., k-dimensional arrays. The kth-order tensor $\boldsymbol{\delta}^k \in \mathbb{R}^{\overbrace{D\times D\times \ldots \times D}^{k \text{ times}}}$ is obtained as a k-fold outer product, denoted by $\otimes$, of the vector $\boldsymbol{\delta} \in \mathbb{R}^D$. For example,

A vector can be implemented as a one-dimensional array, a matrix as a two-dimensional array.

$$\boldsymbol{\delta}^2 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} = \boldsymbol{\delta}\boldsymbol{\delta}^\top, \quad \boldsymbol{\delta}^2[i,j] = \delta[i]\delta[j] \tag{5.153}$$

$$\boldsymbol{\delta}^3 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} \otimes \boldsymbol{\delta}\,, \quad \boldsymbol{\delta}^3[i,j,k] = \delta[i]\delta[j]\delta[k]\,. \tag{5.154}$$

Figure 5.13 visualizes two such outer products. In general, we obtain the terms

$$D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)\boldsymbol{\delta}^k = \sum_{i_1=1}^{D} \cdots \sum_{i_k=1}^{D} D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)[i_1,\ldots,i_k]\delta[i_1]\cdots\delta[i_k] \tag{5.155}$$

in the Taylor series, where $D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)\boldsymbol{\delta}^k$ contains k-th order polynomials.

Now that we defined the Taylor series for vector fields, let us explicitly write down the first terms $D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)\boldsymbol{\delta}^k$ of the Taylor series expansion for $k = 0,\ldots,3$ and $\boldsymbol{\delta} := \boldsymbol{x} - \boldsymbol{x}_0$:

$$k = 0 : D_{\boldsymbol{x}}^0 f(\boldsymbol{x}_0)\boldsymbol{\delta}^0 = f(\boldsymbol{x}_0) \in \mathbb{R} \tag{5.156}$$

```
np.einsum(
'i,i',Df1,d)
```

$$k = 1 : D_{\boldsymbol{x}}^1 f(\boldsymbol{x}_0)\boldsymbol{\delta}^1 = \underbrace{\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_0)}_{1\times D}\underbrace{\boldsymbol{\delta}}_{D\times 1} = \sum_{i=1}^{D} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_0)[i]\delta[i] \in \mathbb{R} \tag{5.157}$$

```
np.einsum(
'ij,i,j',
Df2,d,d)
```

$$k = 2 : D_{\boldsymbol{x}}^2 f(\boldsymbol{x}_0)\boldsymbol{\delta}^2 = \mathrm{tr}\big(\underbrace{\boldsymbol{H}(\boldsymbol{x}_0)}_{D\times D}\underbrace{\boldsymbol{\delta}}_{D\times 1}\underbrace{\boldsymbol{\delta}^\top}_{1\times D}\big) = \boldsymbol{\delta}^\top \boldsymbol{H}(\boldsymbol{x}_0)\boldsymbol{\delta} \tag{5.158}$$

```
np.einsum(
'ijk,i,j,k',
Df3,d,d,d)
```

$$= \sum_{i=1}^{D}\sum_{j=1}^{D} H[i,j]\delta[i]\delta[j] \in \mathbb{R} \tag{5.159}$$

$$k = 3 : D_{\boldsymbol{x}}^3 f(\boldsymbol{x}_0)\boldsymbol{\delta}^3 = \sum_{i=1}^{D}\sum_{j=1}^{D}\sum_{k=1}^{D} D_x^3 f(\boldsymbol{x}_0)[i,j,k]\delta[i]\delta[j]\delta[k] \in \mathbb{R} \tag{5.160}$$

Here, $\boldsymbol{H}(\boldsymbol{x}_0)$ is the Hessian of f evaluated at $\boldsymbol{x}_0$.

Example 5.15 (Taylor Series Expansion of a Function with Two Variables)
Consider the function

$$f(x,y) = x^2 + 2xy + y^3\,. \tag{5.161}$$

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 in (5.161) 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 of (5.151) for an exact alternative representation of (5.161).

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

$$f(1,2) = 13 \tag{5.162}$$

$$\frac{\partial f}{\partial x} = 2x + 2y \implies \frac{\partial f}{\partial x}(1,2) = 6 \tag{5.163}$$
$$\frac{\partial f}{\partial y} = 2x + 3y^2 \implies \frac{\partial f}{\partial y}(1,2) = 14\,. \tag{5.164}$$

Therefore, we obtain

$$D^1_{x,y} f(1,2) = \nabla_{x,y} f(1,2) = \begin{bmatrix} \frac{\partial f}{\partial x}(1,2) & \frac{\partial f}{\partial y}(1,2) \end{bmatrix} = \begin{bmatrix} 6 & 14 \end{bmatrix} \in \mathbb{R}^{1\times 2} \tag{5.165}$$

such that

$$\frac{D^1_{x,y} f(1,2)}{1!}\boldsymbol{\delta} = \begin{bmatrix} 6 & 14 \end{bmatrix} \begin{bmatrix} x-1 \\ y-2 \end{bmatrix} = 6(x-1) + 14(y-2)\,. \tag{5.166}$$

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

$$\frac{\partial^2 f}{\partial x^2} = 2 \implies \frac{\partial^2 f}{\partial x^2}(1,2) = 2 \tag{5.167}$$
$$\frac{\partial^2 f}{\partial y^2} = 6y \implies \frac{\partial^2 f}{\partial y^2}(1,2) = 12 \tag{5.168}$$
$$\frac{\partial^2 f}{\partial y \partial x} = 2 \implies \frac{\partial^2 f}{\partial y \partial x}(1,2) = 2 \tag{5.169}$$
$$\frac{\partial^2 f}{\partial x \partial y} = 2 \implies \frac{\partial^2 f}{\partial x \partial y}(1,2) = 2\,. \tag{5.170}$$

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

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 6y \end{bmatrix}, \tag{5.171}$$

such that

$$\boldsymbol{H}(1,2) = \begin{bmatrix} 2 & 2 \\ 2 & 12 \end{bmatrix} \in \mathbb{R}^{2\times 2}\,. \tag{5.172}$$

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

$$\frac{D^2_{x,y} f(1,2)}{2!}\boldsymbol{\delta}^2 = \frac{1}{2}\boldsymbol{\delta}^\top \boldsymbol{H}(1,2)\boldsymbol{\delta} \tag{5.173a}$$
$$= \frac{1}{2}\begin{bmatrix} x-1 & y-2 \end{bmatrix} \begin{bmatrix} 2 & 2 \\ 2 & 12 \end{bmatrix} \begin{bmatrix} x-1 \\ y-2 \end{bmatrix} \tag{5.173b}$$
$$= (x-1)^2 + 2(x-1)(y-2) + 6(y-2)^2\,. \tag{5.173c}$$

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

$$D^3_{x,y} f = \begin{bmatrix} \frac{\partial \boldsymbol{H}}{\partial x} & \frac{\partial \boldsymbol{H}}{\partial y} \end{bmatrix} \in \mathbb{R}^{2\times 2\times 2}\,, \tag{5.174}$$

$$D^3_{x,y} f[:,:,1] = \frac{\partial \boldsymbol{H}}{\partial x} = \begin{bmatrix} \frac{\partial^3 f}{\partial x^3} & \frac{\partial^3 f}{\partial x^2 \partial y} \\ \frac{\partial^3 f}{\partial x \partial y \partial x} & \frac{\partial^3 f}{\partial x \partial y^2} \end{bmatrix}\,, \tag{5.175}$$

$$D^3_{x,y} f[:,:,2] = \frac{\partial \boldsymbol{H}}{\partial y} = \begin{bmatrix} \frac{\partial^3 f}{\partial y \partial x^2} & \frac{\partial^3 f}{\partial y \partial x \partial y} \\ \frac{\partial^3 f}{\partial y^2 \partial x} & \frac{\partial^3 f}{\partial y^3} \end{bmatrix}\,. \tag{5.176}$$

Since most second-order partial derivatives in the Hessian in (5.171) are constant, the only nonzero third-order partial derivative is

$$\frac{\partial^3 f}{\partial y^3} = 6 \implies \frac{\partial^3 f}{\partial y^3}(1,2) = 6\,. \tag{5.177}$$

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

$$D^3_{x,y} f[:,:,1] = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}\,, \quad D^3_{x,y} f[:,:,2] = \begin{bmatrix} 0 & 0 \\ 0 & 6 \end{bmatrix} \tag{5.178}$$

and

$$\frac{D^3_{x,y} f(1,2)}{3!}\boldsymbol{\delta}^3 = (y-2)^3\,, \tag{5.179}$$

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

$$f(x) = f(1,2) + D^1_{x,y} f(1,2)\boldsymbol{\delta} + \frac{D^2_{x,y} f(1,2)}{2!}\boldsymbol{\delta}^2 + \frac{D^3_{x,y} f(1,2)}{3!}\boldsymbol{\delta}^3 \tag{5.180a}$$

$$\begin{aligned} &= f(1,2) + \frac{\partial f(1,2)}{\partial x}(x-1) + \frac{\partial f(1,2)}{\partial y}(y-2) \\ &\quad + \frac{1}{2!}\left(\frac{\partial^2 f(1,2)}{\partial x^2}(x-1)^2 + \frac{\partial^2 f(1,2)}{\partial y^2}(y-2)^2\right. \\ &\quad \left. + 2\frac{\partial^2 f(1,2)}{\partial x \partial y}(x-1)(y-2)\right) + \frac{1}{6}\frac{\partial^3 f(1,2)}{\partial y^3}(y-2)^3 \end{aligned} \tag{5.180b}$$

$$\begin{aligned} &= 13 + 6(x-1) + 14(y-2) \\ &\quad + (x-1)^2 + 6(y-2)^2 + 2(x-1)(y-2) + (y-2)^3\,. \end{aligned} \tag{5.180c}$$

In this case, we obtained an exact Taylor series expansion of the polynomial in (5.161), i.e., the polynomial in (5.180c) is identical to the original polynomial in (5.161). In this particular example, this result is not surprising 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 in (5.180c).