and the gradient is obtained by the matrix multiplication

$$\frac{\mathrm{d}f}{\mathrm{d}(s,t)} = \frac{\partial f}{\partial \boldsymbol{x}}\frac{\partial \boldsymbol{x}}{\partial(s,t)} = \underbrace{\begin{bmatrix}\frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2}\end{bmatrix}}_{=\frac{\partial f}{\partial \boldsymbol{x}}} \underbrace{\begin{bmatrix} \frac{\partial x_1}{\partial s} & \frac{\partial x_1}{\partial t}\\ \frac{\partial x_2}{\partial s} & \frac{\partial x_2}{\partial t}\end{bmatrix}}_{=\frac{\partial \boldsymbol{x}}{\partial(s,t)}} . \tag{5.53}$$

This compact way of writing the chain rule as a matrix multiplication only makes sense if the gradient is defined as a row vector. Otherwise, we will need to start transposing gradients for the matrix dimensions to match. This may still be straightforward as long as the gradient is a vector or a matrix; however, when the gradient becomes a tensor (we will discuss this in the following), the transpose is no longer a triviality.

The chain rule can be written as a matrix multiplication.

Remark (Verifying the Correctness of a Gradient Implementation). The definition of the partial derivatives as the limit of the corresponding difference quotient (see (5.39)) can be exploited when numerically checking the correctness of gradients in computer programs: When we compute gradients and implement them, we can use finite differences to numerically test our computation and implementation: We choose the value h to be small (e.g., $h = 10^{-4}$) and compare the finite-difference approximation from (5.39) with our (analytic) implementation of the gradient. If the error is small, our gradient implementation is probably correct. "Small" could mean that $\sqrt{\frac{\sum_i (dh_i - df_i)^2}{\sum_i (dh_i + df_i)^2}} < 10^{-6}$, where dh_i is the finite-difference approximation and df_i is the analytic gradient of f with respect to the ith variable x_i. ♢

Gradient checking

5.3 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

$$\boldsymbol{f}(\boldsymbol{x}) = \begin{bmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_m(\boldsymbol{x}) \end{bmatrix} \in \mathbb{R}^m . \tag{5.54}$$

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 in Section 5.2.

Therefore, the partial derivative of a vector-valued function $\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^m$ with respect to $x_i \in \mathbb{R}$, $i = 1, \ldots n$, is given as the vector

$$\frac{\partial \boldsymbol{f}}{\partial x_i} = \begin{bmatrix} \frac{\partial f_1}{\partial x_i} \\ \vdots \\ \frac{\partial f_m}{\partial x_i} \end{bmatrix} = \begin{bmatrix} \lim_{h \to 0} \frac{f_1(x_1, \ldots, x_{i-1}, x_i + h, x_{i+1}, \ldots x_n) - f_1(\boldsymbol{x})}{h} \\ \vdots \\ \lim_{h \to 0} \frac{f_m(x_1, \ldots, x_{i-1}, x_i + h, x_{i+1}, \ldots x_n) - f_m(\boldsymbol{x})}{h} \end{bmatrix} \in \mathbb{R}^m . \tag{5.55}$$

From (5.40), we know that the gradient of $\boldsymbol{f}$ with respect to a vector is the row vector of the partial derivatives. In (5.55), 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:

$$\frac{\mathrm{d}\boldsymbol{f}(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}} = \left[\boxed{\frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_1}} \cdots \boxed{\frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_n}} \right] \tag{5.56a}$$

$$= \left[\boxed{\begin{matrix} \frac{\partial f_1(\boldsymbol{x})}{\partial x_1} \\ \vdots \\ \frac{\partial f_m(\boldsymbol{x})}{\partial x_1} \end{matrix}} \begin{matrix} \cdots \\ \\ \cdots \end{matrix} \boxed{\begin{matrix} \frac{\partial f_1(\boldsymbol{x})}{\partial x_n} \\ \vdots \\ \frac{\partial f_m(\boldsymbol{x})}{\partial x_n} \end{matrix}} \right] \in \mathbb{R}^{m \times n} . \tag{5.56b}$$

Jacobian

The gradient of a function $\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^m$ is a matrix of size $m \times n$.

Definition 5.6 (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:

$$\boldsymbol{J} = \nabla_{\boldsymbol{x}} \boldsymbol{f} = \frac{\mathrm{d}\boldsymbol{f}(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}} = \begin{bmatrix} \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_n} \end{bmatrix} \tag{5.57}$$

$$= \begin{bmatrix} \frac{\partial f_1(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial f_1(\boldsymbol{x})}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_m(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial f_m(\boldsymbol{x})}{\partial x_n} \end{bmatrix} , \tag{5.58}$$

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} , \quad J(i, j) = \frac{\partial f_i}{\partial x_j} . \tag{5.59}$$

As a special case of (5.58), a function $f : \mathbb{R}^n \to \mathbb{R}^1$, which maps a vector $\boldsymbol{x} \in \mathbb{R}^n$ onto a scalar (e.g., $f(\boldsymbol{x}) = \sum_{i=1}^n x_i$), possesses a Jacobian that is a row vector (matrix of dimension $1 \times n$); see (5.40).

numerator layout

Remark. In this book, we use the *numerator layout* of the derivative, i.e., the derivative $\mathrm{d}\boldsymbol{f}/\mathrm{d}\boldsymbol{x}$ of $\boldsymbol{f} \in \mathbb{R}^m$ with respect to $\boldsymbol{x} \in \mathbb{R}^n$ is an $m \times n$ matrix, where the elements of $\boldsymbol{f}$ define the rows and the elements of $\boldsymbol{x}$ define the columns of the corresponding Jacobian; see (5.58). There

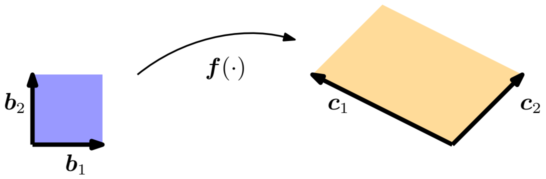


Figure 5.5 The determinant of the Jacobian of $\boldsymbol{f}$ can be used to compute the magnifier between the blue and orange area.

exists also the *denominator layout*, which is the transpose of the numerator layout. In this book, we will use the numerator layout. ♢

denominator layout

We will see how the Jacobian is used in the change-of-variable method for probability distributions in Section 6.7. The amount of scaling due to the transformation of a variable is provided by the determinant.

In Section 4.1, we saw that the determinant can be used to compute the area of a parallelogram. If we are given two vectors $\boldsymbol{b}_1 = [1, 0]^\top$, $\boldsymbol{b}_2 = [0, 1]^\top$ as the sides of the unit square (blue; see Figure 5.5), the area of this square is

$$\left|\det\left(\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\right)\right| = 1\,. \tag{5.60}$$

If we take a parallelogram with the sides $\boldsymbol{c}_1 = [-2, 1]^\top$, $\boldsymbol{c}_2 = [1, 1]^\top$ (orange in Figure 5.5), its area is given as the absolute value of the determinant (see Section 4.1)

$$\left|\det\left(\begin{bmatrix}-2 & 1\\ 1 & 1\end{bmatrix}\right)\right| = |-3| = 3\,, \tag{5.61}$$

i.e., the area of this is exactly three times the area of the unit square. We can find this scaling factor by finding a mapping that transforms the unit square into the other square. In linear algebra terms, we effectively perform a variable transformation from $(\boldsymbol{b}_1, \boldsymbol{b}_2)$ to $(\boldsymbol{c}_1, \boldsymbol{c}_2)$. In our case, the mapping is linear and the absolute value of the determinant of this mapping gives us exactly the scaling factor we are looking for.

We will describe two approaches to identify this mapping. First, we exploit that the mapping is linear so that we can use the tools from Chapter 2 to identify this mapping. Second, we will find the mapping using partial derivatives using the tools we have been discussing in this chapter.

Approach 1 To get started with the linear algebra approach, we identify both $\{\boldsymbol{b}_1, \boldsymbol{b}_2\}$ and $\{\boldsymbol{c}_1, \boldsymbol{c}_2\}$ as bases of $\mathbb{R}^2$ (see Section 2.6.1 for a recap). What we effectively perform is a change of basis from $(\boldsymbol{b}_1, \boldsymbol{b}_2)$ to $(\boldsymbol{c}_1, \boldsymbol{c}_2)$, and we are looking for the transformation matrix that implements the basis change. Using results from Section 2.7.2, we identify the desired basis change matrix as

$$\boldsymbol{J} = \begin{bmatrix}-2 & 1\\ 1 & 1\end{bmatrix}, \tag{5.62}$$

such that $\boldsymbol{J}\boldsymbol{b}_1 = \boldsymbol{c}_1$ and $\boldsymbol{J}\boldsymbol{b}_2 = \boldsymbol{c}_2$. The absolute value of the determinant of $\boldsymbol{J}$, which yields the scaling factor we are looking for, is given as $|\det(\boldsymbol{J})| = 3$, i.e., the area of the square spanned by $(\boldsymbol{c}_1, \boldsymbol{c}_2)$ is three times greater than the area spanned by $(\boldsymbol{b}_1, \boldsymbol{b}_2)$.

Approach 2 The linear algebra approach works for linear transformations; for nonlinear transformations (which become relevant in Section 6.7), we follow a more general approach using partial derivatives.

For this approach, we consider a function $\boldsymbol{f} : \mathbb{R}^2 \to \mathbb{R}^2$ that performs a variable transformation. In our example, $\boldsymbol{f}$ maps the coordinate representation of any vector $\boldsymbol{x} \in \mathbb{R}^2$ with respect to $(\boldsymbol{b}_1, \boldsymbol{b}_2)$ onto the coordinate representation $\boldsymbol{y} \in \mathbb{R}^2$ with respect to $(\boldsymbol{c}_1, \boldsymbol{c}_2)$. We want to identify the mapping so that we can compute how an area (or volume) changes when it is being transformed by $\boldsymbol{f}$. For this, we need to find out how $\boldsymbol{f}(\boldsymbol{x})$ changes if we modify $\boldsymbol{x}$ a bit. This question is exactly answered by the Jacobian matrix $\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{2\times 2}$. Since we can write

$$y_1 = -2x_1 + x_2 \tag{5.63}$$

$$y_2 = x_1 + x_2 \tag{5.64}$$

we obtain the functional relationship between $\boldsymbol{x}$ and $\boldsymbol{y}$, which allows us to get the partial derivatives

$$\frac{\partial y_1}{\partial x_1} = -2\,, \quad \frac{\partial y_1}{\partial x_2} = 1\,, \quad \frac{\partial y_2}{\partial x_1} = 1\,, \quad \frac{\partial y_2}{\partial x_2} = 1 \tag{5.65}$$

and compose the Jacobian as

$$\boldsymbol{J} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} -2 & 1 \\ 1 & 1 \end{bmatrix}. \tag{5.66}$$

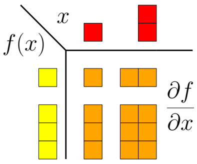
Geometrically, the Jacobian determinant gives the magnification/ scaling factor when we transform an area or volume.

Jacobian determinant

The Jacobian represents the coordinate transformation we are looking for. It is exact if the coordinate transformation is linear (as in our case), and (5.66) recovers exactly the basis change matrix in (5.62). If the coordinate transformation is nonlinear, the Jacobian approximates this nonlinear transformation locally with a linear one. The absolute value of the *Jacobian determinant* $|\det(\boldsymbol{J})|$ is the factor by which areas or volumes are scaled when coordinates are transformed. Our case yields $|\det(\boldsymbol{J})| = 3$.

The Jacobian determinant and variable transformations will become relevant in Section 6.7 when we transform random variables and probability distributions. These transformations are extremely relevant in machine learning in the context of training deep neural networks using the *reparametrization trick*, also called *infinite perturbation analysis*.

Figure 5.6 Dimensionality of (partial) derivatives.



In this chapter, we encountered derivatives of functions. Figure 5.6 summarizes the dimensions of those derivatives. If $f : \mathbb{R} \to \mathbb{R}$ the gradient is simply a scalar (top-left entry). For $f : \mathbb{R}^D \to \mathbb{R}$ the gradient is a $1 \times D$ row vector (top-right entry). For $\boldsymbol{f} : \mathbb{R} \to \mathbb{R}^E$, the gradient is an $E \times 1$ column vector, and for $\boldsymbol{f} : \mathbb{R}^D \to \mathbb{R}^E$ the gradient is an $E \times D$ matrix.

Example 5.9 (Gradient of a Vector-Valued Function)
We are given

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}\,, \qquad \boldsymbol{f}(\boldsymbol{x}) \in \mathbb{R}^M, \quad \boldsymbol{A} \in \mathbb{R}^{M\times N}, \quad \boldsymbol{x} \in \mathbb{R}^N\,.$$

To compute the gradient $\mathrm{d}\boldsymbol{f}/\mathrm{d}\boldsymbol{x}$ we first determine the dimension of $\mathrm{d}\boldsymbol{f}/\mathrm{d}\boldsymbol{x}$: Since $\boldsymbol{f} : \mathbb{R}^N \to \mathbb{R}^M$, it follows that $\mathrm{d}\boldsymbol{f}/\mathrm{d}\boldsymbol{x} \in \mathbb{R}^{M\times N}$. Second, to compute the gradient we determine the partial derivatives of f with respect to every x_j:

$$f_i(\boldsymbol{x}) = \sum_{j=1}^{N} A_{ij}x_j \implies \frac{\partial f_i}{\partial x_j} = A_{ij} \tag{5.67}$$

We collect the partial derivatives in the Jacobian and obtain the gradient

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} = \begin{bmatrix} A_{11} & \cdots & A_{1N} \\ \vdots & & \vdots \\ A_{M1} & \cdots & A_{MN} \end{bmatrix} = \boldsymbol{A} \in \mathbb{R}^{M\times N}\,. \tag{5.68}$$

Example 5.10 (Chain Rule)
Consider the function $h : \mathbb{R} \to \mathbb{R}$, $h(t) = (f \circ g)(t)$ with

$$f : \mathbb{R}^2 \to \mathbb{R} \tag{5.69}$$

$$g : \mathbb{R} \to \mathbb{R}^2 \tag{5.70}$$

$$f(\boldsymbol{x}) = \exp(x_1 x_2^2)\,, \tag{5.71}$$

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = g(t) = \begin{bmatrix} t\cos t \\ t\sin t \end{bmatrix} \tag{5.72}$$

and compute the gradient of h with respect to t. Since $f : \mathbb{R}^2 \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}^2$ we note that

$$\frac{\partial f}{\partial \boldsymbol{x}} \in \mathbb{R}^{1\times 2}\,, \quad \frac{\partial g}{\partial t} \in \mathbb{R}^{2\times 1}\,. \tag{5.73}$$

The desired gradient is computed by applying the chain rule:

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \frac{\partial f}{\partial \boldsymbol{x}} \frac{\partial \boldsymbol{x}}{\partial t} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial t} \end{bmatrix} \tag{5.74a}$$

$$= \begin{bmatrix} \exp(x_1 x_2^2) x_2^2 & 2\exp(x_1 x_2^2) x_1 x_2 \end{bmatrix} \begin{bmatrix} \cos t - t\sin t \\ \sin t + t\cos t \end{bmatrix} \tag{5.74b}$$

$$= \exp(x_1 x_2^2)\big(x_2^2(\cos t - t\sin t) + 2x_1 x_2(\sin t + t\cos t)\big)\,, \tag{5.74c}$$

where $x_1 = t\cos t$ and $x_2 = t\sin t$; see (5.72).

Example 5.11 (Gradient of a Least-Squares Loss in a Linear Model)

We will discuss this model in much more detail in Chapter 9 in the context of linear regression, where we need derivatives of the least-squares loss L with respect to the parameters $\boldsymbol{\theta}$.

Let us consider the linear model

$$\boldsymbol{y} = \boldsymbol{\Phi}\boldsymbol{\theta}\,, \tag{5.75}$$

where $\boldsymbol{\theta} \in \mathbb{R}^D$ is a parameter vector, $\boldsymbol{\Phi} \in \mathbb{R}^{N\times D}$ are input features and $\boldsymbol{y} \in \mathbb{R}^N$ are the corresponding observations. We define the functions

$$L(\boldsymbol{e}) := \|\boldsymbol{e}\|^2\,, \tag{5.76}$$

$$\boldsymbol{e}(\boldsymbol{\theta}) := \boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta}\,. \tag{5.77}$$

least-squares loss

We seek $\frac{\partial L}{\partial \boldsymbol{\theta}}$, and we will use the chain rule for this purpose. L is called a *least-squares loss* function.

Before we start our calculation, we determine the dimensionality of the gradient as

$$\frac{\partial L}{\partial \boldsymbol{\theta}} \in \mathbb{R}^{1\times D}\,. \tag{5.78}$$

The chain rule allows us to compute the gradient as

$$\frac{\partial L}{\partial \boldsymbol{\theta}} = \frac{\partial L}{\partial \boldsymbol{e}}\frac{\partial \boldsymbol{e}}{\partial \boldsymbol{\theta}}\,, \tag{5.79}$$

```
dLdtheta =
np.einsum(
'n,nd',
dLde,dedtheta)
```

where the dth element is given by

$$\frac{\partial L}{\partial \boldsymbol{\theta}}[1, d] = \sum_{n=1}^{N} \frac{\partial L}{\partial \boldsymbol{e}}[n]\frac{\partial \boldsymbol{e}}{\partial \boldsymbol{\theta}}[n, d]\,. \tag{5.80}$$

We know that $\|\boldsymbol{e}\|^2 = \boldsymbol{e}^\top \boldsymbol{e}$ (see Section 3.2) and determine

$$\frac{\partial L}{\partial \boldsymbol{e}} = 2\boldsymbol{e}^\top \in \mathbb{R}^{1\times N}\,. \tag{5.81}$$

Furthermore, we obtain

$$\frac{\partial \boldsymbol{e}}{\partial \boldsymbol{\theta}} = -\boldsymbol{\Phi} \in \mathbb{R}^{N\times D}\,, \tag{5.82}$$

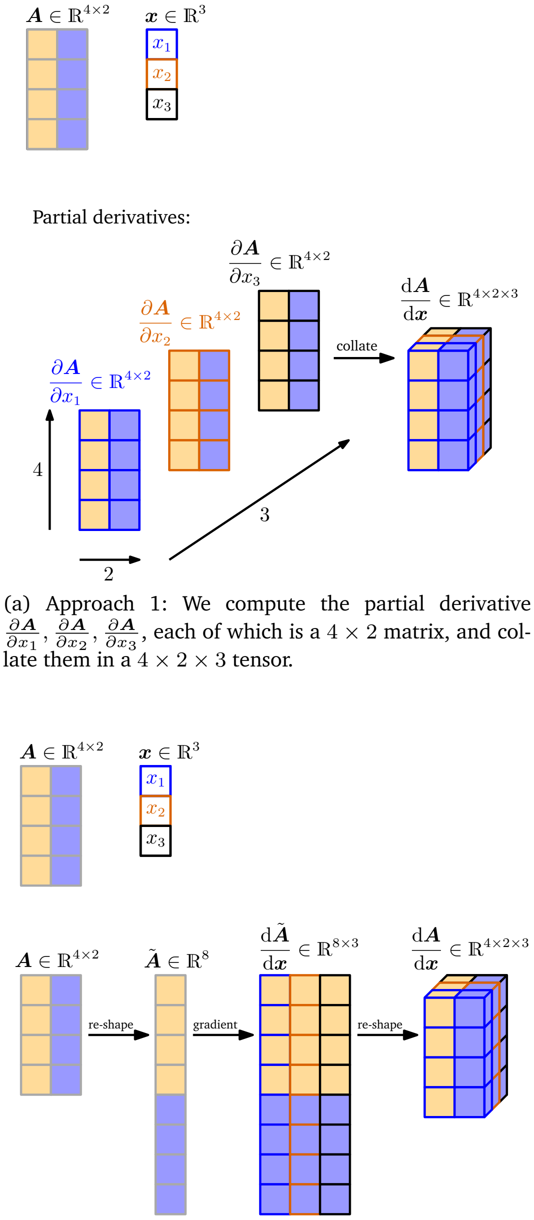
such that our desired derivative is

$$\frac{\partial L}{\partial \boldsymbol{\theta}} = -2\boldsymbol{e}^\top \boldsymbol{\Phi} \overset{(5.77)}{=} -\underbrace{2(\boldsymbol{y}^\top - \boldsymbol{\theta}^\top\boldsymbol{\Phi}^\top)}_{1\times N}\underbrace{\boldsymbol{\Phi}}_{N\times D} \in \mathbb{R}^{1\times D}\,. \tag{5.83}$$

Remark. We would have obtained the same result without using the chain rule by immediately looking at the function

$$L_2(\boldsymbol{\theta}) := \|\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta}\|^2 = (\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta})^\top(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta})\,. \tag{5.84}$$

This approach is still practical for simple functions like L_2 but becomes impractical for deep function compositions. ◇


$\boldsymbol{A} \in \mathbb{R}^{4\times 2}$
$\boldsymbol{x} \in \mathbb{R}^{3}$
x_1
x_2
x_3
Partial derivatives:
$\frac{\partial \boldsymbol{A}}{\partial x_3} \in \mathbb{R}^{4\times 2}$
$\frac{\partial \boldsymbol{A}}{\partial x_2} \in \mathbb{R}^{4\times 2}$
$\frac{\partial \boldsymbol{A}}{\partial x_1} \in \mathbb{R}^{4\times 2}$
$\frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{4\times 2\times 3}$
collate
4
2
3
$\tilde{\boldsymbol{A}} \in \mathbb{R}^{8}$
$\frac{\mathrm{d}\tilde{\boldsymbol{A}}}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{8\times 3}$
re-shape
gradient
re-shape

(a) Approach 1: We compute the partial derivative $\frac{\partial \boldsymbol{A}}{\partial x_1}, \frac{\partial \boldsymbol{A}}{\partial x_2}, \frac{\partial \boldsymbol{A}}{\partial x_3}$, each of which is a 4×2 matrix, and collate them in a $4 \times 2 \times 3$ tensor.

(b) Approach 2: We re-shape (flatten) $\boldsymbol{A} \in \mathbb{R}^{4\times 2}$ into a vector $\tilde{\boldsymbol{A}} \in \mathbb{R}^{8}$. Then, we compute the gradient $\frac{\mathrm{d}\tilde{\boldsymbol{A}}}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{8\times 3}$. We obtain the gradient tensor by re-shaping this gradient as illustrated above.

Figure 5.7 Visualization of gradient computation of a matrix with respect to a vector. We are interested in computing the gradient of $\boldsymbol{A} \in \mathbb{R}^{4\times 2}$ with respect to a vector $\boldsymbol{x} \in \mathbb{R}^{3}$. We know that gradient $\frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{4\times 2\times 3}$. We follow two equivalent approaches to arrive there: (a) collating partial derivatives into a Jacobian tensor;
(b) flattening of the matrix into a vector, computing the Jacobian matrix, re-shaping into a Jacobian tensor.

5.4 Gradients of Matrices

We will encounter situations where we need to take gradients of matrices with respect to vectors (or other matrices), which results in a multidimensional tensor. We can think of this tensor as a multidimensional array that

We can think of a tensor as a multidimensional array.

collects partial derivatives. For example, if we compute the gradient of an $m \times n$ matrix $\boldsymbol{A}$ with respect to a $p \times q$ matrix $\boldsymbol{B}$, the resulting Jacobian would be $(m\times n)\times(p\times q)$, i.e., a four-dimensional tensor $\boldsymbol{J}$, whose entries are given as $J_{ijkl} = \partial A_{ij}/\partial B_{kl}$.

Since matrices represent linear mappings, we can exploit the fact that there is a vector-space isomorphism (linear, invertible mapping) between the space $\mathbb{R}^{m\times n}$ of $m \times n$ matrices and the space $\mathbb{R}^{mn}$ of mn vectors. Therefore, we can re-shape our matrices into vectors of lengths mn and pq, respectively. The gradient using these mn vectors results in a Jacobian of size $mn \times pq$. Figure 5.7 visualizes both approaches. In practical applications, it is often desirable to re-shape the matrix into a vector and continue working with this Jacobian matrix: The chain rule (5.48) boils down to simple matrix multiplication, whereas in the case of a Jacobian tensor, we will need to pay more attention to what dimensions we need to sum out.

Matrices can be transformed into vectors by stacking the columns of the matrix ("flattening").

Example 5.12 (Gradient of Vectors with Respect to Matrices)
Let us consider the following example, where

$$\boldsymbol{f} = \boldsymbol{A}\boldsymbol{x}\,, \quad \boldsymbol{f} \in \mathbb{R}^{M}, \quad \boldsymbol{A} \in \mathbb{R}^{M\times N}, \quad \boldsymbol{x} \in \mathbb{R}^{N} \tag{5.85}$$

and where we seek the gradient $\mathrm{d}\boldsymbol{f}/\mathrm{d}\boldsymbol{A}$. Let us start again by determining the dimension of the gradient as

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{A}} \in \mathbb{R}^{M\times(M\times N)}\,. \tag{5.86}$$

By definition, the gradient is the collection of the partial derivatives:

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{A}} = \begin{bmatrix} \frac{\partial f_1}{\partial \boldsymbol{A}} \\ \vdots \\ \frac{\partial f_M}{\partial \boldsymbol{A}} \end{bmatrix}, \quad \frac{\partial f_i}{\partial \boldsymbol{A}} \in \mathbb{R}^{1\times(M\times N)}\,. \tag{5.87}$$

To compute the partial derivatives, it will be helpful to explicitly write out the matrix vector multiplication:

$$f_i = \sum_{j=1}^{N} A_{ij}x_j, \quad i = 1, \dots, M\,, \tag{5.88}$$

and the partial derivatives are then given as

$$\frac{\partial f_i}{\partial A_{iq}} = x_q\,. \tag{5.89}$$

This allows us to compute the partial derivatives of f_i with respect to a row of $\boldsymbol{A}$, which is given as

$$\frac{\partial f_i}{\partial A_{i,:}} = \boldsymbol{x}^\top \in \mathbb{R}^{1\times1\times N}\,, \tag{5.90}$$

$$\frac{\partial f_i}{\partial A_{k\neq i,:}} = \mathbf{0}^\top \in \mathbb{R}^{1\times 1\times N} \tag{5.91}$$

where we have to pay attention to the correct dimensionality. Since f_i maps onto $\mathbb{R}$ and each row of $\boldsymbol{A}$ is of size $1 \times N$, we obtain a $1 \times 1 \times N$-sized tensor as the partial derivative of f_i with respect to a row of $\boldsymbol{A}$.

We stack the partial derivatives (5.91) and get the desired gradient in (5.87) via

$$\frac{\partial f_i}{\partial \boldsymbol{A}} = \begin{bmatrix} \mathbf{0}^\top \\ \vdots \\ \mathbf{0}^\top \\ \boldsymbol{x}^\top \\ \mathbf{0}^\top \\ \vdots \\ \mathbf{0}^\top \end{bmatrix} \in \mathbb{R}^{1\times(M\times N)} . \tag{5.92}$$

Example 5.13 (Gradient of Matrices with Respect to Matrices)
Consider a matrix $\boldsymbol{R} \in \mathbb{R}^{M\times N}$ and $\boldsymbol{f} : \mathbb{R}^{M\times N} \to \mathbb{R}^{N\times N}$ with

$$\boldsymbol{f}(\boldsymbol{R}) = \boldsymbol{R}^\top \boldsymbol{R} =: \boldsymbol{K} \in \mathbb{R}^{N\times N} , \tag{5.93}$$

where we seek the gradient $\mathrm{d}\boldsymbol{K}/\mathrm{d}\boldsymbol{R}$.

To solve this hard problem, let us first write down what we already know: The gradient has the dimensions

$$\frac{\mathrm{d}\boldsymbol{K}}{\mathrm{d}\boldsymbol{R}} \in \mathbb{R}^{(N\times N)\times(M\times N)} , \tag{5.94}$$

which is a tensor. Moreover,

$$\frac{\mathrm{d}K_{pq}}{\mathrm{d}\boldsymbol{R}} \in \mathbb{R}^{1\times M\times N} \tag{5.95}$$

for $p, q = 1, \ldots, N$, where K_{pq} is the (p, q)th entry of $\boldsymbol{K} = \boldsymbol{f}(\boldsymbol{R})$. Denoting the ith column of $\boldsymbol{R}$ by $\boldsymbol{r}_i$, every entry of $\boldsymbol{K}$ is given by the dot product of two columns of $\boldsymbol{R}$, i.e.,

$$K_{pq} = \boldsymbol{r}_p^\top \boldsymbol{r}_q = \sum_{m=1}^{M} R_{mp} R_{mq} . \tag{5.96}$$

When we now compute the partial derivative $\frac{\partial K_{pq}}{\partial R_{ij}}$ we obtain

$$\frac{\partial K_{pq}}{\partial R_{ij}} = \sum_{m=1}^{M} \frac{\partial}{\partial R_{ij}} R_{mp} R_{mq} = \partial_{pqij} , \tag{5.97}$$

$$\partial_{pqij} = \begin{cases} R_{iq} & \text{if } j = p,\ p \neq q \\ R_{ip} & \text{if } j = q,\ p \neq q \\ 2R_{iq} & \text{if } j = p,\ p = q \\ 0 & \text{otherwise} \end{cases} . \tag{5.98}$$

From (5.94), we know that the desired gradient has the dimension $(N \times N) \times (M \times N)$, and every single entry of this tensor is given by ∂_{pqij} in (5.98), where $p, q, j = 1, \dots, N$ and $i = 1, \dots, M$.

5.5 Useful Identities for Computing Gradients

In the following, we list some useful gradients that are frequently required in a machine learning context (Petersen and Pedersen, 2012). Here, we use $\text{tr}(\cdot)$ as the trace (see Definition 4.4), $\det(\cdot)$ as the determinant (see Section 4.1) and $\boldsymbol{f}(\boldsymbol{X})^{-1}$ as the inverse of $\boldsymbol{f}(\boldsymbol{X})$, assuming it exists.

$$\frac{\partial}{\partial \boldsymbol{X}} \boldsymbol{f}(\boldsymbol{X})^\top = \left(\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\right)^\top \tag{5.99}$$

$$\frac{\partial}{\partial \boldsymbol{X}} \text{tr}(\boldsymbol{f}(\boldsymbol{X})) = \text{tr}\left(\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\right) \tag{5.100}$$

$$\frac{\partial}{\partial \boldsymbol{X}} \det(\boldsymbol{f}(\boldsymbol{X})) = \det(\boldsymbol{f}(\boldsymbol{X}))\text{tr}\left(\boldsymbol{f}(\boldsymbol{X})^{-1}\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\right) \tag{5.101}$$

$$\frac{\partial}{\partial \boldsymbol{X}} \boldsymbol{f}(\boldsymbol{X})^{-1} = -\boldsymbol{f}(\boldsymbol{X})^{-1}\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\boldsymbol{f}(\boldsymbol{X})^{-1} \tag{5.102}$$

$$\frac{\partial \boldsymbol{a}^\top \boldsymbol{X}^{-1} \boldsymbol{b}}{\partial \boldsymbol{X}} = -(\boldsymbol{X}^{-1})^\top \boldsymbol{a}\boldsymbol{b}^\top (\boldsymbol{X}^{-1})^\top \tag{5.103}$$

$$\frac{\partial \boldsymbol{x}^\top \boldsymbol{a}}{\partial \boldsymbol{x}} = \boldsymbol{a}^\top \tag{5.104}$$

$$\frac{\partial \boldsymbol{a}^\top \boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{a}^\top \tag{5.105}$$

$$\frac{\partial \boldsymbol{a}^\top \boldsymbol{X} \boldsymbol{b}}{\partial \boldsymbol{X}} = \boldsymbol{a}\boldsymbol{b}^\top \tag{5.106}$$

$$\frac{\partial \boldsymbol{x}^\top \boldsymbol{B} \boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{x}^\top(\boldsymbol{B} + \boldsymbol{B}^\top) \tag{5.107}$$

$$\frac{\partial}{\partial \boldsymbol{s}} (\boldsymbol{x} - \boldsymbol{A}\boldsymbol{s})^\top \boldsymbol{W} (\boldsymbol{x} - \boldsymbol{A}\boldsymbol{s}) = -2(\boldsymbol{x} - \boldsymbol{A}\boldsymbol{s})^\top \boldsymbol{W}\boldsymbol{A} \quad \text{for symmetric } \boldsymbol{W} \tag{5.108}$$

Remark. In this book, we only cover traces and transposes of matrices. However, we have seen that derivatives can be higher-dimensional tensors, in which case the usual trace and transpose are not defined. In these cases, the trace of a $D \times D \times E \times F$ tensor would be an $E \times F$-dimensional matrix. This is a special case of a tensor contraction. Similarly, when we