The Elements of Differentiable Programming

Mathieu Blondel
Google DeepMind
mblondel@google.com

Vincent Roulet
Google DeepMind
vroulet@google.com

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Mathieu Blondel[1] and Vincent Roulet[1]

[1] *Google DeepMind*

ABSTRACT

Artificial intelligence has recently experienced remarkable advances, fueled by large models, vast datasets, accelerated hardware, and, last but not least, the transformative power of differentiable programming. This new programming paradigm enables end-to-end differentiation of complex computer programs (including those with control flows and data structures), making gradient-based optimization of program parameters possible.

As an emerging paradigm, differentiable programming builds upon several areas of computer science and applied mathematics, including automatic differentiation, graphical models, optimization and statistics. This book presents a comprehensive review of the fundamental concepts useful for differentiable programming. We adopt two main perspectives, that of optimization and that of probability, with clear analogies between the two.

Differentiable programming is not merely the differentiation of programs, but also the thoughtful design of programs intended for differentiation. By making programs differentiable, we inherently introduce probability distributions over their execution, providing a means to quantify the uncertainty associated with program outputs.

Notation

Table 1: Naming conventions

Notation	Description
$\mathcal{X} \subseteq \mathbb{R}^D$	Input space (e.g., features)
$\mathcal{Y} \subseteq \mathbb{R}^M$	Output space (e.g., classes)
$\mathcal{S}_k \subseteq \mathbb{R}^{D_k}$	Output space on layer or state k
$\mathcal{W} \subseteq \mathbb{R}^P$	Weight space
$\Lambda \subseteq \mathbb{R}^Q$	Hyperparameter space
$\Theta \subseteq \mathbb{R}^R$	Distribution parameter space, logit space
N	Number of training samples
T	Number of optimization iterations
$\boldsymbol{x} \in \mathcal{X}$	Input vector
$\boldsymbol{y} \in \mathcal{Y}$	Target vector
$\boldsymbol{s}_k \in \mathcal{S}_k$	State vector k
$\boldsymbol{w} \in \mathcal{W}$	Network (model) weights
$\boldsymbol{\lambda} \in \Lambda$	Hyperparameters
$\boldsymbol{\theta} \in \Theta$	Distribution parameters, logits
$\pi \in [0, 1]$	Probability value
$\boldsymbol{\pi} \in \triangle^M$	Probability vector

Table 2: Naming conventions (continued)

Notation	Description
f	Network function
$f(\cdot\,;\boldsymbol{x})$	Network function with $\boldsymbol{x}$ fixed
L	Objective function
ℓ	Loss function
κ	Kernel function
ϕ	Output embedding, sufficient statistic
step	Heaviside step function
logistic_σ	Logistic function with temperature σ
logistic	Shorthand for logistic_1
$p_{\boldsymbol{\theta}}$	Model distribution with parameters $\boldsymbol{\theta}$
ρ	Data distribution over $\mathcal{X} \times \mathcal{Y}$
$\rho_{\mathcal{X}}$	Data distribution over $\mathcal{X}$
$\boldsymbol{\mu}, \sigma^2$	Mean and variance
Z	Random noise variable

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Introduction

1.1 What is differentiable programming?

A computer program is a sequence of elementary instructions for performing a task. In traditional programming, the program is typically hand-written by a programmer. However, for certain tasks, such as image recognition or text generation, hand-writing a program to perform such tasks is nearly impossible.

This has motivated the need for statistical approaches based on machine learning. With differentiable programming, while the overall structure of the program is typically designed by a human, parameters of the program (such as weights in a neural network) can be automatically adjusted to achieve a task or optimize a criterion. This paradigm has also been referred to as "software 2.0". We give an informal definition.

> **Definition 1.1** (Differentiable programming). Differentiable programming is a programming paradigm in which complex computer programs (including those with control flows and data structures) can be differentiated end-to-end automatically, enabling gradient-based optimization of parameters in the program.

In differentiable programming, a program is also defined as the

composition of elementary operations, forming a **computation graph**. The key difference with classical computer programming is that the program can be differentiated end-to-end, using **automatic differentiation** (autodiff). Typically, it is assumed that the program defines a **mathematically valid function** (a.k.a. pure function): the function should return identical values for identical arguments and should not have any side effects. Moreover, the function should have **well-defined derivatives**, ensuring that it can be used in a gradient-based optimization algorithm. Therefore, differentiable programming is not only the art of differentiating through programs but also of **designing** meaningful differentiable programs.

Why are derivatives important?

Machine learning typically boils down to optimizing a certain objective function, which is the composition of a loss function and a model (network) function. Derivative-free optimization is called **zero-order optimization**. It only assumes that we can evaluate the objective function that we wish to optimize. Unfortunately, it is known to suffer from the **curse of dimensionality**, i.e., it only scales to small dimensional problems, such as less than 10 dimensions. Derivative-based optimization, on the other hand, is much more efficient and can scale to millions or billions of parameters. Algorithms that use first and second derivatives are known as **first-order** and **second-order** algorithms, respectively.

Why is autodiff important?

Before the autodiff revolution, researchers and practitioners needed to manually implement the gradient of the functions they wished to optimize. Manually deriving gradients can become very tedious for complicated functions. Moreover, every time the function is changed (for example, for trying out a new idea), the gradient needs to be re-derived. Autodiff is a game changer because it allows users to focus on quickly and creatively experimenting with functions for their tasks.

Differentiable programming is not just deep learning

While there is clearly overlap between deep learning and differentiable programming, their focus is different. Deep learning studies artificial neural networks composed of multiple layers, able to learn **intermediate representations** of the data. Neural network architectures have been proposed with various **inductive biases**. For example, convolutional neural networks are designed for images and transformers are designed for sequences. On the other hand, differentiable programming studies the techniques to differentiate through complex programs. It is useful beyond deep learning: for instance in reinforcement learning, probabilistic programming and scientific computing in general.

Differentiable programming is not just autodiff

While autodiff is a key ingredient of differentiable programming, this is not the only one. Differentiable programming is also concerned with the design of principled differentiable operations. In fact, much research on differentiable programming has been devoted to make classical computer programming operations compatible with autodiff. As we shall see, many differentiable relaxations can be interpreted in a probabilistic framework. A core theme of this book is the interplay between optimization, probability and differentiation. Differentiation is useful for optimization and conversely, optimization can be used to design differentiable operators.

1.2   Book goals and scope

The present book aims to provide an comprehensive introduction to differentiable programming with an emphasis on **core mathematical tools**.

- In Part I, we review **fundamentals**: differentiation and probabilistic learning.

- In Part II, we review **differentiable programs**. This includes neural networks, sequence networks and control flows.

- In Part III, we review how to **differentiate through programs**. This includes automatic differentiation, but also differentiating through optimization and integration (in particular, expectations).

- In Part IV, we review **smoothing programs**. We focus on two main techniques: infimal convolution, which comes from the world of optimization and convolution, which comes from the world of integration. We also strive to spell out the connections between them.

- In Part V, we review **optimizing programs**: basic optimization concepts, first-order algorithms, second-order-algorithms and duality.

Our goal is to present the fundamental techniques useful for differentiable programming, **not** to survey how these techniques have been used in various applications.

1.3 Intended audience

This book is intended to be a graduate-level introduction to differentiable programming. Our pedagogical choices are made with the machine learning community in mind. Some familiarity with calculus, linear algebra, probability theory and machine learning is beneficial.

1.4 How to read this book?

This book does not need to be read linearly chapter by chapter. When needed, we indicate at the beginning of a chapter what chapters are recommended to be read as a prerequisite.

1.5 Related work

Differentiable programming builds upon a variety of connected topics. We review in this section relevant textbooks, tutorials and software.

Standard textbooks on backpropagation and automatic differentiation are that of Werbos (1994) and Griewank and Walther (2008).

A tutorial with a focus on machine learning is provided by Baydin *et al.* (2018). Automatic differentiation is also reviewed as part of more general textbooks, such as those of Deisenroth *et al.* (2020), Murphy (2022) (from a linear algebra perspective) and Murphy (2023) (from a functional perspective; autodiff section authored by Roy Frostig). The present book was also influenced by Peyré (2020)'s textbook on data science. The history of reverse-mode autodiff is reviewed by Griewank (2012).

A tutorial on different perspectives of backpropagation is "There and Back Again: A Tale of Slopes and Expectations" (link), by Deisenroth and Ong. A tutorial on implicit differentiation is "Deep Implicit Layers - Neural ODEs, Deep Equilibirum Models, and Beyond" (link), by Kolter, Duvenaud, and Johnson.

The standard reference on inference in graphical models and its connection with exponential families is that of Wainwright and Jordan (2008). Differential programming is also related to probabilistic programming; see, e.g., Meent *et al.* (2018).

A review of smoothing from the infimal convolution perspective is provided by Beck and Teboulle (2012). A standard textbook on convex optimization is that of Nesterov (2018). A textbook on first-order optimization methods is that of Beck (2017).

Autodiff implementations that accelerated the autodiff revolution in machine learning are Theano (Bergstra *et al.*, 2010) and Autograd (Maclaurin *et al.*, 2015). Major modern implementations of autodiff include Tensorflow (Abadi *et al.*, 2016), JAX (Bradbury *et al.*, 2018), and PyTorch (Paszke *et al.*, 2019). We in particular acknowledge the JAX team for influencing our view of autodiff.

Part I

Fundamentals

2

Differentiation

In this chapter, we review key differentiation concepts. In particular, we emphasize on the fundamental role played by linear maps.

2.1 Univariate functions

2.1.1 Derivatives

Before studying derivatives, we briefly recall the definition of function **continuity**.

Definition 2.1 (Continuous function). A function $f : \mathbb{R} \to \mathbb{R}$ is continuous at a point $w \in \mathbb{R}$ if

$$\lim_{v \to w} f(v) = f(w).$$

A function f is said to be continuous if it is continuous at all points in its domain.

In the following, we use Landau's little o notation. We write

$$g(v) = o(f(v)) \text{ as } v \to w$$

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if

$$\lim_{v \to w} \frac{|g(v)|}{|f(v)|} = 0.$$

That is, the function f dominates g in the limit $v \to w$. For example, f is continuous at w if and only if

$$f(w + \delta) = f(w) + o(1) \text{ as } \delta \to 0.$$

We now explain derivatives. Consider a function $f : \mathbb{R} \to \mathbb{R}$. As illustrated in Fig. 2.1, its value on an interval $[w_0, w_0 + \delta]$ can be approximated by the secant between its values $f(w_0)$ and $f(w_0 + \delta)$, a linear function with slope $(f(w_0 + \delta) - f(w_0))/\delta$. In the limit of an infinitesimal variation δ around w_0, the secant converges to the **tangent** of f at w_0 and the resulting slope defines the derivative of f at w_0. The definition below formalizes this intuition.

Definition 2.2 (Derivative)**.** The **derivative** of $f : \mathbb{R} \to \mathbb{R}$ at $w \in \mathbb{R}$ is defined as

$$f'(w) := \lim_{\delta \to 0} \frac{f(w + \delta) - f(w)}{\delta}, \tag{2.1}$$

provided that the limit exists. If $f'(w)$ is well-defined at a particular w, we say that the function f is **differentiable** at w.

Here, and in the following definitions, if f is differentiable at any $w \in \mathbb{R}$, we say that it is **differentiable everywhere** or differentiable for short. If f is differentiable at a given w, then it is necessarily **continuous** at w.

Proposition 2.1 (Differentiability implies continuity)**.** If $f : \mathbb{R} \to \mathbb{R}$ is differentiable at $w \in \mathbb{R}$, then it is continuous at $w \in \mathbb{R}$.

Proof. In little o notation, f is differentiable at w if there exists $f'(w) \in \mathbb{R}$, such that

$$f(w + \delta) = f(w) + f'(w)\delta + o(\delta) \text{ as } \delta \to 0.$$

Since $f'(w)\delta + o(\delta) = o(1)$ as $\delta \to 0$, f is continuous at w. $\qquad\square$
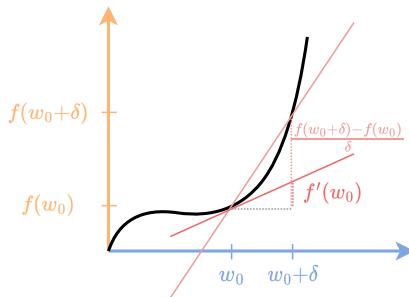
Figure 2.1: A function f can be locally approximated around a point w_0 by a secant, a linear function $w \mapsto aw + b$ with slope a and intercept b, crossing f at w_0 with value $y_0 = f(w_0)$ and crossing at $w_0 + \delta$ with value $u_\delta = f(w_0 + \delta)$. Using $u_0 = aw_0 + b$ and $u_\delta = a(w_0 + \delta) + b$, we find that its slope is $a = (f(w_0 + \delta) - f(w_0))/\delta$ and the intercept is $b = f(w_0) - aw_0$. The derivative $f'(w)$ of a function f at a point w_0 is then defined as the limit of the slope a when $\delta \to 0$. It is the slope of the tangent of f at w_0. The value $f(w)$ of the function at w can then be locally approximated around w_0 by $w \mapsto f'(w_0)w + f(w_0) - f'(w_0)w_0 = f(w_0) + f'(w_0)(w - w_0)$.

In addition to enabling the construction of a linear approximation of f in a neighborhood of w, since it is the slope of the tangent of f at w, the derivative f' informs us about the **monotonicity** of f around w. If $f'(w)$ is positive, the function is increasing around w. Conversely, if $f'(w)$ is negative, the function is decreasing. Such information can be used to develop iterative algorithms seeking to minimize f by computing iterates of the form $w_{t+1} = w_t - \gamma f'(w_t)$ for $\gamma > 0$, which move along descent directions of f around w_t.

For several elementary functions such as w^n, e^w, $\ln w$, $\cos w$ or $\sin w$, their derivatives can be obtained directly by applying the definition of the derivative in Eq. (2.1) as illustrated in Example 2.1.

Example 2.1 (Derivative of power function). Consider $f(w) = w^n$

for $w \in \mathbb{R}$, $n \in \mathbb{N} \setminus \{0\}$. For any $\delta \in \mathbb{R}$, we have

$$\frac{f(w+\delta) - f(w)}{\delta} = \frac{(w+\delta)^n - w^n}{\delta}$$

$$= \frac{\sum_{k=0}^{n} \binom{n}{k} \delta^k w^{n-k} - w^n}{\delta}$$

$$= \sum_{k=1}^{n} \binom{n}{k} \delta^{k-1} w^{n-k}$$

$$= \binom{n}{1} w^{n-1} + \sum_{k=2}^{n} \binom{n}{k} \delta^{k-1} w^{n-k},$$

where, in the second line, we used the binomial theorem. Since $\binom{n}{1} = n$ and $\lim_{\delta \to 0} \sum_{k=2}^{n} \binom{n}{k} \delta^{k-1} w^{n-k} = 0$, we get $f'(w) = nw^{n-1}$.

Remark 2.1 (Functions on a subset $\mathcal{U}$ of $\mathbb{R}$). For simplicity, we presented the definition of the derivative for a function defined on the whole set of real numbers $\mathbb{R}$. If a function $f : \mathcal{U} \to \mathbb{R}$ is defined on a subset $\mathcal{U} \subseteq \mathbb{R}$ of the real numbers, as it is the case for $f(w) = \sqrt{w}$ defined on $\mathcal{U} = \mathbb{R}_+$, the derivative of f at $w \in \mathcal{U}$ is defined by the limit in (2.1) provided that the function f is well defined on a neighborhood of w, that is, there exists $r > 0$ such that $w + \delta \in \mathcal{U}$ for any $|\delta| \leq r$. The function f is then said **differentiable everywhere** or differentiable for short if it is differentiable at any point w in the **interior** of $\mathcal{U}$, the set of points $w \in \mathcal{U}$ such that $\{w + \delta : |\delta| \leq r\} \subseteq \mathcal{U}$ for r sufficiently small. For points lying at the boundary of $\mathcal{U}$ (such as a and b if $\mathcal{U} = [a, b]$), one may define the right and left derivatives of f at a and b, meaning that the limit is taken by approaching a from the right or b from the left.

2.1.2 Calculus rules

For a given $w \in \mathbb{R}$ and two functions $f : \mathbb{R} \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}$, the derivative of elementary operations on f and g such as their sums, products or compositions can easily be derived from the definition of the derivative, under appropriate conditions on the differentiability properties of f and g at w. For example, if the derivative of f and g

exist at w then the derivative of their weighted sum or the derivatives or their products exist and lead to the following rules

$$\forall a, b \in \mathbb{R}, \ (af + bg)'(w) = af'(w) + bg'(w) \qquad \text{(Linearity)}$$
$$(fg)'(w) = f'(w)g(w) + f(w)g'(w), \quad \text{(Product rule)}$$

where $(fg)(w) = f(w)g(w)$. The linearity can be verified directly from the linearity of the limits. For the product rule, in little o notation, we have, as $\delta \to 0$,

$$(fg)(w + \delta) = (f(w) + f'(w)\delta + o(\delta))(g(w) + g'(w)\delta + o(\delta))$$
$$= f(w)g(w) + f'(w)g(w)\delta + f(w)g'(w)\delta + o(\delta),$$

hence the result.

If the derivatives of g at w and of f at $g(w)$ exist, then the derivative of the composition $(f \circ g)(w) := f(g(w))$ at w exist and is given by

$$(f \circ g)'(w) = f'(g(w))g'(w). \qquad \text{(Chain rule)}$$

We prove this result more generally in Proposition 2.2. As seen in the sequel, the linearity and the product rule can be seen as byproducts of the chain rule, making the chain rule the cornerstone of differentiation.

For now, consider a function that can be expressed as sums, products or compositions of elementary functions such as $f(w) = e^w \ln w + \cos w^2$. Its derivative can be computed by applying the aforementioned rules on the decomposition of f into elementary operations and functions, as illustrated in Example 2.2.

Example 2.2 (Applying rules of differentiation). Consider $f(w) = e^w \ln w + \cos w^2$. The derivative of f on $w > 0$ can be computed

step by step as follows, denoting $\mathrm{sq}(w) := w^2$,

$$f'(w) = (\exp \cdot \ln)'(w) + (\cos \circ \mathrm{sq})'(w) \qquad \text{(Linearity)}$$
$$(\exp \cdot \ln)'(w) = \exp'(w) \cdot \ln(w) + \exp(w) \cdot \ln'(w) \qquad \text{(Product rule)}$$
$$(\cos \circ \mathrm{sq})'(w) = \cos'(\mathrm{sq}(w)) \, \mathrm{sq}'(w) \qquad \text{(Chain rule)}$$
$$\exp'(w) = \exp(w), \qquad \ln'(w) = 1/w, \qquad \text{(Elem. func.)}$$
$$\mathrm{sq}'(w) = 2w, \qquad \cos'(w) = -\sin(w). \qquad \text{(Elem. func.)}$$

We obtain then that $f'(w) = e^w \ln w + e^w/w - 2w \sin w^2$.

Such a process is purely mechanical and lends itself to an automated procedure, which is the main idea of automatic differentiation presented in Chapter 7.

2.1.3 Leibniz's notation

The notion of derivative was first introduced independently by Newton and Leibniz in the 18th century (Ball, 1960). The latter considered derivatives as the quotient of infinitesimal variations. Namely, denoting $u = f(w)$ a variable depending on w through f, Leibniz considered the derivative of f as the quotient

$$f' = \frac{du}{dw} \quad \text{with} \quad f'(w) = \frac{du}{dw}\bigg|_w$$

where du and dw denote infinitesimal variations of u and w respectively and the symbol $|_w$ denotes the evaluation of the derivative at a given point w. This notation simplifies the statement of the chain rule first discovered by Leibniz (Rodriguez and Lopez Fernandez, 2010) as we have for $v = g(w)$ and $u = f(v)$

$$\frac{du}{dw} = \frac{du}{dv} \cdot \frac{dv}{dw}.$$

This hints that derivatives are multiplied when considering compositions. At evaluation, the chain rule in Leibniz notation recovers the formula presented above as

$$\frac{du}{dw}\bigg|_w = \frac{du}{dv}\bigg|_{g(w)} \frac{dv}{dw}\bigg|_w = f'(g(w))g'(w) = (f \circ g)'(w).$$

The ability of Leibniz's notation to capture the chain rule as a mere product of quotients made it popular throughout the centuries, especially in mechanics (Ball, 1960). The rationale behind Leibniz's notation, that is, the concept of "infinitesimal variations" was questioned by later mathematicians for its potential logical issues (Ball, 1960). The notation $f'(w)$ first introduced by Euler and further popularized by Lagrange (Cajori, 1993) has then taken over in numerous mathematical textbooks. The concept of infinitesimal variations has been rigorously defined by considering the set of hyperreal numbers. They extend the set of real numbers by considering each number as a sum of a non-infinitesimal part and an infinitesimal part (Hewitt, 1948). The formalism of infinitesimal variations further underlies the development of automatic differentiation algorithms through the concept of dual numbers.

2.2 Multivariate functions

2.2.1 Directional derivatives

Let us now consider a function $f : \mathbb{R}^P \to \mathbb{R}$ of multiple inputs $\boldsymbol{w} = (w_1, \ldots, w_P) \in \mathbb{R}^P$. The most important example in machine learning is a function which, to the parameters $\boldsymbol{w} \in \mathbb{R}^P$ of a neural network, associates a loss value in $\mathbb{R}$. Variations of f need to be defined along specific directions, such as the variation $f(\boldsymbol{w} + \delta\boldsymbol{v}) - f(\boldsymbol{w})$ of f around $\boldsymbol{w} \in \mathbb{R}^P$ in the direction $\boldsymbol{v} \in \mathbb{R}^P$ by an amount $\delta > 0$. This consideration naturally leads to the definition of the directional derivative.

> **Definition 2.3** (Directional derivative)**.** The **directional derivative** of f at $\boldsymbol{w}$ in the **direction** $\boldsymbol{v}$ is given by
> $$\partial f(\boldsymbol{w})[\boldsymbol{v}] \coloneqq \lim_{\delta \to 0} \frac{f(\boldsymbol{w} + \delta\boldsymbol{v}) - f(\boldsymbol{w})}{\delta},$$
> provided that the limit exists.

One example of directional derivative consists in computing the derivative of a function f at $\boldsymbol{w}$ in any of the canonical directions
$$\boldsymbol{e}_i \coloneqq (0, \ldots, 0, \underbrace{1}_{i}, 0, \ldots, 0).$$

This allows us to define the notion of **partial derivatives**, denoted for $i \in [P]$

$$\partial_i f(\boldsymbol{w}) := \partial f(\boldsymbol{w})[\boldsymbol{e}_i] = \lim_{\delta \to 0} \frac{f(\boldsymbol{w} + \delta \boldsymbol{e}_i) - f(\boldsymbol{w})}{\delta}.$$

This is also denoted in Leibniz's notation as $\partial_i f(\boldsymbol{w}) = \frac{\partial f(\boldsymbol{w})}{\partial w_i}$ or $\partial_i f(\boldsymbol{w}) = \partial_{w_i} f(\boldsymbol{w})$. By moving along only the ith coordinate of the function, the partial derivative is akin to using the function $\phi(\omega_i) = f(w_1, \ldots, \omega_i, \ldots, w_P)$ around ω_i, letting all other coordinates fixed at their values $\boldsymbol{w}_i$.

2.2.2 Gradients

We now introduce the gradient vector, which gathers the partial derivatives. We first recall the definitions of linear map and linear form.

> **Definition 2.4** (Linear map, linear form). A function $l : \mathbb{R}^P \to \mathbb{R}^M$ is a **linear map** if for any $a_1, a_2 \in \mathbb{R}$, $\boldsymbol{v}_1, \boldsymbol{v}_2 \in \mathbb{R}^D$,
>
> $$l[a_1 \boldsymbol{v}_1 + a_2 \boldsymbol{v}_2] = a_1 l(\boldsymbol{v}_1) + a_2 l[\boldsymbol{v}_2].$$
>
> A linear map with values in $\mathbb{R}$, $l : \mathbb{R}^P \to \mathbb{R}$, is called a **linear form**.

Linearity plays a crucial role in the differentiability of a function.

> **Definition 2.5** (Differentiability, single-output case). A function $f : \mathbb{R}^P \to \mathbb{R}$ is **differentiable** at $\boldsymbol{w} \in \mathbb{R}^P$ if its directional derivative is defined along any direction, linear in any direction, and if
>
> $$\lim_{\|\boldsymbol{v}\|_2 \to 0} \frac{|f(\boldsymbol{w} + \boldsymbol{v}) - f(\boldsymbol{w}) - \partial f(\boldsymbol{w})[\boldsymbol{v}]|}{\|\boldsymbol{v}\|_2} = 0.$$

We can now introduce the gradient.

> **Definition 2.6** (Gradient). The **gradient** of a differentiable function $f : \mathbb{R}^P \to \mathbb{R}$ at a point $\boldsymbol{w} \in \mathbb{R}^P$ is defined as the vector of partial derivatives
>
> $$\nabla f(\boldsymbol{w}) := \begin{pmatrix} \partial_1 f(\boldsymbol{w}) \\ \vdots \\ \partial_P f(\boldsymbol{w}) \end{pmatrix} = \begin{pmatrix} \partial f(\boldsymbol{w})[\boldsymbol{e}_1] \\ \vdots \\ \partial f(\boldsymbol{w})[\boldsymbol{e}_P] \end{pmatrix}.$$

By linearity, the directional derivative of f at $\boldsymbol{w}$ in the direction $\boldsymbol{v} = \sum_{i=1}^{P} v_i \boldsymbol{e}_i$ is then given by

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] = \sum_{i=1}^{P} v_i \partial f(\boldsymbol{w})[\boldsymbol{e}_i] = \langle \boldsymbol{v}, \nabla f(\boldsymbol{w}) \rangle.$$

In the definition above, the fact that the gradient can be used to compute the directional derivative is a mere consequence of the linearity. However, in more abstract cases presented in later sections, the gradient is defined through this property.

As a simple example, any linear function of the form $f(\boldsymbol{w}) = \boldsymbol{a}^\top \boldsymbol{w} = \sum_{i=1}^{P} a_i w_i$ is differentiable as we have $(\boldsymbol{a}^\top(\boldsymbol{w}+\boldsymbol{v}) - \boldsymbol{a}^\top \boldsymbol{w} - \boldsymbol{a}^\top \boldsymbol{v})/\|\boldsymbol{v}\|_2 = 0$ for any $\boldsymbol{v}$ and in particular for $\|\boldsymbol{v}\| \to 0$. Moreover, its gradient is naturally given by $\nabla f(\boldsymbol{w}) = \boldsymbol{a}$.

Generally, to show that a function is differentiable and find its gradient, one approach is to approximate $f(\boldsymbol{w} + \boldsymbol{v})$ around $\boldsymbol{v} = 0$. If we can find a vector $\boldsymbol{g}$ such that

$$f(\boldsymbol{w} + \boldsymbol{v}) = f(\boldsymbol{w}) + \langle \boldsymbol{g}, \boldsymbol{v} \rangle + o(\|\boldsymbol{v}\|_2),$$

then f is differentiable at $\boldsymbol{w}$ since $\langle \boldsymbol{g}, \cdot \rangle$ is linear. Moreover, $\boldsymbol{g}$ is then the gradient of f at $\boldsymbol{w}$.

Remark 2.2 (Gateaux and Fréchet differentiability)**.** Multiple definitions of differentiability exist. The one presented in Definition 2.5 is about **Fréchet differentiable** functions. Alternatively, if $f : \mathbb{R}^P \to \mathbb{R}$ has well-defined directional derivatives along any directions then the function is **Gateaux differentiable**. Note that the existence of directional derivatives in any directions is not a sufficient condition for the function to be differentiable. In other words, any Fréchet differentiable function is Gateaux differentiable, but the converse is not true. As a counter-example, one can verify that the function $f(x_1, x_2) = x_1^3/(x_1^2 + x_2^2)$ is Gateaux differentiable at 0 but not (Fréchet) differentiable at 0 (because the directional derivative at 0 is not linear).

Some authors also require Gateaux differentiable functions to have linear directional derivatives along any direction. These are

still not Fréchet differentiable functions. Indeed, the limit in Definition 2.5 is over any vectors tending to 0 (potentially in a pathological way), while directional derivatives look at such limits uniquely in terms of a single direction.

In the remainder of this chapter, all definitions of differentiability are in terms of Fréchet differentiability.

Example 2.3 illustrates how to compute the gradient of the logistic loss and validate its differentiability.

Example 2.3 (Gradient of logistic loss). Consider the logistic loss $\ell(\boldsymbol{\theta}, \boldsymbol{y}) := -\boldsymbol{y}^\top \boldsymbol{\theta} + \log \sum_{i=1}^M e^{\theta_i}$, that measures the prediction error of the logits $\boldsymbol{\theta} \in \mathbb{R}^M$ w.r.t. the correct label $\boldsymbol{y} \in \{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_M\}$. Let us compute the gradient of this loss w.r.t. $\boldsymbol{\theta}$ for fixed $\boldsymbol{y}$, i.e., we want to compute the gradient of $f(\boldsymbol{\theta}) := \ell(\boldsymbol{\theta}, \boldsymbol{y})$. Let us decompose f as $f = l + \text{logsumexp}$ with $l(\boldsymbol{\theta}) := \langle -\boldsymbol{y}, \boldsymbol{\theta} \rangle$ and

$$\text{logsumexp}(\boldsymbol{\theta}) := \log \sum_{i=1}^M e^{\theta_i},$$

the log-sum-exp function. The function l is linear so differentiable with gradient $\nabla l(\theta) = -\boldsymbol{y}$. We therefore focus on logsumexp. Denoting $\exp(\boldsymbol{\theta}) = (\exp(\theta_1), \ldots, \exp(\theta_M))$, and using that $\exp(1 + x) = 1 + x + o(x)$, and $\log(1 + x) = x + o(x)$, we get

$$\begin{aligned} \text{logsumexp}(\boldsymbol{\theta} + \boldsymbol{v}) &= \log(\langle \exp(\boldsymbol{\theta} + \boldsymbol{v}), \boldsymbol{1} \rangle) \\ &= \log(\langle \exp(\boldsymbol{\theta}), \boldsymbol{1} \rangle + \langle \exp(\boldsymbol{\theta}), \boldsymbol{v} \rangle + o(\|\boldsymbol{v}\|_2)) \\ &= \log(\langle \exp(\boldsymbol{\theta}), \boldsymbol{1} \rangle) + \left\langle \frac{\exp(\boldsymbol{\theta})}{\langle \exp(\boldsymbol{\theta}), \boldsymbol{1} \rangle}, \boldsymbol{v} \right\rangle + o(\|\boldsymbol{v}\|_2), \end{aligned}$$

The above decomposition of $\text{logsumexp}(\boldsymbol{\theta} + \boldsymbol{v})$ shows that it is differentiable, and that $\nabla \text{logsumexp}(\boldsymbol{\theta}) = \text{softargmax}(\boldsymbol{\theta})$, where

$$\text{softargmax}(\boldsymbol{\theta}) := \left(e^{\theta_1} / \left(\sum_{j=1}^M e^{\theta_j} \right), \ldots, e^{\theta_M} / \left(\sum_{j=1}^M e^{\theta_j} \right) \right).$$

In total, we then get that $\nabla f(\boldsymbol{\theta}) = -\boldsymbol{y} + \text{softargmax}(\boldsymbol{\theta})$.

Linearity of gradients

The notion of differentiability for multi-inputs functions naturally inherits from the linearity of derivatives for single-input functions. For any $u_1, \ldots, u_M \in \mathbb{R}$ and any multi-inputs functions $f_1, \ldots, f_M$ differentiable at $\boldsymbol{w}$, the function $u_1 f_1 + \ldots + u_M f_M$ is differentiable at $\boldsymbol{w}$ and its gradient is

$$\nabla(u_1 f_1 + \ldots + u_M f_M)(\boldsymbol{w}) = u_1 \nabla f_1(\boldsymbol{w}) + \ldots + u_M \nabla f_M(\boldsymbol{w}).$$

Why is the gradient useful?

The gradient defines the steepest ascent direction of f from $\boldsymbol{w}$. To see why, notice that

$$\underset{\boldsymbol{v} \in \mathbb{R}^P, \|\boldsymbol{v}\|_2 \leq 1}{\arg\max} \partial f(\boldsymbol{w})[\boldsymbol{v}] = \underset{\boldsymbol{v} \in \mathbb{R}^P, \|\boldsymbol{v}\|_2 \leq 1}{\arg\max} \langle \boldsymbol{v}, \nabla f(\boldsymbol{w}) \rangle = \nabla f(\boldsymbol{w}) / \|\nabla f(\boldsymbol{w})\|_2,$$

where we assumed $\nabla f(\boldsymbol{w}) \neq \boldsymbol{0}$. The gradient $\nabla f(\boldsymbol{w})$ is orthogonal to the level set of the function (the set of points $\boldsymbol{w}$ sharing the same value $f(\boldsymbol{w})$) and points towards higher values of f as illustrated in Fig. 2.2. Conversely, the negated gradient $-\nabla f(\boldsymbol{w})$ points towards lower values of f. This observation motivates the development of optimization algorithms such as gradient descent. It is based on iteratively performing the update $\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \gamma \nabla f(\boldsymbol{w}_t)$, for $\gamma > 0$. It therefore seeks for a minimizer of f by moving along the direction of steepest descent around $\boldsymbol{w}_t$ given, up to a multiplicative factor, by $-\nabla f(\boldsymbol{w}_t)$.

2.2.3   Jacobians

Let us now consider a multi-output function $f : \mathbb{R}^P \to \mathbb{R}^M$ defined by $f(\boldsymbol{w}) := (f_1(\boldsymbol{w}), \ldots, f_M(\boldsymbol{w}))$, where $f_j : \mathbb{R}^P \to \mathbb{R}$. A typical example in machine learning is a neural network. The notion of directional derivative can be extended to such function by defining it as the vector composed of the coordinate-wise directional derivatives:

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] := \lim_{\delta \to 0} \frac{f(\boldsymbol{w} + \delta \boldsymbol{v}) - f(\boldsymbol{w})}{\delta} = \lim_{\delta \to 0} \begin{pmatrix} \frac{f_1(\boldsymbol{w} + \delta \boldsymbol{v}) - f_1(\boldsymbol{w})}{\delta} \\ \vdots \\ \frac{f_M(\boldsymbol{w} + \delta \boldsymbol{v}) - f_M(\boldsymbol{w})}{\delta} \end{pmatrix} \in \mathbb{R}^M,$$
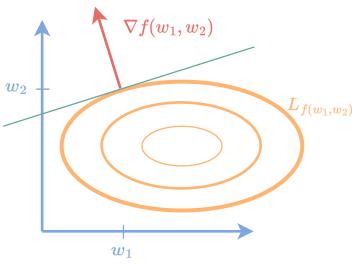
Figure 2.2: The gradient of a function $f : \mathbb{R}^2 \to \mathbb{R}$ at (w_1, w_2) is the normal vector to the tangent space of the level set $L_{f(w_1,w_2)} = \{(w_1', w_2') : f(w_1', w_2') = f(w_1, w_2)\}$ and points towards points with higher function values.
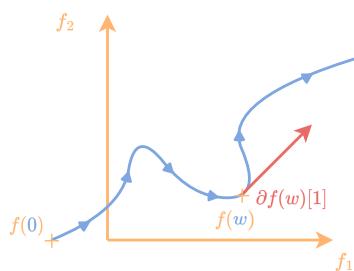
Figure 2.3: The directional derivative of a parameterized curve $f : \mathbb{R} \to \mathbb{R}^2$ at t is the tangent to the curve at the point $f(w) \in \mathbb{R}^2$.

where the limits (provided that they exist) are applied coordinate-wise. The directional derivative of f in the direction $\boldsymbol{v} \in \mathbb{R}^P$ is therefore the vector that gathers the directional derivative of each f_j, i.e., $\partial f(\boldsymbol{w})[\boldsymbol{w}] = (\partial f_j(\boldsymbol{v})[\boldsymbol{v}])_{j=1}^M$. In particular, we can define the **partial derivatives** of f at $\boldsymbol{w}$ as the vectors

$$\partial_i f(\boldsymbol{w}) := \partial f(\boldsymbol{w})[\boldsymbol{e}_i] = \begin{pmatrix} \partial_i f_1(\boldsymbol{w}) \\ \vdots \\ \partial_i f_M(\boldsymbol{w}) \end{pmatrix} \in \mathbb{R}^M.$$

As for the usual definition of the derivative, the directional derivative can provide a linear approximation of a function around a current input as illustrated in Fig. 2.3 for a parameterized curve $f : \mathbb{R} \to \mathbb{R}^2$.

Just as in the single-output case, differentiability is defined not only as the existence of directional derivatives in any direction but also by the linearity in the chosen direction.

Definition 2.7 (Differentiability, multi-output case). A function $f : \mathbb{R}^P \to \mathbb{R}^M$ is (Fréchet) **differentiable** at a point $\boldsymbol{w} \in \mathbb{R}^P$ if its directional derivative is defined along any directions, linear along

any directions, and,

$$\lim_{\|\boldsymbol{v}\|_2 \to 0} \frac{\|f(\boldsymbol{w} + \boldsymbol{v}) - f(\boldsymbol{w}) - \partial f(\boldsymbol{w})[\boldsymbol{v}]\|_2}{\|\boldsymbol{v}\|_2} = 0.$$

The partial derivatives of all function coordinates are gathered in the **Jacobian matrix**.

Definition 2.8 (Jacobian). The **Jacobian** of a differentiable function $f : \mathbb{R}^P \to \mathbb{R}^M$ at $\boldsymbol{w}$ is defined as the matrix of all partial derivatives of all coordinate functions provided they exist,

$$\boldsymbol{\partial} f(\boldsymbol{w}) := \begin{pmatrix} \partial_1 f_1(\boldsymbol{w}) & \dots & \partial_P f_1(\boldsymbol{w}) \\ \vdots & \ddots & \vdots \\ \partial_1 f_M(\boldsymbol{w}) & \dots & \partial_P f_M(\boldsymbol{w}) \end{pmatrix} \in \mathbb{R}^{M \times P}.$$

The Jacobian can be represented by stacking columns of partial derivatives or rows of gradients,

$$\boldsymbol{\partial} f(\boldsymbol{w}) = \big(\partial_1 f(\boldsymbol{w}), \dots, \partial_P f(\boldsymbol{w})\big) = \begin{pmatrix} \nabla f_1(\boldsymbol{w})^\top \\ \vdots \\ \nabla f_M(\boldsymbol{w})^\top \end{pmatrix}.$$

By linearity, the directional derivative of f at $\boldsymbol{w}$ along any input direction $\boldsymbol{v} = \sum_{i=1}^P v_i \boldsymbol{e}_i \in \mathbb{R}^P$ is then given by

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] = \sum_{i=1}^P v_i \partial_i f(\boldsymbol{w}) = \boldsymbol{\partial} f(\boldsymbol{w}) \boldsymbol{v} \in \mathbb{R}^M.$$

Notice that we use bold $\boldsymbol{\partial}$ to indicate the Jacobian matrix. The Jacobian matrix naturally generalizes the concepts of derivatives and gradients presented earlier. As for the single input case, to show that a function is differentiable, one approach is to approximate $f(\boldsymbol{w} + \boldsymbol{v})$ around $\boldsymbol{v} = \boldsymbol{0}$. If we find a linear map l such that

$$f(\boldsymbol{w} + \boldsymbol{v}) = f(\boldsymbol{w}) + l[\boldsymbol{v}] + o(\|\boldsymbol{v}\|_2),$$

then f is differentiable at $\boldsymbol{w}$. Moreover, if l is represented by matrix $\boldsymbol{J}$ such that $l[\boldsymbol{v}] = \boldsymbol{J}\boldsymbol{v}$ then $\boldsymbol{J} = \boldsymbol{\partial} f(\boldsymbol{w})$.

As a simple example, any linear function $f(\boldsymbol{w}) = \boldsymbol{A}\boldsymbol{w}$ for $\boldsymbol{A} \in \mathbb{R}^{M \times P}$ is differentiable, since all its coordinate-wise components are single-output linear functions, and the Jacobian of f at any $\boldsymbol{w}$ is given by $\boldsymbol{\partial} f(\boldsymbol{w}) = \boldsymbol{A}$.

Remark 2.3 (Special cases of the Jacobian)**.** For single-output functions $f : \mathbb{R}^P \to \mathbb{R}$, i.e., $M = 1$, the Jacobian matrix reduces to a row vector identified as the transpose of the gradient, i.e.,

$$\boldsymbol{\partial} f(\boldsymbol{w}) = \nabla f(\boldsymbol{w})^\top \in \mathbb{R}^{1 \times P}.$$

For a single-input function $f : \mathbb{R} \to \mathbb{R}^M$, the Jacobian reduces to a single column vector of directional derivatives, denoted

$$\boldsymbol{\partial} f(w) = f'(w) := \begin{pmatrix} f_1'(w) \\ \vdots \\ f_M'(w) \end{pmatrix} \in \mathbb{R}^{M \times 1}.$$

For a single-input single-output function $f : \mathbb{R} \to \mathbb{R}$, the Jacobian reduces to the derivative of f, i.e.,

$$\boldsymbol{\partial} f(w) = f'(w) \in \mathbb{R}.$$

Example 2.4 illustrates the form of the Jacobian matrix for the element-wise application of a differentiable function such as the softplus activation. This example already shows that the Jacobian takes a simple diagonal matrix form. As a consequence, the directional derivative associated with this function is simply given by an element-wise product rather than a full matrix-vector product as suggested in Definition 2.8. We will revisit this point in Section 2.3.

Example 2.4 (Jacobian matrix of the softplus activation)**.** Consider the element-wise application of the softplus defined for $\boldsymbol{w} \in \mathbb{R}^P$ by

$$f(\boldsymbol{w}) := \begin{pmatrix} \sigma(w_1) \\ \vdots \\ \sigma(w_P) \end{pmatrix} \in \mathbb{R}^P \quad \text{where} \quad \sigma(w) := \log(1 + e^w).$$

Since σ is differentiable, each coordinate of this function is differentiable and the overall function is differentiable. The jth coordinate of f is independent of the ith coordinate of $\boldsymbol{w}$ for $i \neq j$, so $\partial_i f_j(\boldsymbol{w}) = 0$ for $i \neq j$. For $i = j$, the result boils down to the derivative of σ at w_j. That is, $\partial_j f_j(\boldsymbol{w}) = \sigma'(w_j)$, where $\sigma'(w) = e^w/(1 + e^w)$. The Jacobian of f is therefore a diagonal matrix

$$\boldsymbol{\partial} f(\boldsymbol{w}) = \mathbf{diag}(\sigma'(w_1), \ldots, \sigma'(w_P)) := \begin{pmatrix} \sigma'(w_1) & 0 & \ldots & & 0 \\ 0 & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & & \ldots & 0 & \sigma'(w_P) \end{pmatrix}.$$

Variations along outputs

Rather than considering variations of f along an **input** direction $\boldsymbol{v} \in \mathbb{R}^P$, we may also consider the variations of f along an **output** direction $\boldsymbol{u} \in \mathbb{R}^M$, namely, computing the gradients $\nabla(\boldsymbol{u}^\top f)(\boldsymbol{w})$ of single-output functions, where we defined

$$(\boldsymbol{u}^\top f)(\boldsymbol{w}) := \boldsymbol{u}^\top f(\boldsymbol{w}) \in \mathbb{R}.$$

In particular, we may consider computing the gradients $\nabla f_j(\boldsymbol{w})$ of each function coordinate $f_j = \boldsymbol{e}_j^\top f$ at $\boldsymbol{w}$, where $\boldsymbol{e}_j$ is the jth canonical vector in $\mathbb{R}^M$. The infinitesimal variations of f at $\boldsymbol{w}$ along any output direction $\boldsymbol{u} = \sum_{j=1}^M u_j \boldsymbol{e}_j \in \mathbb{R}^M$ are given by

$$\nabla(\boldsymbol{u}^\top f)(\boldsymbol{w}) = \sum_{j=1}^M u_j \nabla f_j(\boldsymbol{w}) = \boldsymbol{\partial} f(\boldsymbol{w})^\top \boldsymbol{u} \in \mathbb{R}^P,$$

where $\boldsymbol{\partial} f(\boldsymbol{w})^\top$ is the Jacobian's transpose. Using the definition of derivative as a limit, we obtain for $i \in [P]$

$$\nabla_i(\boldsymbol{u}^\top f)(\boldsymbol{w}) = [\boldsymbol{\partial} f(\boldsymbol{w})^\top \boldsymbol{u}]_i = \lim_{\delta \to 0} \frac{\boldsymbol{u}^\top (f(\boldsymbol{w} + \delta \boldsymbol{e}_i) - f(\boldsymbol{w}))}{\delta}.$$

Chain rule

Equipped with a generic definition of differentiability and the associated objects, gradients and Jacobians, we can now generalize the chain rule,

previously introduced for single-input single-output functions.

Proposition 2.2 (Chain rule)**.** Consider $f : \mathbb{R}^P \to \mathbb{R}^M$ and $g : \mathbb{R}^M \to \mathbb{R}^R$. If f is differentiable at $\boldsymbol{w} \in \mathbb{R}^P$ and g is differentiable at $f(\boldsymbol{w}) \in \mathbb{R}^M$, then the composition $g \circ f$ is differentiable at $\boldsymbol{w} \in \mathbb{R}^P$ and its Jacobian is given by

$$\boldsymbol{\partial}(g \circ f)(\boldsymbol{w}) = \boldsymbol{\partial}g(f(\boldsymbol{w}))\boldsymbol{\partial}f(\boldsymbol{w}).$$

Proof. We progressively approximate $g \circ f(\boldsymbol{w} + \boldsymbol{v})$ using the differentiability of f at $\boldsymbol{w}$ and g at $f(\boldsymbol{w})$,

$$g(f(\boldsymbol{w} + \boldsymbol{v})) = g(f(\boldsymbol{w}) + \boldsymbol{\partial}f(\boldsymbol{w})\boldsymbol{v} + o(\|\boldsymbol{v}\|))$$
$$= g(f(\boldsymbol{w})) + \boldsymbol{\partial}g(f(\boldsymbol{w}))\boldsymbol{\partial}f(\boldsymbol{w})\boldsymbol{v} + o(\|\boldsymbol{v}\|).$$

Hence, $g \circ f$ is differentiable at $\boldsymbol{w}$ with Jacobian $\boldsymbol{\partial}g(f(\boldsymbol{w}))\boldsymbol{\partial}f(\boldsymbol{w})$. $\quad\square$

Proposition 2.2 can be seen as the cornerstone of any derivative computations. For example, it can be used to rederive the linearity or the product rule associated to the derivatives of single-input single-outptut functions.

When g is scalar-valued, combined with Remark 2.3, we obtain a simple expression for $\nabla(g \circ f)$.

Proposition 2.3 (Chain rule, scalar-valued case)**.** Consider $f : \mathbb{R}^P \to \mathbb{R}^M$ and $g : \mathbb{R}^M \to \mathbb{R}$. The gradient of the composition is given by

$$\nabla(g \circ f)(\boldsymbol{w}) = \boldsymbol{\partial}f(\boldsymbol{w})^\top \nabla g(f(\boldsymbol{w})).$$

This is illustrated with linear regression in Example 2.5.

Example 2.5 (Linear regression)**.** Consider the squared residuals of a linear regression of N inputs $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^D$ onto N targets $y_1, \ldots, y_N \in \mathbb{R}$ with a vector $\boldsymbol{w} \in \mathbb{R}^D$, that is, $f(\boldsymbol{w}) = \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|_2^2 = \sum_{i=1}^N (\boldsymbol{x}_i^\top \boldsymbol{w} - y_i)^2$ for $\boldsymbol{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)^\top \in \mathbb{R}^{N \times D}$ and $\boldsymbol{y} = (y_1, \ldots, y_N)^\top \in \mathbb{R}^N$.

The function f can be decomposed into a linear mapping $f_1(\boldsymbol{w}) = \boldsymbol{X}\boldsymbol{w}$ and a squared error $f_2(\boldsymbol{p}) = \|\boldsymbol{p} - \boldsymbol{y}\|_2^2$, so that $f = f_2 \circ f_1$. We can then apply the chain rule in Proposition 2.3 to

get

$$\nabla f(\boldsymbol{w}) = \boldsymbol{\partial} f_1(\boldsymbol{w})^\top \nabla f_2(f_1(\boldsymbol{w}))$$

provided that f_1, f_2 are differentiable at $\boldsymbol{w}$ and $f_1(\boldsymbol{w})$, respectively.

The function f_1 is linear so differentiable with Jacobian $\boldsymbol{\partial} f_1(\boldsymbol{w}) = \boldsymbol{X}$. On the other hand the partial derivatives of f_2 are given by $\partial_j f_2(\boldsymbol{p}) = 2(p_j - y_j)$ for $j \in \{1, \dots, N\}$. Therefore, f_2 is differentiable at any $\boldsymbol{p}$ and its gradient is $\nabla f_2(\boldsymbol{p}) = 2(\boldsymbol{p} - \boldsymbol{y})$. By combining the computations of the Jacobian of f_1 and the gradient of f_2, we then get the gradient of f as

$$\nabla f(\boldsymbol{w}) = 2\boldsymbol{X}^\top (f_1(\boldsymbol{w}) - \boldsymbol{y}) = 2\boldsymbol{X}^\top (\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}).$$

2.3   Linear differentiation maps

The Jacobian matrix is useful as a representation of the partial derivatives. However, the core idea underlying the definition of differentiable functions, as well as their implementation in an autodiff framework, lies in the access to two key **linear maps**. These two maps encode infinitesimal variations along **input** or **output** directions and are referred to, respectively, as **Jacobian-vector product** (JVP) and **Vector-jacobian product** (VJP). This section formalizes these notions, in the context of Euclidean spaces.

2.3.1   The need for linear maps

So far, we have focused on functions $f \colon \mathbb{R}^P \to \mathbb{R}^M$, that take a vector as input and produce a vector as output. However, functions that use matrix or even tensor inputs/outputs are common place in neural networks. For example, consider the function of matrices of the form $f(\boldsymbol{W}) = \boldsymbol{W}\boldsymbol{x}$, where $\boldsymbol{x} \in \mathbb{R}^D$ and $\boldsymbol{W} \in \mathbb{R}^{M \times D}$. This function takes a matrix as input, not a vector. Of course, a matrix $\boldsymbol{W} \in \mathbb{R}^{M \times D}$ can always be "flattened" into a vector $\boldsymbol{w} \in \mathbb{R}^{MD}$, by stacking the columns of $\boldsymbol{W}$. We denote this operation by $\boldsymbol{w} = \text{vec}(\boldsymbol{W})$ and its inverse by $\boldsymbol{W} = \text{vec}^{-1}(\boldsymbol{w})$. We can then equivalently write $f(\boldsymbol{W})$ as $\tilde{f}(\boldsymbol{w}) = f(\text{vec}^{-1}(\boldsymbol{w})) = \text{vec}^{-1}(\boldsymbol{w})\boldsymbol{x}$, so that the previous framework applies. However, we will now see that this would be inefficient.

Indeed, the resulting Jacobian of $\tilde{f}$ at any $\boldsymbol{w}$ consists in a matrix of size $\mathbb{R}^{M \times MD}$, which, after some computations, can be observed to be mostly filled with zeros. Getting the directional derivative of f at $\boldsymbol{W} \in \mathbb{R}^{M \times D}$ in a direction $\boldsymbol{V} \in \mathbb{R}^{M \times D}$ would consist in (i) vectorizing $\boldsymbol{V}$ into $\boldsymbol{v} = \text{vec}(\boldsymbol{V})$, (ii) computing the matrix-vector product $\partial \tilde{f}(\boldsymbol{w})\boldsymbol{v}$ at a cost of $M^3 D^2$ computations (ignoring the fact that the Jacobian has zero entries), (iii) re-shaping the result into a matrix.

On the other hand, since f is linear in its matrix input, we can infer that the directional derivative of f at any $\boldsymbol{W} \in \mathbb{R}^{M \times D}$ in any direction $\boldsymbol{V} \in \mathbb{R}^{M \times D}$ is simply given by the function itself applied on $\boldsymbol{V}$. Namely, we have $\partial f(\boldsymbol{W})[\boldsymbol{V}] = f(\boldsymbol{V}) = \boldsymbol{V}\boldsymbol{x}$, which is simple to implement and clearly only requires MD^2 operations. Note that the cost would have been the same, had we ignored the non-zero entries of $\partial \tilde{f}(\boldsymbol{w})$. The point here is that by considering the operations associated to the differentiation of a function as linear maps rather than using the associated representation as a Jacobian matrix, we can streamline the associated implementations and exploit the structures of the underlying input or output space. To that end, we now recall the main abstractions necessary to extend the previous definitions in the context of Euclidean spaces.

2.3.2 Euclidean spaces

Linear spaces, a.k.a. **vector spaces**, are spaces equipped (and closed under) an addition rule compatible with multiplication by a scalar (we limit ourselves to the field of reals). Namely, in a vector space $\mathcal{E}$, there exists the operations $+$ and $\cdot$, such that for any $\boldsymbol{u}$, $\boldsymbol{v} \in \mathcal{E}$, and $a \in \mathbb{R}$, we have $\boldsymbol{u} + \boldsymbol{v} \in \mathcal{E}$ and $a \cdot \boldsymbol{u} \in \mathcal{E}$. **Euclidean spaces** are linear spaces equipped with a basis $\boldsymbol{e}_1, \ldots, \boldsymbol{e}_P \in \mathcal{E}$. Any element $\boldsymbol{v} \in \mathcal{E}$ can be decomposed as $\boldsymbol{v} = \sum_{i=1}^{P} v_i \boldsymbol{e}_i$ for some unique scalars $v_1, \ldots, v_P \in \mathbb{R}$. A canonical example of Euclidean space is the set $\mathbb{R}^P$ of all vectors of size P that we already covered. The set of matrices $\mathbb{R}^{P_1 \times P_2}$ of size $P_1 \times P_2$ is also naturally a Euclidean space generated by the set of canonical matrices $\boldsymbol{E}_{ij} \in \{0, 1\}^{P_1 \times P_2}$ for $i \in [P_1], j \in [P_2]$ filled with zero except at the $(i, j)^{\text{th}}$ entry filled with one. For example, $\boldsymbol{W} \in \mathbb{R}^{P_1 \times P_2}$ can be written $\boldsymbol{W} = \sum_{i,j=1}^{P_1, P_2} W_{ij} \boldsymbol{E}_{ij}$.

Euclidean spaces are naturally equipped with a notion of inner product defined below.

Definition 2.9 (Inner product)**.** An **inner product** on a vector space $\mathcal{E}$ is a function $\langle \cdot, \cdot \rangle : \mathcal{E} \times \mathcal{E} \to \mathbb{R}$ that is

- bilinear, that is, $\boldsymbol{x} \mapsto \langle \boldsymbol{x}, \boldsymbol{w} \rangle$ and $\boldsymbol{y} \mapsto \langle \boldsymbol{v}, \boldsymbol{y} \rangle$ are linear for any $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{E}$

- symmetric, that is, $\langle \boldsymbol{w}, \boldsymbol{v} \rangle = \langle \boldsymbol{w}, \boldsymbol{v} \rangle$ for any $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{E}$

- positive definite, that is, $\langle \boldsymbol{w}, \boldsymbol{w} \rangle \geq 0$ for any $\boldsymbol{w} \in \mathcal{E}$, and $\langle \boldsymbol{w}, \boldsymbol{w} \rangle = 0$ if and only if $\boldsymbol{w} = 0$.

An inner product defines a norm $\|\boldsymbol{w}\| := \sqrt{\langle \boldsymbol{w}, \boldsymbol{w} \rangle}$.

The norm induced by an inner product defines a distance $\|\boldsymbol{w} - \boldsymbol{v}\|$ between $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{E}$, and therefore a notion of convergence.

For vectors, where $\mathcal{E} = \mathbb{R}^P$, the inner product is the usual one $\langle \boldsymbol{w}, \boldsymbol{v} \rangle = \sum_{i=1}^{P} w_i v_i$. For matrices, where $\mathcal{E} = \mathbb{R}^{P_1 \times P_2}$, the inner product is the so-called Frobenius inner product. It is defined for any $\boldsymbol{W}, \boldsymbol{V} \in \mathbb{R}^{P_1 \times P_2}$ by

$$\langle \boldsymbol{W}, \boldsymbol{V} \rangle := \langle \mathrm{vec}(\boldsymbol{W}), \mathrm{vec}(\boldsymbol{V}) \rangle = \sum_{i,j=1}^{P_1, P_2} W_{ij} V_{ij} = \mathrm{tr}(\boldsymbol{W}^\top \boldsymbol{V}),$$

where $\mathrm{tr}(\boldsymbol{Z}) := \sum_{i=1}^{P} Z_{ii}$ is the trace operator defined for square matrices $\boldsymbol{Z} \in \mathbb{R}^{P \times P}$. For tensors of order R, which generalize matrices to $\mathcal{E} = \mathbb{R}^{P_1 \times \ldots \times P_R}$, the inner product is defined similarly for $\mathsf{W}, \mathsf{V} \in \mathbb{R}^{P_1 \times \ldots \times P_R}$ by

$$\langle \mathsf{W}, \mathsf{V} \rangle := \langle \mathrm{vec}(\mathsf{W}), \mathrm{vec}(\mathsf{V}) \rangle = \sum_{i_1, \ldots, i_R = 1}^{P_1, \ldots, P_R} \mathsf{W}_{i_1 \ldots i_R} \mathsf{V}_{i_1 \ldots i_R},$$

where $\mathsf{W}_{i_1 \ldots i_R}$ is the $(i_1, \ldots, i_R)^{\mathrm{th}}$ entry of W.

2.3.3 Linear maps and their adjoints

The notion of linear map defined in Definition 2.4 naturally extends to Euclidean spaces. Namely, a function $l : \mathcal{E} \to \mathcal{F}$ from a Euclidean

space $\mathcal{E}$ onto a Euclidean space $\mathcal{F}$ is a **linear map** if for any $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{E}$ and $a, b \in \mathbb{R}$, we have $l[a\boldsymbol{w} + b\boldsymbol{v}] = a \cdot l[\boldsymbol{w}] + b \cdot l[\boldsymbol{v}]$. When $\mathcal{E} = \mathbb{R}^P$ and $\mathcal{F} = \mathbb{R}^M$, there always exists a matrix $\boldsymbol{A} \in \mathbb{R}^{M \times P}$ such that $l[\boldsymbol{x}] = \boldsymbol{A}\boldsymbol{x}$. Therefore, we can think of $\boldsymbol{A}$ as the "materialization" of l.

We can define the adjoint operator of a linear map.

> **Definition 2.10** (Adjoint operator). Given two Euclidean spaces $\mathcal{E}$ and $\mathcal{F}$ equipped with inner products $\langle \cdot, \cdot \rangle_\mathcal{E}$ and $\langle \cdot, \cdot \rangle_\mathcal{F}$, the **adjoint** of a linear map $l : \mathcal{E} \to \mathcal{F}$ is the unique linear map $l^* : \mathcal{F} \to \mathcal{E}$ such that for any $\boldsymbol{v} \in \mathcal{E}$ and $\boldsymbol{u} \in \mathcal{F}$,
>
> $$\langle l[\boldsymbol{v}], \boldsymbol{u} \rangle_\mathcal{F} = \langle \boldsymbol{v}, l^*[\boldsymbol{u}] \rangle_\mathcal{E}.$$

The adjoint can be thought as the counterpart of the matrix transpose for linear maps. When $l[\boldsymbol{v}] = \boldsymbol{A}\boldsymbol{v}$, we have $l^*[\boldsymbol{u}] = \boldsymbol{A}^\top \boldsymbol{u}$ since

$$\langle l[\boldsymbol{v}], \boldsymbol{u} \rangle_\mathcal{F} = \langle \boldsymbol{A}\boldsymbol{v}, \boldsymbol{u} \rangle_\mathcal{F} = \langle \boldsymbol{v}, \boldsymbol{A}^\top \boldsymbol{u} \rangle_\mathcal{E} = \langle \boldsymbol{v}, l^*[\boldsymbol{u}] \rangle_\mathcal{E}.$$

2.3.4 Jacobian-vector products

We now define the directional derivative using linear maps, leading to the notion of Jacobian-vector product (JVP). This can be used to facilitate the treatment of functions on matrices or be used for further extensions to infinite-dimensional spaces. In the following, $\mathcal{E}$ and $\mathcal{F}$ denote two Euclidean spaces equipped with norms $\langle \cdot, \cdot \rangle_\mathcal{E}$ and $\langle \cdot, \cdot \rangle_\mathcal{F}$. We start by defining differentiability in general Euclidean spaces.

> **Definition 2.11** (Differentiability in Euclidean spaces). A function $f : \mathcal{E} \to \mathcal{F}$ is **differentiable** at a point $\boldsymbol{w} \in \mathcal{E}$ if the **directional derivative** along $\boldsymbol{v} \in \mathcal{E}$
>
> $$\partial f(\boldsymbol{w})[\boldsymbol{v}] := \lim_{\delta \to 0} \frac{f(\boldsymbol{w} + \delta\boldsymbol{v}) - f(\boldsymbol{w})}{\delta} = l[\boldsymbol{v}],$$
>
> is well-defined for any $\boldsymbol{v} \in \mathcal{E}$, linear in $\boldsymbol{v}$ and if
>
> $$\lim_{\|\boldsymbol{v}\|_2 \to 0} \frac{\|f(\boldsymbol{w} + \boldsymbol{v}) - f(\boldsymbol{w}) - l[\boldsymbol{v}]\|_2}{\|\boldsymbol{v}\|_2} = 0.$$

We can now formally define the Jacobian-vector product.

Definition 2.12 (Jacobian-vector product)**.** For a differentiable function $f : \mathcal{E} \to \mathcal{F}$, the **linear map** $\partial f(\boldsymbol{w}) : \mathcal{E} \to \mathcal{F}$, mapping $\boldsymbol{v}$ to $\partial f(\boldsymbol{w})[\boldsymbol{v}]$ is called the **Jacobian-vector product** (JVP) by analogy with Definition 2.8. Note that $\partial f \colon \mathcal{E} \to (\mathcal{E} \to \mathcal{F})$.

Strictly speaking, $\boldsymbol{v}$ belongs to $\mathcal{E}$. Therefore it may not be a vector, if for instance $\mathcal{E}$ is the set of real matrices. We adopt the name JVP, as it is standard in the literature.

Recovering the gradient

Previously, we saw that for differentiable functions with vector input and scalar output, the directional derivative is equal to the inner product between the direction and the gradient. The same applies when considering differentiable functions from a Euclidean space with single outputs, except that the gradient is now an element of the input space and the inner product is the one associated with the input space.

Proposition 2.4 (Gradient)**.** If a function $f : \mathcal{E} \to \mathbb{R}$ is differentiable at $\boldsymbol{w} \in \mathcal{E}$, then there exists $\nabla f(\boldsymbol{w}) \in \mathcal{E}$, called the **gradient** of f at $\boldsymbol{w}$ such that the directional derivative of f at $\boldsymbol{w}$ along any input direction $\boldsymbol{v} \in \mathcal{E}$ is given by

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] = \langle \nabla f(\boldsymbol{w}), \boldsymbol{v} \rangle_{\mathcal{E}}.$$

In Euclidean spaces, the existence of the gradient can simply be shown by decomposing the partial derivative along a basis of $\mathcal{E}$. Such a definition generalizes to infinite-dimensional (e.g., Hilbert spaces) spaces as seen in Section 2.3.9.

2.3.5   Vector-Jacobian products

For functions with vector input and vector outputs, we already discussed infinitesimal variations along output directions. The same approach applies for Euclidean spaces and is tied to the adjoint of the JVP as detailed in Proposition 2.5.

Proposition 2.5 (Vector-Jacobian product). If a function $f : \mathcal{E} \to \mathcal{F}$ is differentiable at $\boldsymbol{w} \in \mathcal{E}$, then its infinitesimal variation along an output direction $\boldsymbol{u} \in \mathcal{F}$ is given by the **adjoint map** $\partial f(\boldsymbol{w})^* \colon \mathcal{F} \to \mathcal{E}$ of the JVP, called the **vector-Jacobian product** (VJP). It satisfies

$$\nabla \langle \boldsymbol{u}, f \rangle_{\mathcal{F}}(\boldsymbol{w}) = \partial f(\boldsymbol{w})^*[\boldsymbol{u}],$$

where we denoted $\langle \boldsymbol{u}, f \rangle_{\mathcal{F}}(\boldsymbol{w}) \coloneqq \langle \boldsymbol{u}, f(\boldsymbol{w}) \rangle_{\mathcal{F}}$. Note that $\partial f(\cdot)^* \colon \mathcal{E} \to (\mathcal{F} \to \mathcal{E})$.

Proof. The chain rule presented in Proposition 2.2 naturally generalizes to Euclidean spaces (see Proposition 2.6). Since $\langle \boldsymbol{u}, \cdot \rangle$ is linear, its directional derivative is itself. Therefore, the directional derivative of $\langle \boldsymbol{u}, f \rangle_{\mathcal{F}}$ is

$$\begin{aligned}
\partial(\langle \boldsymbol{u}, f \rangle_{\mathcal{F}})(\boldsymbol{w})[\boldsymbol{v}] &= \langle \boldsymbol{u}, \partial f(\boldsymbol{w})[\boldsymbol{v}] \rangle_{\mathcal{F}} \\
&= \langle \partial f(\boldsymbol{w})^*[\boldsymbol{u}], \boldsymbol{v} \rangle_{\mathcal{F}}.
\end{aligned}$$

As this is true for any $\boldsymbol{v} \in \mathcal{E}$, $\partial f(\boldsymbol{w})^*[\boldsymbol{u}]$ is the gradient of $\langle \boldsymbol{u}, f \rangle_{\mathcal{F}}$ per Proposition 2.4. □

2.3.6 Chain rule

The chain rule presented before in terms of Jacobian matrices can readily be formulated in terms of linear maps to take advantage of the implementations of the JVP and VJP as linear maps.

Proposition 2.6 (Chain rule, general case). Consider $f : \mathcal{E} \to \mathcal{F}$ and $g : \mathcal{F} \to \mathcal{G}$ for $\mathcal{E}, \mathcal{F}, \mathcal{G}$ some Euclidean spaces. If f is differentiable at $\boldsymbol{w} \in \mathcal{E}$ and g is differentiable at $f(\boldsymbol{w}) \in \mathcal{F}$, then the composition $g \circ f$ is differentiable at $\boldsymbol{w} \in \mathcal{E}$. Its JVP is given by

$$\partial(g \circ f)(\boldsymbol{w})[\boldsymbol{v}] = \partial g(f(\boldsymbol{w}))[\partial f(\boldsymbol{w})[\boldsymbol{v}]]$$

and its VJP is given by

$$\partial(g \circ f)(\boldsymbol{w})^*[\boldsymbol{u}] = \partial f(\boldsymbol{w})^*[\partial g(f(\boldsymbol{w}))^*[\boldsymbol{u}]].$$

The proof follows the one of Proposition 2.2. When the last function is scalar-valued, which is often the case in machine learning, we obtain the following simplified result.

Proposition 2.7 (Chain rule, scalar case). Consider $f : \mathcal{E} \to \mathcal{F}$ and $g : \mathcal{F} \to \mathbb{R}$, the gradient of the composition is given by

$$\nabla(g \circ f)(\boldsymbol{w}) = \partial f(\boldsymbol{w})^*[\nabla g(f(\boldsymbol{w}))].$$

2.3.7   Functions of multiple inputs (fan-in)

Oftentimes, the inputs of a function do not belong to only one Euclidean space but to a product of them. An example is $f(\boldsymbol{x}, \boldsymbol{W}) = \boldsymbol{W}\boldsymbol{x}$, which is defined on $\mathcal{E} = \mathbb{R}^D \times \mathbb{R}^{M \times D}$. In such a case, it is convenient to generalize the notion of partial derivatives to handle blocks of inputs.

Consider a function $f(\boldsymbol{w}_1, \ldots, \boldsymbol{w}_S)$ defined on $\mathcal{E} = \mathcal{E}_1 \times \ldots \times \mathcal{E}_S$, where $\boldsymbol{w}_i \in \mathcal{E}_i$. We denote the partial derivative with respect to the ith input $\boldsymbol{w}_i$ along $\boldsymbol{v}_i \in \mathcal{E}_i$ as $\partial_i f(\boldsymbol{w}_1, \ldots, \boldsymbol{w}_S)[\boldsymbol{v}_i]$. Equipped with this notation, we can analyze how JVPs or VJPs are decomposed along several inputs.

Proposition 2.8 (Multiple inputs). Consider a differentiable function of the form $f(\boldsymbol{w}) = f(\boldsymbol{w}_1, \ldots, \boldsymbol{w}_S)$ with signature $f : \mathcal{E} \to \mathcal{F}$, where $\boldsymbol{w} := (\boldsymbol{w}_1, \ldots, \boldsymbol{w}_S) \in \mathcal{E}$ and $\mathcal{E} := \mathcal{E}_1 \times \cdots \times \mathcal{E}_S$. Then the JVP with the input direction $\boldsymbol{v} = (\boldsymbol{v}_1, \ldots, \boldsymbol{v}_S) \in \mathcal{E}$ is given by

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] = \partial f(\boldsymbol{w}_1, \ldots, \boldsymbol{w}_S)[\boldsymbol{v}_1, \ldots, \boldsymbol{v}_S] \in \mathcal{F}$$
$$= \sum_{i=1}^{S} \partial_i f(\boldsymbol{w}_1, \ldots, \boldsymbol{w}_S)[\boldsymbol{v}_i].$$

The VJP with the output direction $\boldsymbol{u} \in \mathcal{F}$ is given by

$$\partial f(\boldsymbol{w})^*[\boldsymbol{u}] = \partial f(\boldsymbol{w}_1, \ldots, \boldsymbol{w}_S)^*[\boldsymbol{u}] \in \mathcal{E}$$
$$= (\partial_1 f(\boldsymbol{w}_1, \ldots, \boldsymbol{w}_S)^*[\boldsymbol{u}], \ldots, \partial_S f(\boldsymbol{w}_1, \ldots, \boldsymbol{w}_S)^*[\boldsymbol{u}]).$$

Example 2.6 (Matrix-vector product). Consider $f(\boldsymbol{x}, \boldsymbol{W}) = \boldsymbol{W}\boldsymbol{x}$, where $\boldsymbol{W} \in \mathbb{R}^{M \times D}$ and $\boldsymbol{x} \in \mathbb{R}^D$. This corresponds to setting $\mathcal{E} = \mathcal{E}_1 \times \mathcal{E}_2 = \mathbb{R}^D \times \mathbb{R}^{M \times D}$ and $\mathcal{F} = \mathbb{R}^M$. For the JVP, letting $\boldsymbol{v} \in \mathbb{R}^D$ and $\boldsymbol{V} \in \mathbb{R}^{M \times D}$, we obtain

$$\partial f(\boldsymbol{x}, \boldsymbol{W})[\boldsymbol{v}, \boldsymbol{V}] = \boldsymbol{W}\boldsymbol{v} + \boldsymbol{V}\boldsymbol{x} \in \mathcal{F}.$$

We can also access the individual JVPs as

$$\partial_1 f(\boldsymbol{x}, \boldsymbol{W})[\boldsymbol{v}] = \boldsymbol{W}\boldsymbol{v} \in \mathcal{F},$$
$$\partial_2 f(\boldsymbol{x}, \boldsymbol{W})[\boldsymbol{V}] = \boldsymbol{V}\boldsymbol{x} \in \mathcal{F}.$$

For the VJP, letting $\boldsymbol{u} \in \mathbb{R}^M$, we obtain

$$\partial f(\boldsymbol{x}, \boldsymbol{W})^*[\boldsymbol{u}] = (\boldsymbol{W}^\top \boldsymbol{u}, \boldsymbol{u}\boldsymbol{x}^\top) \in \mathcal{E}.$$

We can access the individual VJPs by

$$\partial_1 f(\boldsymbol{x}, \boldsymbol{W})^*[\boldsymbol{u}] = \boldsymbol{W}^\top \boldsymbol{u} \in \mathcal{E}_1,$$
$$\partial_2 f(\boldsymbol{x}, \boldsymbol{W})^*[\boldsymbol{u}] = \boldsymbol{u}\boldsymbol{x}^\top \in \mathcal{E}_2.$$

Remark 2.4 (Nested inputs). It is sometimes convenient to group inputs in meaningful parts. For instance, if the input is naturally broken down into two parts $\boldsymbol{x} = (\boldsymbol{x}_1, \boldsymbol{x}_2)$, where $\boldsymbol{x}_1$ is a text part and $\boldsymbol{x}_2$ is an image part, and the network parameters are naturally grouped into three layers $\boldsymbol{w} = (\boldsymbol{w}_1, \boldsymbol{w}_2, \boldsymbol{w}_3)$, we can write $f(\boldsymbol{x}, \boldsymbol{w}) = f((\boldsymbol{x}_1, \boldsymbol{x}_2), (\boldsymbol{w}_1, \boldsymbol{w}_2, \boldsymbol{w}_3))$. This is mostly a convenience and we can again reduce it to a function of a single input, thanks to the linear map perspective in Euclidean spaces.

Remark 2.5 (Hiding away inputs). It will often be convenient to ignore inputs when differentiating. We use the semicolon for this

purpose. For instance, a function of the form $L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y})$ (notice the semicolon) has signature $L \colon \mathcal{W} \to \mathbb{R}$ because we treat $\boldsymbol{x}$ and $\boldsymbol{y}$ as constants. Therefore, the gradient is $\nabla L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}) \in \mathcal{W}$. On the other hand, the function $L(\boldsymbol{w}, \boldsymbol{x}, \boldsymbol{y})$ (notice the comma) has signature $L \colon \mathcal{W} \times \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ so its gradient is $\nabla L(\boldsymbol{w}, \boldsymbol{x}, \boldsymbol{y}) \in \mathcal{W} \times \mathcal{X} \times \mathcal{Y}$. If we need to access partial gradients, we use indexing, e.g., $\nabla_1 L(\boldsymbol{w}, \boldsymbol{x}, \boldsymbol{y}) \in \mathcal{W}$ or $\nabla_{\boldsymbol{w}} L(\boldsymbol{w}, \boldsymbol{x}, \boldsymbol{y}) \in \mathcal{W}$ when there is no ambiguity.

2.3.8 Functions of multiple outputs (fan-out)

Similarly, it is often convenient to deal with functions of multiple outputs.

Proposition 2.9 (Multiple outputs). Consider a differentiable function of the form $f(\boldsymbol{w}) = (f_1(\boldsymbol{w}), \ldots, f_T(\boldsymbol{w}))$, with signatures $f \colon \mathcal{E} \to \mathcal{F}$ and $f_i \colon \mathcal{E} \to \mathcal{F}_i$, where $\mathcal{F} := \mathcal{F}_1 \times \cdots \times \mathcal{F}_T$. Then the JVP with the input direction $\boldsymbol{v} \in \mathcal{E}$ is given by

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] = (\partial f_1(\boldsymbol{w})[\boldsymbol{v}], \ldots, \partial f_T(\boldsymbol{w})[\boldsymbol{v}]) \in \mathcal{F}.$$

The VJP with the output direction $\boldsymbol{u} = (\boldsymbol{u}_1, \ldots, \boldsymbol{u}_T) \in \mathcal{F}$ is

$$\partial f(\boldsymbol{w})^*[\boldsymbol{u}] = \partial f(\boldsymbol{w})^*[\boldsymbol{u}_1, \ldots, \boldsymbol{u}_T] \in \mathcal{E}$$
$$= \sum_{i=1}^{T} \partial f_i(\boldsymbol{w})^*[\boldsymbol{u}_i].$$

Combined with the chain rule, we obtain that the Jacobian of

$$\boldsymbol{h}(\boldsymbol{w}) := g(f(\boldsymbol{w})) = g(f_1(\boldsymbol{w}), \ldots, f_T(\boldsymbol{w}))$$

is $\partial \boldsymbol{h}(\boldsymbol{w}) = \sum_{i=1}^{T} \partial_i f(g(\boldsymbol{w})) \circ \partial g_i(\boldsymbol{w})$ and therefore the JVP is

$$\partial \boldsymbol{h}(\boldsymbol{w})[\boldsymbol{v}] = \sum_{i=1}^{T} \partial_i f(g(\boldsymbol{w}))[\partial g_i(\boldsymbol{w})[\boldsymbol{v}]].$$

2.3.9 Extensions to non-Euclidean linear spaces

We focused on Euclidean spaces, i.e., linear spaces with a finite basis. However, the notions introduced earlier can be defined in more generic

spaces.

For example, **directional derivatives** (see Definition 2.11) can be defined in any linear space equipped with a norm and complete with respect to this norm. Such spaces are called **Banach spaces**. Completeness is a technical assumption that requires that any Cauchy sequence converges (a Cauchy sequence is a sequence whose elements become arbitrarily close to each other as the sequence progresses). A function $f : \mathcal{E} \to \mathcal{F}$ defined from a Banach space $\mathcal{E}$ onto a Banach space $\mathcal{F}$ is then called **Gateaux differentiable** if its directional derivative is defined along any direction (where limits are defined w.r.t. the norm in $\mathcal{F}$). Some authors also require the directional derivative to be linear to define a Gateaux differentiable function.

Fréchet differentiability can also naturally be generalized to Banach spaces. The only difference is that, in generic Banach spaces, the linear map l satisfying Definition 2.11 must be continuous, i.e., there must exist $C > 0$, such that $l[\boldsymbol{v}] \leq C\|\boldsymbol{v}\|$, where $\|\cdot\|$ is the norm in the Banach space $\mathcal{E}$.

The definitions of gradient and VJPs require in addition a notion of inner product. They can be defined in **Hilbert spaces**, that is, linear spaces equipped with an inner product and complete with respect to the norm induced by the inner product (they could also be defined in a Banach space by considering operations in the dual space, see, e.g. (Clarke *et al.*, 2008)). The existence of the gradient is ensured by **Riesz's representation theorem** which states that any continuous linear form in a Hilbert space can be represented by the inner product with a vector. Since for a differentiable function $f : \mathcal{E} \to \mathbb{R}$, the JVP $\partial f(\boldsymbol{w}) : \mathcal{E} \to \mathbb{R}$ is a linear form, Riesz's representation theorem ensures the existence of the gradient as the element $g \in \mathcal{E}$ such that $\partial f(\boldsymbol{w})\boldsymbol{v} = \langle g, \boldsymbol{v}\rangle$ for any $\boldsymbol{v} \in \mathcal{E}$. The VJP is also well-defined as the adjoint of the JVP w.r.t. the inner product of the Hilbert space.

As an example, the space of squared integrable functions on $\mathbb{R}$ is a Hilbert space equipped with the inner product $\langle a, b\rangle := \int a(x)b(x)dx$. Here, we cannot find a finite number of functions that can express all possible functions on $\mathbb{R}$. Therefore, this space is not a mere Euclidean space. Nevertheless, we can consider functions on this Hilbert space (called **functionals** to distinguish them from the elements of the space).

The associated directional derivatives and gradients, can be defined and are called respectively, **functional derivative** and **functional gradient**, see, e.g., Frigyik *et al.* (2008) and references therein.

2.4 Second-order differentiation

2.4.1 Second derivatives

For a single-input, single-output differentiable function $f : \mathbb{R} \to \mathbb{R}$, its derivative at any point is itself a function $f' : \mathbb{R} \to \mathbb{R}$. We may then consider the derivative of the derivative at any point: the **second derivative**.

Definition 2.13 (Second derivative)**.** The **second derivative** $f^{(2)}(w)$ of a differentiable function $f : \mathbb{R} \to \mathbb{R}$ at $w \in \mathbb{R}$ is defined as the derivative of f' at w, that is,

$$f^{(2)}(w) := \lim_{\delta \to 0} \frac{f'(w + \delta) - f'(w)}{\delta},$$

provided that the limit is well-defined. If the second derivative of a function f is well-defined at w, the function is said **twice differentiable** at w.

If f has a small second derivative at a given w, the derivative around w is almost constant. That is, the function behaves like a line around w, as illustrated in Fig. 2.4. Hence, the second derivative is usually interpreted as the **curvature** of the function at a given point.

2.4.2 Second directional derivatives

For a multi-input function $f : \mathbb{R}^P \to \mathbb{R}$, we saw that the directional derivative encodes infinitesimal variations of f along a given direction. To analyze the second derivative, the curvature of the function at a given point $\boldsymbol{w}$, we can consider the variations along a pair of directions, as defined below.

Definition 2.14 (Second directional derivative)**.** The **second directional derivative** of $f : \mathbb{R}^P \to \mathbb{R}$ at $\boldsymbol{w} \in \mathbb{R}^P$ along $\boldsymbol{v}, \boldsymbol{v}' \in \mathbb{R}^P$
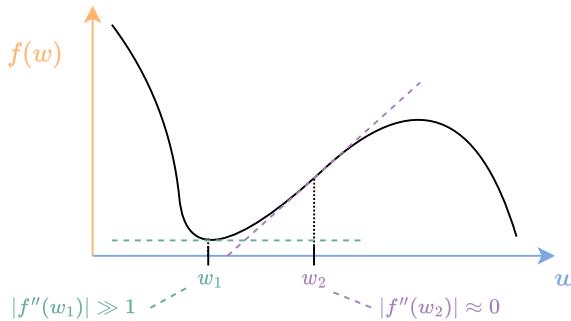
Figure 2.4: Points at which the second derivative is small are points along which the function is well approximated by its tangent line. On the other hand, point with large second derivative tend to be badly approximated by the tangent line.

is defined as the directional derivative of $\boldsymbol{w} \mapsto \partial f(\boldsymbol{w})[\boldsymbol{v}]$ along $\boldsymbol{v}'$, that is,

$$\partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}'] := \lim_{\delta \to 0} \frac{\partial f(\boldsymbol{w} + \delta \boldsymbol{v}')[\boldsymbol{v}] - \partial f(\boldsymbol{w})[\boldsymbol{v}]}{\delta},$$

provided that $\partial f(\boldsymbol{w})[\boldsymbol{v}]$ is well-defined around $\boldsymbol{w}$ and that the limit exists.

Of particular interest are the variations of a function around the canonical directions: the **second partial derivatives**, defined as

$$\partial_{ij}^2 f(\boldsymbol{w}) := \partial^2 f(\boldsymbol{w})[\boldsymbol{e}_i, \boldsymbol{e}_j]$$

for $\boldsymbol{e}_i$, $\boldsymbol{e}_j$ the ith and j^{th} canonical directions in $\mathbb{R}^P$, respectively. In Leibniz notation, the second partial derivatives are denoted

$$\partial_{ij}^2 f(\boldsymbol{w}) = \frac{\partial^2 f(\boldsymbol{w})}{\partial w_i \partial w_j}.$$

2.4.3 Hessians

For a multi-input function, twice differentiability is simply defined as the differentiability of any directional derivative $\partial f(\boldsymbol{w})[\boldsymbol{v}]$ w.r.t. $\boldsymbol{w}$.

Definition 2.15 (Twice differentiability). A function $f : \mathbb{R}^P \to \mathbb{R}$ is twice differentiable at $\boldsymbol{w} \in \mathbb{R}^P$ if it is differentiable and $\partial f : \mathbb{R}^P \to (\mathbb{R}^P \to \mathbb{R})$ is also differentiable at $\boldsymbol{w}$.

As a result, the second directional derivative is a bilinear form.

Definition 2.16 (Bilinear map, bilinear form). A function $b : \mathbb{R}^P \times \mathbb{R}^P \to \mathbb{R}^M$ is a **bilinear map** if $b[\boldsymbol{v}, \cdot] : \mathbb{R}^P \to \mathbb{R}$ is linear for any $\boldsymbol{v}$ and $b[\cdot, \boldsymbol{v}']$ is linear for any $\boldsymbol{v}'$. That is,

$$b[\boldsymbol{v}, \boldsymbol{v}'] = \sum_{i=1}^{P} v_i b[\boldsymbol{e}_i, \boldsymbol{v}'] = \sum_{i=1}^{P} \sum_{j=1}^{P} v_i v_j' b[\boldsymbol{e}_i, \boldsymbol{e}_j],$$

for $\boldsymbol{v} = \sum_{i=1}^{P} v_i \boldsymbol{e}_i$ and $\boldsymbol{v}' = \sum_{i=1}^{P} v_i' \boldsymbol{e}_i$. A bilinear map with values in $\mathbb{R}$, $b : \mathbb{R}^P \times \mathbb{R}^P \to \mathbb{R}$, is called a **bilinear form**.

The second directional derivative can be computed along any two directions from the knowledge of the second partial derivatives gathered in the **Hessian**.

Definition 2.17 (Hessian). The **Hessian** of a twice differentiable function $f : \mathbb{R}^P \to \mathbb{R}$ at $\boldsymbol{w}$ is the $P \times P$ matrix gathering all second partial derivatives:

$$\nabla^2 f(\boldsymbol{w}) := \begin{pmatrix} \partial_{11} f(\boldsymbol{w}) & \dots & \partial_{1P} f(\boldsymbol{w}) \\ \vdots & \ddots & \vdots \\ \partial_{P1} f(\boldsymbol{w}) & \dots & \partial_{PP} f(\boldsymbol{w}) \end{pmatrix},$$

provided that all second partial derivatives are well-defined.

The second directional derivative at $\boldsymbol{w}$ is bilinear in any directions $\boldsymbol{v} = \sum_{i=1}^{P} v_i \boldsymbol{e}_i$ and $\boldsymbol{v}' = \sum_{i=1}^{P} v_i' \boldsymbol{e}_i$. Therefore,

$$\partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}'] = \sum_{i,j=1}^{P} v_i v_j' \partial^2 f(\boldsymbol{w})[\boldsymbol{e}_i, \boldsymbol{e}_j] = \langle \boldsymbol{v}, \nabla^2 f(\boldsymbol{w}) \boldsymbol{v}' \rangle.$$

Given the gradient of f, the Hessian is equivalent to the transpose of the Jacobian of the gradient. By slightly generalizing the notation ∇ to denote the transpose of the Jacobian of a function (which matches

its definition for single-output functions), we have that the Hessian can be expressed as $\nabla^2 f(\boldsymbol{w}) = \nabla(\nabla f)(\boldsymbol{w})$, which justifies its notation.

Similarly as for the differentiability of a function f, twice differentiability of f at $\boldsymbol{w}$ is equivalent to having the second partial derivatives not only defined but also continuous in a neighborhood of $\boldsymbol{w}$. Remarkably, by requiring twice differentiability, i.e., continuous second partial derivatives, the Hessian is guaranteed to be symmetric (Schwarz, 1873).

> **Proposition 2.10** (Symmetry of the Hessian). If a function $f : \mathbb{R}^P \to \mathbb{R}$ is twice differentiable at $\boldsymbol{w}$, then its Hessian $\nabla^2 f(\boldsymbol{w})$ is symmetric, that is, $\partial^2_{ij} f(\boldsymbol{w}) = \partial^2_{ji} f(\boldsymbol{w})$ for any $i, j \in \{1, \dots P\}$.

The symmetry of the Hessian means that it can alternatively be written as $\nabla^2 f(\boldsymbol{w}) = (\partial^2_{ji} f(\boldsymbol{w}))^P_{i,j=1} = \boldsymbol{\partial}(\nabla f)(\boldsymbol{w})$, i.e., the Jacobian of the gradient of f.

2.4.4 Hessian-vector products

Similarly to the Jacobian, we can exploit the formal definition of the Hessian as a bilinear form to extend its definition for Euclidean spaces. In particular, we can define the notion of Hessian-vector product.

> **Definition 2.18** (Hessian-vector product). If a function $f : \mathcal{E} \to \mathbb{R}$ defined on a Euclidean space $\mathcal{E}$ with inner product $\langle \cdot, \cdot \rangle$, is twice differentiable at $\boldsymbol{w} \in \mathcal{E}$, then for any $\boldsymbol{v} \in \mathcal{E}$, there exists $\nabla^2 f(\boldsymbol{w})[\boldsymbol{v}]$, called the **Hessian-vector product** (HVP) of f at $\boldsymbol{w}$ along $\boldsymbol{v}$ such that for any $\boldsymbol{v}' \in \mathcal{E}$,
> $$\partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}'] = \langle \boldsymbol{v}', \nabla^2 f(\boldsymbol{w})[\boldsymbol{v}] \rangle.$$
> In particular for $\mathcal{E} = \mathbb{R}^P$, the HVP is $\nabla^2 f(\boldsymbol{w})[\boldsymbol{v}] = (\partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{e}_i])^P_{i=1}$.

From an autodiff point of view, the HVP can be implemented in four different ways, as explained in Section 8.1.

2.4.5 Second-order Jacobians

The previous definitions naturally extend to multi-output functions $f : \mathcal{E} \to \mathcal{F}$, where $f := (f_1, \dots, f_M)$, $f_j : \mathcal{E} \to \mathcal{F}_j$ and $\mathcal{F} := \mathcal{F}_1 \times \cdots \times \mathcal{F}_M$.

The second directional derivative is defined by gathering the second derivatives of all coordinates, that is, for $\boldsymbol{w}, \boldsymbol{v}, \boldsymbol{v}' \in \mathcal{E}$,

$$\partial f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}'] = (\partial f_j(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}'])_{j=1}^M \in \mathcal{F}.$$

The function f is twice differentiable if and only if all its coordinates are twice differentiable. The second directional derivative is then a **bilinear map**. We can then compute second directional derivatives as

$$\partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}'] = \sum_{i,j=1}^P v_i v_j' \partial^2 f(\boldsymbol{w})[\boldsymbol{e}_i, \boldsymbol{e}_j] = (\langle \boldsymbol{v}, \nabla^2 f_j(\boldsymbol{w}) \boldsymbol{v}' \rangle)_{j=1}^M.$$

When $\mathcal{E} = \mathbb{R}^P$ and $\mathcal{F}_j = \mathbb{R}$, so that $\mathcal{F} = \mathbb{R}^M$, the bilinear map can be materialized as a tensor

$$\partial^2 f(\boldsymbol{w}) = (\partial^2 f(\boldsymbol{w})[\boldsymbol{e}_i, \boldsymbol{e}_j])_{i,j=1}^P \in \mathbb{R}^{M \times P \times P},$$

the "second-order Jacobian" of f. However, similarly to the Hessian, it is usually more convenient to apply the bilinear map to prescribed vectors $\boldsymbol{v}$ and $\boldsymbol{v}'$ than to materialize as a tensor.

2.5   Higher-order differentiation

2.5.1   Higher-order derivatives

Derivatives can be extended to any order. Formally, the nth derivative can be defined inductively as follows for a single-input, single-output function.

Definition 2.19 (n^{th} order derivative). The nth derivative $f^{(n)}$ of a function $f : \mathbb{R} \to \mathbb{R}$ at $w \in \mathbb{R}$ is defined as

$$f^{(n)}(w) := (f^{(n-1)})'(w) = \lim_{\delta \to 0} \frac{f^{(n-1)}(w + \delta) - f^{(n-1)}(w)}{\delta}$$

provided that f^{n-1} is differentiable around w and that the limit exists. In such a case, the function is said n times differentiable at w.

2.5.2 Higher-order directional derivatives

For a multi-input function f, we can naturally extend the notion of directional derivative as follows.

Definition 2.20 (n^{th} order directional derivative). The nth directional derivative of $f : \mathbb{R}^P \to \mathbb{R}$ at $\boldsymbol{w} \in \mathbb{R}^P$ along $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n$ is defined as

$$
\partial^n f(\boldsymbol{w})[\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n]
$$
$$
= \partial(\partial^{n-1} f(\cdot)[\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{n-1}])[\boldsymbol{v}_n]
$$
$$
= \lim_{\delta \to 0} \frac{\partial f(\boldsymbol{w} + \delta \boldsymbol{v}_n)[\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{n-1}] - \partial f(\boldsymbol{w})[\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{n-1}]}{\delta}
$$

A multi-input function f is n-times differentiable if it is $n - 1$ differentiable and its $n - 1$ directional derivative along any direction is differentiable. As a consequence the nth directional derivative is a **multilinear form**.

Definition 2.21 (Multilinear map, multilinear form). A function $c : \otimes_{i=1}^{n} \mathbb{R}^P \to \mathbb{R}^M$ is a **multilinear map** if it is linear in each coordinate given all others fixed, that is, if $\boldsymbol{v}_j \mapsto c[\boldsymbol{v}_1, \ldots, \boldsymbol{v}_j, \ldots, \boldsymbol{v}_n]$ is linear in $\boldsymbol{v}_j$ for any $j \in [n]$. It is a **multilinear form** if it has values in $\mathbb{R}$.

The nth order directional derivative is then given by

$$
\partial^n f(\boldsymbol{w})[\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n] = \sum_{i_1, \ldots, i_n = 1}^{P} v_{1,i_1} \ldots v_{n,i_n} \partial^n f(\boldsymbol{w})[\boldsymbol{e}_{i_1}, \ldots, \boldsymbol{e}_{i_n}].
$$

Its materialization is an nth order tensor

$$
\nabla^n f(\boldsymbol{w}) = (\partial^n f(\boldsymbol{w})[\boldsymbol{e}_{i_1}, \ldots, \boldsymbol{e}_{i_n}])_{i_1, \ldots, i_n = 1}^{P} \in \mathbb{R}^{P \times \ldots \times P}.
$$

2.5.3 Higher-order Jacobians

All above definitions extend directly to the case of multi-output functions $f : \mathcal{E} \to \mathcal{F}$, where $\mathcal{F} = \mathcal{F}_1 \times \cdots \times \mathcal{F}_M$. The nth directional derivatives

$$
\partial^n f(\boldsymbol{w})[\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n] = (\partial^n f_j(\boldsymbol{w})[\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n])_{j=1}^{M}.
$$

The function f is then n times differentiable if if it is $n-1$ differentiable and its $n-1$ directional derivative along any direction is differentiable. As a consequence, the nth directional derivative is a **multilinear map**. The nth directional derivative can be decomposed into partial derivatives as

$$\partial^n f(\boldsymbol{w})[\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n] = \sum_{i_1,\ldots,i_n=1}^{P} v_{1,i_1} \ldots v_{n,i_n} \partial^n f(\boldsymbol{w})[\boldsymbol{e}_{i_1}, \ldots, \boldsymbol{e}_{i_n}].$$

When $\mathcal{E} = \mathbb{R}^P$ and $\mathcal{F} = \mathbb{R}^M$, it is materialized by an $n + 1^{\text{th}}$ order tensor

$$\partial^n f(\boldsymbol{w}) = (\partial^n f_j(\boldsymbol{w})[\boldsymbol{e}_{i_1}, \ldots, \boldsymbol{e}_{i_n}])_{j=1,i_1,\ldots,i_n=1}^{M,P,\ldots,P} \in \mathbb{R}^{M \times P \times \ldots \times P}.$$

2.5.4 Taylor expansions

With Landau's little o notation, we have seen that if a function is differentiable it is approximated by a linear function in $\boldsymbol{v}$,

$$f(\boldsymbol{w} + \boldsymbol{v}) = f(\boldsymbol{w}) + \langle \nabla f(\boldsymbol{w}), \boldsymbol{v} \rangle + o(\|\boldsymbol{v}\|_2).$$

Such an expansion of the function up to its first derivative is called the **first-order Taylor expansion** of f around $\boldsymbol{w}$.

If the function f is twice differentiable, we can approximate it by a quadratic in $\boldsymbol{v}$, leading to the **second-order Taylor expansion** of f around $\boldsymbol{w}$,

$$f(\boldsymbol{w} + \boldsymbol{v}) = f(\boldsymbol{w}) + \langle \nabla f(\boldsymbol{w}), \boldsymbol{v} \rangle + \frac{1}{2} \langle \boldsymbol{v}, \nabla^2 f(\boldsymbol{w}) \boldsymbol{v} \rangle + o(\|\boldsymbol{v}\|_2^2).$$

Compared to the first-order Taylor approximation, it is naturally more accurate around $\boldsymbol{w}$, as reflected by the fact that $\|\boldsymbol{v}\|_2^3 \le \|\boldsymbol{v}\|_2^2$ for $\|\boldsymbol{v}\|_2 \le 1$.

More generally, we can build the $\boldsymbol{n}^{\text{th}}$ **order Taylor expansion** of a n times differentiable function $f \colon \mathbb{R}^P \to \mathbb{R}^M$ around $\boldsymbol{w} \in \mathbb{R}^P$ by

$$f(\boldsymbol{w} + \boldsymbol{v}) = f(\boldsymbol{w}) + \partial f(\boldsymbol{w})[\boldsymbol{v}] + \frac{1}{2} \partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}] + \ldots$$
$$+ \frac{1}{n!} \partial^n f(\boldsymbol{w}) [\underbrace{\boldsymbol{v}, \ldots, \boldsymbol{v}}_{n \text{ times}}] + o(\|\boldsymbol{v}\|_2^n).$$

Note that, using the change of variable $\boldsymbol{w}' = \boldsymbol{w} + \boldsymbol{v} \iff \boldsymbol{v} = \boldsymbol{w}' - \boldsymbol{w}$, it is often convenient to write the nth Taylor expansion of $f(\boldsymbol{w}')$ around $\boldsymbol{w}$ as

$$f(\boldsymbol{w}') = f(\boldsymbol{w}) + \sum_{j=1}^{n} \frac{1}{j!} \partial^j f(\boldsymbol{w}) \underbrace{[\boldsymbol{w}' - \boldsymbol{w}, \ldots, \boldsymbol{w}' - \boldsymbol{w}]}_{j \text{ times}} + o(\|\boldsymbol{w}' - \boldsymbol{w}\|_2^n).$$

Taylor expansions will prove useful in Chapter 6 for computing derivatives by finite differences.

2.6 Differential geometry

In this chapter, we progressively generalized the notion of derivative from real numbers to vectors and variables living in a linear space (a.k.a. vector space), either finite dimensional or infinite dimensional. We can further generalize these notions by considering a local notion of linearity. This is formalized by smooth manifolds in **differential geometry**, whose terminology is commonly adopted in the automatic differentiation literature and software. In this section, we give a brief overview of derivatives on smooth manifolds (simply referred as manifolds), and refer to Boumal (2023) for a complete introduction.

2.6.1 Differentiability on manifolds

Essentially, a manifold is a set that can be locally approximated by a Euclidean space. The most common example is a sphere like the Earth. Seen from the Moon, the Earth is not a plane, but locally, at a human level, it can be seen as a flat surface. Euclidean spaces are also trivial examples of manifold. A formal characterization of the sphere as a manifold is presented in Example 2.7. For now, we may think of a "manifold" as some set (e.g., the sphere) contained in some ambient Euclidean space; note however that manifolds can be defined generally without being contained in a Euclidean space (Boumal, 2023, Chapter 8). Differentiability in manifolds is simply inherited from the notion of differentiability in the ambient Euclidean space.

Definition 2.22 (Differentiability of restricted functions). Let $\mathcal{M}$ and $\mathcal{N}$ be manifolds. A function $f : \mathcal{M} \to \mathcal{N}$ defined from $\mathcal{M} \subseteq \mathcal{E}$ to $\mathcal{N} \subseteq \mathcal{F}$, with $\mathcal{E}$ and $\mathcal{F}$ Euclidean spaces, is differentiable if f is the restriction of a differentiable function $\bar{f} : \mathcal{E} \to \mathcal{F}$, so that f coincides with $\bar{f}$ on $\mathcal{M}$.

Our objective is to formalize the directional derivatives and gradients for functions defined on manifolds. This formalization leads to the definitions of tangent spaces and cotangent spaces, and the associated generalizations of JVP and VJP operators as pushforward and pullback operators, respectively.

2.6.2   Tangent spaces and pushforward operators

To generalize the notion of directional derivatives of a function f, the one property we want to preserve is the chain rule. Rather than starting from the variations of f at a given point along a direction, we start with the variations of f along curves. Namely, on a manifold like the sphere $\mathcal{S}^P$ in $\mathbb{R}^P$, we can look at curves $\alpha : \mathbb{R} \to \mathcal{S}^P$ passing by $\boldsymbol{w} \in \mathcal{S}^P$ at time 0, that is, $\alpha(0) = \boldsymbol{w}$. For single-input functions like α, we denoted for simplicity $\alpha'(0) := (\alpha'_1(0), \ldots, \alpha'_P(0))$. The directional derivative of f must typically serve to define the derivative of $f \circ \alpha$ at 0, such that $(f \circ \alpha)'(0) = \partial f(\boldsymbol{w})[\alpha'(0)]$. In the case of the sphere, as illustrated in Fig. 2.5, the derivative $\alpha'(0)$ of a curve α passing through a point $\boldsymbol{w}$ is always **tangent** to the sphere at $\boldsymbol{w}$. The tangent plane to the sphere at $\boldsymbol{w}$, then captures all possible relevant vectors to pass to the JVP we are building. To define the directional derivative of a function f on a manifold, we therefore restrict ourselves to an operator defined on the **tangent space** $\mathcal{T}_{\boldsymbol{w}}\mathcal{M}$, whose definition below is simplified for our purposes.

Definition 2.23 (Tangent space). The **tangent space** of a manifold $\mathcal{M}$ at $\boldsymbol{w} \in \mathcal{M}$ is defined as

$$\mathcal{T}_{\boldsymbol{w}}\mathcal{M} := \{\boldsymbol{v} = \alpha'(0) \text{ for any } \alpha : \mathbb{R} \to \mathcal{M} \text{ differentiable s.t. } \alpha(0) = \boldsymbol{w}\}.$$

In the case of the sphere in Fig. 2.5, the tangent space is a plane, that is, a Euclidean space. This property is generally true: tangent spaces
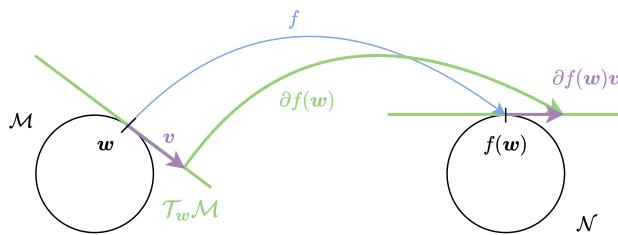
Figure 2.5: A differentiable function f defined from a sphere $\mathcal{M}$ to a sphere $\mathcal{N}$ defines a push-forward operator that maps tangent vectors (derivatives of functions on the sphere passing by $\boldsymbol{w}$) in the tangent space $\mathcal{T}_{\boldsymbol{w}}\mathcal{M}$ of $\mathcal{M}$ at $\boldsymbol{w}$ to tangent vectors of $\mathcal{N}$ at $f(\boldsymbol{w})$ in the tangent space $\mathcal{T}_{f(\boldsymbol{w})}\mathcal{N}$.

are Euclidean spaces such that we will be able to define directional derivatives as linear operators. Now, if f is differentiable and goes from a manifold $\mathcal{M}$ to a manifold $\mathcal{N}$, then $f \circ \alpha$ is a differentiable curve in $\mathcal{N}$. Therefore, $(f \circ \alpha)'(0)$ is the derivative of a curve passing through $f(\boldsymbol{w})$ at 0 and is tangent to $\mathcal{N}$ at $f(\boldsymbol{w})$. Hence, the directional derivative of $f : \mathcal{M} \to \mathcal{N}$ at $\boldsymbol{w}$ can be defined as a function from the tangent space $\mathcal{T}_{\boldsymbol{w}}\mathcal{M}$ of $\mathcal{M}$ at $\boldsymbol{w}$ onto the tangent space $\mathcal{T}_{f(\boldsymbol{w})}\mathcal{N}$ of $\mathcal{N}$ at $f(\boldsymbol{w})$. Overall, we built the directional derivative (JVP) by considering how a composition of f with any curve α pushes forward the derivative of α into the derivative of $f \circ \alpha$. The resulting JVP is called a **pushforward operator** in differentiable geometry.

> **Definition 2.24** (Pushforward operator). Given two manifolds $\mathcal{M}$ and $\mathcal{N}$, the **pushforward operator** of a differentiable function $f : \mathcal{M} \to \mathcal{N}$ at $\boldsymbol{w} \in \mathcal{M}$ is the linear map $\partial f(\boldsymbol{w}) : \mathcal{T}_{\boldsymbol{w}}\mathcal{M} \to \mathcal{T}_{f(\boldsymbol{w})}\mathcal{N}$ defined by
>
> $$\partial f(\boldsymbol{w})[\boldsymbol{v}] \coloneqq (f \circ \alpha)'(0),$$
>
> for any $\boldsymbol{v} \in \mathcal{T}_{\boldsymbol{w}}\mathcal{M}$ such that $\boldsymbol{v} = \alpha'(0)$, for a differerentiable curve $\alpha : \mathbb{R} \to \mathcal{M}$, passing by $\boldsymbol{w}$ at 0, i.e., $\alpha(0) = \boldsymbol{w}$.

2.6.3 Cotangent spaces and pullback operators

To generalize the JVP, we composed $f : \mathcal{M} \to \mathcal{N}$ with any single-input function $\alpha : \mathbb{R} \to \mathcal{M}$ giving values on the manifold. The derivative of

any such α is then pushed forward from $\mathcal{T}_{\boldsymbol{w}}\mathcal{M}$ to $\mathcal{T}_{f(\boldsymbol{w})}\mathcal{N}$ by the action of f. To define the VJP, we take a symmetric approach. We consider all single-output differentiable functions $\beta : \mathcal{N} \to \mathbb{R}$ defined on $\boldsymbol{y} \in \mathcal{N}$ with $\boldsymbol{y} = f(\boldsymbol{w})$ for some $\boldsymbol{w} \in \mathcal{M}$. We then want to pull back the derivatives of β when precomposing it by f. Therefore, the space on which the VJP acts is the space of directional derivatives of any $\beta : \mathcal{N} \to \mathbb{R}$ at $\boldsymbol{y}$, defining the **cotangent space**.

> **Definition 2.25** (Cotangent space). The **cotangent space** of a manifold $\mathcal{N}$ at $\boldsymbol{y} \in \mathcal{N}$ is defined as
>
> $$\begin{aligned} \mathcal{T}_{\boldsymbol{y}}^{*}\mathcal{N} &= \{u = \partial\beta(\boldsymbol{y}) \text{ for any } \beta : \mathcal{N} \to \mathbb{R} \text{ differentiable}\} \\ &= \{u : \mathcal{T}_{\boldsymbol{y}}\mathcal{N} \to \mathbb{R} \text{ for any linear map } u\}, \end{aligned}$$

Note that elements of the cotangent space are linear mappings, not vectors. This distinction is important to define the pullback operator as an operator on functions as done in measure theory. From a linear algebra viewpoint, the cotangent space is exactly the **dual space** of $\mathcal{T}_{\boldsymbol{y}}\mathcal{N}$, that is, the set of linear maps from $\mathcal{T}_{\boldsymbol{y}}\mathcal{N}$ to $\mathbb{R}$, called **linear forms**. As $\mathcal{T}_{\boldsymbol{y}}\mathcal{N}$ is a Euclidean space, its dual space $\mathcal{T}_{\boldsymbol{y}}^{*}\mathcal{N}$ is also a Euclidean space. The **pullback** operator is then defined as the operator that gives access to directional derivatives of $\beta \circ f$ given the directional derivative of β at $f(\boldsymbol{w})$.

> **Definition 2.26** (Pullback operator). Given two manifolds $\mathcal{M}$ and $\mathcal{N}$, the **pullback operator** of a differentiable function $f : \mathcal{M} \to \mathcal{N}$ at $\boldsymbol{w} \in \mathcal{M}$ is the linear map $\partial f(\boldsymbol{w})^{\star} : \mathcal{T}_{f(\boldsymbol{w})}^{*}\mathcal{N} \to \mathcal{T}_{\boldsymbol{w}}^{*}\mathcal{M}$ defined by
>
> $$\partial f(\boldsymbol{w})^{\star}u := \partial(\beta \circ f)(\boldsymbol{w}),$$
>
> for any $u \in \mathcal{T}_{f(\boldsymbol{w})}\mathcal{N}^{*}$ such that $\partial\beta(f(\boldsymbol{w})) = u$, for a differentiable function $\beta : \mathcal{N} \to \mathbb{R}$.

Contrary to the pushforward operator that acts on vectors, the pullback operator acts on linear forms. Hence, the slight difference in notation between $\partial f(\boldsymbol{w})^{\star}$ and $\partial f(\boldsymbol{w})^{*}$, the adjoint operator of $\partial f(\boldsymbol{w})$. To properly define the adjoint operator $\partial f(\boldsymbol{w})^{*}$, we need a notion of inner product. Since tangent spaces are Euclidean spaces, we can

define an inner product $\langle \cdot, \cdot \rangle_{\boldsymbol{w}}$ for each $\mathcal{T}_{\boldsymbol{w}}\mathcal{M}$ and $\boldsymbol{w} \in \mathcal{M}$, making $\mathcal{M}$ a **Riemannian manifold**. Equipped with these inner products, the cotangent space can be identified with the tangent space, and we can define gradients.

Definition 2.27 (Gradients in Riemannian manifolds). Let $\mathcal{M}$ be a Riemannian manifold equipped with inner products $\langle \cdot, \cdot \rangle_{\boldsymbol{w}}$. For any **cotangent vector** $u \in \mathcal{T}_{\boldsymbol{w}}^*\mathcal{M}$, with $\boldsymbol{w} \in \mathcal{M}$, there exists a unique **tangent vector** $\boldsymbol{u} \in \mathcal{T}_{\boldsymbol{w}}\mathcal{M}$ such that

$$\forall \boldsymbol{v} \in \mathcal{T}_{\boldsymbol{w}}\mathcal{M}, \ u[\boldsymbol{v}] = \langle \boldsymbol{u}, \boldsymbol{v} \rangle_{\boldsymbol{w}}.$$

In particular for any differentiable function $f : \mathcal{M} \to \mathbb{R}$, we can define the **gradient** of f as the unique tangent vector $\nabla f(\boldsymbol{w}) \in \mathcal{T}_{\boldsymbol{w}}\mathcal{M}$ such that

$$\forall \boldsymbol{v} \in \mathcal{T}_{\boldsymbol{w}}\mathcal{M}, \ \partial f(\boldsymbol{w})[\boldsymbol{v}] = \langle \nabla f(\boldsymbol{w}), \boldsymbol{v} \rangle.$$

Therefore, rather than pulling back directional derivatives, we can pull back gradients. The corresponding operator is then naturally the adjoint $\partial f(\boldsymbol{w})^*$ of the pushforward operator. Namely, given two Riemannian manifolds $\mathcal{M}$ and $\mathcal{N}$, and a differentiable function $f : \mathcal{M} \to \mathcal{N}$, we have

$$\left(\partial f(\boldsymbol{w})^{\star} u \right)[\boldsymbol{v}] = \langle \partial f(\boldsymbol{w})^*[\boldsymbol{u}], \boldsymbol{v} \rangle \text{ for any } \boldsymbol{v} \in \mathcal{T}_{\boldsymbol{w}}\mathcal{M}$$

for $u = \langle \cdot, \boldsymbol{u} \rangle \in \mathcal{T}_{f(\boldsymbol{w})}^*\mathcal{N}$ represented by $\boldsymbol{u} \in \mathcal{T}_{f(\boldsymbol{w})}\mathcal{N}$.

Example 2.7 (The sphere as a manifold). The sphere $\mathcal{S}^P$ in $\mathbb{R}^P$ is defined as the set of points $\boldsymbol{w} \in \mathbb{R}^P$, satisfying $c(\boldsymbol{w}) := \langle \boldsymbol{w}, \boldsymbol{w} \rangle - 1 = 0$, with JVP $\partial c(\boldsymbol{w})[\boldsymbol{v}] = 2\langle \boldsymbol{w}, \boldsymbol{v} \rangle$.

For any $\boldsymbol{v} = (v_1, \ldots, v_{P-1}) \in \mathbb{R}^{P-1}$ close enough to the $P-1$ coordinates of a point $\boldsymbol{w}$ on the sphere, we can define $\psi_1(\boldsymbol{v}) = \sqrt{1 - \langle \boldsymbol{v}, \boldsymbol{v} \rangle}$ such that $\boldsymbol{\psi}(\boldsymbol{v}) = (v_1, \ldots, v_{P-1}, \psi_1(\boldsymbol{v}))$ satisfies $\langle \boldsymbol{\psi}(\boldsymbol{v}), \boldsymbol{\psi}(\boldsymbol{v}) \rangle = 1$, that is $c(\boldsymbol{\psi}(\boldsymbol{w})) = 1$. With the help of the mapping $\boldsymbol{\psi}^{-1}$ from a neighborhood of $\boldsymbol{w}$ in the sphere to $\mathbb{R}^{P-1}$, we can see the sphere locally as a space of dimension $P-1$.

The tangent space can be naturally characterized in terms of

Function		f	$\mathcal{M} \to \mathcal{N}$
Push-forward		$\partial f(\boldsymbol{w})$	$\mathcal{T}_{\boldsymbol{w}}\mathcal{M} \to \mathcal{T}_{f(\boldsymbol{w})}\mathcal{N}$
Pullback		$\partial f(\boldsymbol{w})^{\star}$	$\mathcal{T}_{f(\boldsymbol{w})}^{*}\mathcal{N} \to \mathcal{T}_{\boldsymbol{w}}^{*}\mathcal{M}$
Adjoint of pushforward		$\partial f(\boldsymbol{w})^{*}$	$\mathcal{T}_{f(\boldsymbol{w})}\mathcal{N} \to \mathcal{T}_{\boldsymbol{w}}\mathcal{M}$

Table 2.1: For a differentiable function f defined from a manifold $\mathcal{M}$ onto a manifold $\mathcal{N}$, the JVP is generalized with the notion of pushforward $\partial f(\boldsymbol{w})$. The counterpart of the pushforward is the pullback operation $\partial f(\boldsymbol{w})^{\star}$ that acts on linear forms in the tangent spaces. For Riemannian manifolds, the pullback operation can be identified with the adjoint operator $\partial f(\boldsymbol{w})^{*}$ of the pushforward operator as any linear form is represented by a vector.

the constraining function c. Namely, a curve $\alpha : \mathbb{R} \to \mathcal{M}$ such that $\alpha(0) = \boldsymbol{w}$ satisfies for any $\delta \in \mathbb{R}$, $c(\alpha(\delta)) = \boldsymbol{0}$. Hence, differentiating the implicit equation, we have

$$(c \circ \alpha)'(0) = \partial c(\boldsymbol{w})[\alpha'(0)].$$

That is, $\alpha'(0)$ is in the null space of $\partial c(\boldsymbol{w})$, denoted

$$\mathrm{Null}(\partial c(\boldsymbol{w})) := \{\boldsymbol{v} \in \mathbb{R}^{P} : \partial c(\boldsymbol{w})[\boldsymbol{v}] = 0\}.$$

The tangent space of $\mathcal{M}$ at $\boldsymbol{w}$ is then

$$\begin{aligned}
\mathcal{T}_{\boldsymbol{w}}\mathcal{M} &= \mathrm{Null}(2\langle \boldsymbol{w}, \cdot \rangle) \\
&= \{\boldsymbol{v} \in \mathbb{R}^{P} : \langle \boldsymbol{w}, \boldsymbol{v} \rangle = 0\}
\end{aligned}$$

We recover naturally that the tangent space is a Euclidean space of dimension $P - 1$ defined as the set of points orthogonal to $\boldsymbol{w}$.

2.7   Generalized derivatives

While we largely focus on differentiable functions in this book, it is important to characterize non-differentiable functions. We distinguish here two cases: continuous functions and non-continuous functions. For the former case, there exists generalizations of the notion of directional derivative, gradient and Jacobian, presented below. For non-continuous functions, even if derivatives exist almost everywhere, they may be

uninformative. For example, piecewise constant functions, encountered in e.g. control flows (Chapter 5), are almost everywhere differentiable but with zero derivatives. In such cases, surrogate functions can be defined to ensure the differentiability of a program (Part IV).

2.7.1 Rademacher's theorem

We first recall the definition of locally Lipschitz continuous function.

> **Definition 2.28** (Locally Lipschitz continuous function)**.** A function $f : \mathcal{E} \to \mathcal{F}$, is Lipschitz continuous if there exists $C \geq 0$ such that for any $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{E}$,
>
> $$\|f(\boldsymbol{x}) - f(\boldsymbol{y})\| \leq C\|\boldsymbol{x} - \boldsymbol{y}\|.$$
>
> A function $f : \mathcal{E} \to \mathcal{F}$ is locally Lipschitz-continuous if for any $\boldsymbol{x} \in \mathcal{E}$, there exists a neighborhood $\mathcal{U}$ of $\boldsymbol{x}$ such that f restricted to $\mathcal{U}$ is Lipschitz-continuous.

Rademacher's theorem (Rademacher, 1919) ensures that f is differentiable almost everywhere; see also Morrey Jr (2009) for a standard proof.

> **Proposition 2.11** (Rademacher's theorem)**.** Let $\mathcal{E}$ and $\mathcal{F}$ denote Euclidean spaces. If $f : \mathcal{E} \to \mathcal{F}$ is locally Lipschitz-continuous, then f is almost everywhere differentiable, that is the set of points in $\mathcal{E}$ at which f is not differentiable is of (Lebesgue) measure zero.

2.7.2 Clarke derivatives

Rademacher's theorem hints that the definitions of directional derivatives, gradients and Jacobians may be generalized to locally Lipschitz continuous functions. This is what Clarke (1975) did in his seminal work, which laid the foundation of **nonsmooth analysis**. The first building block is a notion of generalized directional derivative.

Definition 2.29 (Clarke generalized directional derivative)**.** The **Clarke generalized directional derivative** of a locally Lipschitz continuous function $f : \mathcal{E} \to \mathbb{R}$ at $\boldsymbol{w} \in \mathcal{E}$ in the direction $\boldsymbol{v} \in \mathcal{E}$ is

$$\partial_C f(\boldsymbol{w})[\boldsymbol{v}] := \limsup_{\substack{\boldsymbol{u} \to \boldsymbol{w} \\ \delta \searrow 0}} \frac{f(\boldsymbol{u} + \delta \boldsymbol{v}) - f(\boldsymbol{u})}{\delta},$$

provided that the limit exists, where $\delta \searrow 0$ means that δ approaches 0 by non-negative values and the limit superior is defined as

$$\limsup_{\boldsymbol{x} \to \boldsymbol{a}} f(\boldsymbol{x}) := \lim_{\varepsilon \to 0} \sup\{f(\boldsymbol{x}) : \boldsymbol{x} \in B(\boldsymbol{a}, \varepsilon) \setminus \{\boldsymbol{a}\}\}$$

for $B(\boldsymbol{a}, \varepsilon) := \{\boldsymbol{x} \in \mathcal{E} : \|\boldsymbol{x} - \boldsymbol{a}\| \leq \varepsilon\}$ the ball centered at $\boldsymbol{a}$ of radius ε.

There are two differences with the usual definition of a directional derivative: (i) we considered slopes of the function in a neighborhood of the point rather than at the given point, (ii) we took a limit superior rather than a usual limit. The first point is rather natural in the light of Rademacher's theorem: we can properly characterize variations on points where the function is differentiable, therefore we may take the limits of these slopes as a candidate slope for the point of interest. The second point is more technical but essential: it allows us to characterize the directional derivative as the supremum of some linear forms (Clarke *et al.*, 2008). These linear forms in turn define a set of generalized gradients (Clarke *et al.*, 2008, Chapter 2).

Definition 2.30 (Clarke generalized gradient)**.** A **Clarke generalized gradient** of a locally Lipschitz function $f : \mathcal{E} \to \mathbb{R}$ at $\boldsymbol{w} \in \mathcal{E}$ is a point $\boldsymbol{g} \in \mathcal{E}$ such that $\forall \boldsymbol{v} \in \mathcal{E}$

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] \geq \langle \boldsymbol{g}, \boldsymbol{v} \rangle.$$

The set of Clarke generalized gradients is called the **Clarke subdifferential** of f at $\boldsymbol{w}$.

Definition 2.29 and Definition 2.30 can be used in non-Euclidean spaces, such as Banach or Hilbert spaces (Clarke *et al.*, 2008). In Euclidean spaces, the Clarke generalized gradients can be characterized

more simply thanks to Rademacher's theorem (Clarke *et al.*, 2008, Theorem 8.1). Namely, they can be defined as a convex combination of limits of gradients of f evaluated at a sequence in $\mathcal{E} \setminus \Omega$ that converges to $\boldsymbol{w}$ (Proposition 2.12). In the following, the convex hull of a set $S \subseteq \mathcal{E}$, the set of convex combinations of elements of S, is denoted

$$\operatorname{conv}(S) \coloneqq \{\lambda_1 \boldsymbol{s}_1 + \ldots + \lambda_m \boldsymbol{s}_m \ : m \in \mathbb{N}, \ \lambda_i \geq 0, \sum_{i=1}^{m} \lambda_i = 1, \boldsymbol{s}_i \in S\}.$$

Proposition 2.12 (Characterization of Clarke generalized gradients)**.** Let $f : \mathcal{E} \to \mathbb{R}$ be a locally Lipschitz continuous and denote Ω the set of points at which f is not differentiable (Proposition 2.11). An element $\boldsymbol{g} \in \mathcal{E}$ is a Clarke generalized gradient of f at $\boldsymbol{w} \in \mathcal{E}$ if and only if

$$\boldsymbol{g} \in \operatorname{conv}\left(\left\{\lim_{n \to +\infty} \nabla f(\boldsymbol{v}_n) \colon (\boldsymbol{v}_n)_{n=1}^{+\infty} \text{ s.t. } \boldsymbol{v}_n \in \mathcal{E} \setminus \Omega, \ \boldsymbol{v}_n \underset{n \to +\infty}{\to} \boldsymbol{w}\right\}\right).$$

The Jacobian of a function $f : \mathcal{E} \to \mathcal{F}$ between two Euclidean spaces can be generalized similarly (Clarke *et al.*, 2008, Section 3.3).

Definition 2.31 (Clarke generalized Jacobian)**.** Let $f : \mathcal{E} \to \mathcal{F}$ be a locally Lipschitz continuous and denote Ω the set of points at which f is not differentiable (Proposition 2.11). A **Clarke generalized Jacobian** of f at $\boldsymbol{w} \in \mathcal{E}$ is an element $\mathbf{J}$ of

$$\operatorname{conv}\left(\left\{\lim_{n \to +\infty} \boldsymbol{\partial} f(\boldsymbol{v}_n) \colon (\boldsymbol{v}_n)_{n=1}^{+\infty} \text{ s.t. } \boldsymbol{v}_n \in \mathcal{E} \setminus \Omega, \ \boldsymbol{v}_n \underset{n \to +\infty}{\to} \boldsymbol{w}\right\}\right).$$

For a continuously differentiable function $f : \mathcal{E} \to \mathcal{F}$ or $f : \mathcal{E} \to \mathbb{R}$, there is a unique generalized gradient, that is the usual gradient (Clarke *et al.*, 2008, Proposition 3.1, page 78). The chain-rule can be generalized to these objects (Clarke *et al.*, 2008). Recently, Bolte and Pauwels (2020) and Bolte *et al.* (2022) further generalized Clarke gradients through the definition of conservative gradients to define automatic differentiation schemes for nonsmooth functions.

2.8   Summary

The usual definition of **derivatives** of real-valued univariate functions extends to multivariate functions $f\colon \mathbb{R}^P \to \mathbb{R}$ through the notion of **directional derivative** $\partial f(\boldsymbol{w})[\boldsymbol{v}]$ at $\boldsymbol{w} \in \mathbb{R}^P$ in the direction $\boldsymbol{v} \in \mathbb{R}^P$. To take advantage of the representation of $\boldsymbol{w} = \sum_{j=1}^{P} w_j \boldsymbol{e}_j$ using the canonical bases $\{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_P\}$, the definition of **differentiable** functions requires the **linearity** of the directional derivative w.r.t. the direction $\boldsymbol{v}$. This requirement gives rise to the notion of **gradient** $\nabla f(\boldsymbol{w}) \in \mathbb{R}^P$, the vector that gathers the partial derivatives and further defines the **steepest ascent direction** at $\boldsymbol{w}$. For vector-input, vector-output functions $f\colon \mathbb{R}^P \to \mathbb{R}^M$, the directional derivative leads to the definition of **Jacobian matrix** $\boldsymbol{\partial} f(\boldsymbol{w}) \in \mathbb{R}^{M \times P}$, the matrix which gathers all partial derivatives (notice that we use bold $\boldsymbol{\partial}$). The **chain rule** is then the **product** of Jacobian matrices.

These notions can be extended to general Euclidean spaces, such as the spaces of matrices or tensors. For functions of the form $f\colon \mathcal{E} \to \mathbb{R}$, the gradient is $\nabla f(\boldsymbol{w}) \in \mathcal{E}$. More generally, for functions of the form $f\colon \mathcal{E} \to \mathcal{F}$, the Jacobian $\partial f(\boldsymbol{w})$ can be seen as a **linear map** (notice the non-bold ∂). The directional derivative at $\boldsymbol{w} \in \mathcal{E}$ naturally defines a linear map $\boldsymbol{l}[\boldsymbol{v}] = \partial f(\boldsymbol{w})[\boldsymbol{v}]$, where $\partial f(\boldsymbol{w})\colon \mathcal{E} \to \mathcal{F}$ is called the **Jacobian vector product** (JVP) and captures the infinitesimal variation at $\boldsymbol{w} \in \mathcal{E}$ along the **input** direction $\boldsymbol{v} \in \mathcal{E}$.

Its **adjoint** $\partial f(\boldsymbol{w})^*\colon \mathcal{F} \to \mathcal{E}$ defines another linear map $\boldsymbol{l}[\boldsymbol{u}] = \partial f(\boldsymbol{w})^*[\boldsymbol{u}]$ called the **vector Jacobian product** (VJP) and captures the infinitesimal variation at $\boldsymbol{w} \in \mathcal{E}$ along the **output** direction $\boldsymbol{u} \in \mathcal{F}$. The **chain rule** is then the **composition** of these linear maps. For the particular case when we compose a scalar-valued function ℓ (such as a loss function) with a vector-valued function f (such as a network function), the gradient is given by $\nabla(\ell \circ f)(\boldsymbol{w}) = \partial f(\boldsymbol{w})^* \nabla \ell(f(\boldsymbol{w}))$. This is why being able to apply the adjoint to a gradient, which as we shall see can be done with reverse-mode autodiff, is so pervasive in machine learning.

The definitions of JVP and VJP operators can further be generalized in the context of differentiable geometry. In that framework, the JVP amounts to the **pushforward** operator that acts on **tangent vectors**.

The VJP amounts to the **pullback** operator that acts on **cotangent vectors**.

We also saw that the **Hessian matrix** of a function $f(\boldsymbol{w})$ from $\mathbb{R}^P$ to $\mathbb{R}$ is denoted $\nabla^2 f(\boldsymbol{w}) \in \mathbb{R}^{P \times P}$. It is symmetric if the second partial derivatives are continuous. Seen as linear map, the Hessian leads to the notion of **Hessian-vector product** (HVP), which we saw can be reduced to the JVP or the VJP of $\nabla f(\boldsymbol{w})$.

The main take-away message of this chapter is that computing the directional derivative or the gradient of compositions of functions **does not** require computing intermediate Jacobians but only to evaluate linear maps (JVPs or VJPs) associated with these intermediate functions. The goal of automatic differentiation, presented in Chapter 7, is precisely to provide an efficient implementation of these maps for **computation chains** or more generally for **computation graphs**.

3

Probabilistic learning

In this chapter, we review how to perform probabilistic learning. We also introduce exponential family distributions, as they play a key role in this book.

3.1 Probability distributions

3.1.1 Discrete probability distributions

A discrete probability distribution over a set $\mathcal{Y}$ is specified by its **probability mass function** (PMF) $p\colon \mathcal{Y} \to [0,1]$. The probability of $\boldsymbol{y} \in \mathcal{Y}$ is then defined by

$$\mathbb{P}(Y = \boldsymbol{y}) \coloneqq p(\boldsymbol{y}),$$

where Y denotes a random variable. When Y follows a distribution p, we write $Y \sim p$ (with some abuse of notation, we use the same letter p to denote the distribution and the PMF). The **expectation** of $\phi(Y)$, where $Y \sim p$ and $\phi\colon \mathcal{Y} \to \mathbb{R}^M$, is then

$$\mathbb{E}[\phi(Y)] = \sum_{\boldsymbol{y} \in \mathcal{Y}} p(\boldsymbol{y})\phi(\boldsymbol{y}),$$

its **variance** (for one-dimensional variables) is

$$\mathbb{V}[\phi(Y)] = \mathbb{E}[(\phi(Y) - \mathbb{E}[\phi(Y)])^2] = \sum_{y \in \mathcal{Y}} p(y)(\phi(y) - \mathbb{E}[\phi(Y)])^2$$

and its **mode** is

$$\arg\max_{y \in \mathcal{Y}} p(\boldsymbol{y}).$$

The **Kullback-Leibler** (KL) divergence (also known as relative entropy) between two discrete distributions over $\mathcal{Y}$, with associated PMFs p and q, is the statistical "distance" defined by

$$\mathrm{KL}(p, q) := \sum_{y \in \mathcal{Y}} p(y) \log \left(\frac{p(y)}{q(y)} \right) = \mathbb{E}_{Y \sim p} \log \left(\frac{p(Y)}{q(Y)} \right).$$

3.1.2 Continuous probability distributions

A continuous probability distribution over $\mathcal{Y}$ is specified by its **probability density function** (PDF) $p \colon \mathcal{Y} \to \mathbb{R}_+$. The probability of $\mathcal{A} \subseteq \mathcal{Y}$ is then

$$\mathbb{P}(Y \in \mathcal{A}) = \int_{\mathcal{A}} p(y) dy.$$

The definitions of expectation, variance and KL divergence are defined analogously to the discrete setting, simply replacing $\sum_{y \in \mathcal{Y}}$ with $\int_{\mathcal{Y}}$. Speficially, the expectation of $\phi(Y)$ is

$$\mathbb{E}[\phi(Y)] = \int_{\mathcal{Y}} p(y)\phi(y) dy,$$

the variance is

$$\mathbb{V}[\phi(Y)] = \mathbb{E}[(\phi(Y) - \mathbb{E}[\phi(Y)])^2] = \int_{\mathcal{Y}} p(y)(\phi(y) - \mathbb{E}[\phi(Y)])^2 dy$$

and the KL divergence is

$$\mathrm{KL}(p, q) := \int_{\mathcal{Y}} p(y) \log \left(\frac{p(y)}{q(y)} \right) dy = \mathbb{E}_{Y \sim p} \log \left(\frac{p(Y)}{q(Y)} \right).$$

The mode is defined as the arg maximum of the PDF.

When $\mathcal{Y} = \mathbb{R}$, we can also define the **cumulative distribution function** (CDF)

$$\mathbb{P}(Y \leq b) = \int_{-\infty}^{b} p(y) dy.$$

The probability of Y lying in the semi-closed interval $(a, b]$ is then

$$\mathbb{P}(a < Y \leq b) = \mathbb{P}(Y \leq b) - \mathbb{P}(Y \leq a).$$

3.2   Maximum likelihood estimation

3.2.1   Negative log-likelihood

We saw that a probability distribution over $\mathcal{Y}$ is specified by $p(\boldsymbol{y})$, which is called the probability mass function (PMF) for discrete variables or the probability density function (PDF) for continuous variables. In practice, the true distribution p generating the data is unknown and we wish to approximate it with a distribution $p_{\boldsymbol{\lambda}}$, with parameters $\boldsymbol{\lambda} \in \Lambda$. Given a finite set of observations $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N$, how do we fit $\boldsymbol{\lambda} \in \Lambda$ to the data? This can be done by maximizing the **likelihood** of the data, i.e., we seek to solve

$$\widehat{\boldsymbol{\lambda}}_N := \arg\max_{\boldsymbol{\lambda} \in \Lambda} \prod_{i=1}^{N} p_{\boldsymbol{\lambda}}(\boldsymbol{y}_i).$$

This is known as **maximum likelihood estimation** (MLE). Because the log function is monotonically increasing, this is equivalent to minimizing the **negative log-likelihood**, i.e., we have

$$\widehat{\boldsymbol{\lambda}}_N = \arg\min_{\boldsymbol{\lambda} \in \Lambda} -\sum_{i=1}^{N} \log p_{\boldsymbol{\lambda}}(\boldsymbol{y}_i).$$

Example 3.1 (MLE for the normal distribution). Suppose we set $p_{\boldsymbol{\lambda}}$ to the normal distribution with parameters $\boldsymbol{\lambda} = (\mu, \sigma)$, i.e.,

$$p_{\boldsymbol{\lambda}}(y) := \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{y - \mu}{\sigma}\right)^2\right).$$

Then, given observations $y_1, \ldots, y_N$, the MLE estimators for μ and σ^2 are the sample mean and the sample variance, respectively.

3.2.2   Consistency w.r.t. the Kullback-Leibler divergence

It is well-known that the MLE estimator is **consistent**, in the sense of the Kullback-Leibler divergence. That is, denoting the true distribution

p and

$$\boldsymbol{\lambda}_\infty := \arg\min_{\boldsymbol{\lambda}\in\Lambda} \mathrm{KL}(p, p_{\boldsymbol{\lambda}}) = \mathbb{E}_{Y\sim p}\log\left(\frac{p(Y)}{p_{\boldsymbol{\lambda}}(Y)}\right),$$

then $\widehat{\boldsymbol{\lambda}}_N \to \boldsymbol{\lambda}_\infty$ in expectation over the observations, as $N \to \infty$. This can be seen by using

$$\mathrm{KL}(p, p_{\boldsymbol{\lambda}}) \approx \frac{1}{N}\sum_{i=1}^N \log\left(\frac{p(\boldsymbol{y}_i)}{p_{\boldsymbol{\lambda}}(\boldsymbol{y}_i)}\right) = \frac{1}{N}\sum_{i=1}^N \log p(\boldsymbol{y}_i) - \log p_{\boldsymbol{\lambda}}(\boldsymbol{y}_i)$$

and the law of large numbers.

3.3   Probabilistic supervised learning

3.3.1   Conditional probability distributions

Many times in machine learning, instead of a probability $\mathbb{P}(Y = \boldsymbol{y})$ for some $\boldsymbol{y} \in \mathcal{Y}$, we wish to define a conditional probability $\mathbb{P}(Y = \boldsymbol{y}|X = \boldsymbol{x})$, for some input $\boldsymbol{x} \in \mathcal{X}$. This can be achieved by reduction to an unconditional probability distribution,

$$\mathbb{P}(Y = \boldsymbol{y}|X = \boldsymbol{x}) := p_{\boldsymbol{\lambda}}(\boldsymbol{y})$$

where

$$\boldsymbol{\lambda} := f(\boldsymbol{x}, \boldsymbol{w})$$

and f is a **model function** with **model parameters** $\boldsymbol{w} \in \mathcal{W}$. That is, rather than being a deterministic function from $\mathcal{X}$ to $\mathcal{Y}$, f is a function from $\mathcal{X}$ to Λ, the **distribution parameters** of the output distribution associated with the input.

We emphasize that $\boldsymbol{\lambda}$ could be a single parameter or a collection of parameters. For instance, in the Bernouilli distribution, $\lambda = \pi$, while in the univariate normal distribution, $\boldsymbol{\lambda} = (\mu, \sigma)$.

In Section 3.4 and throughout this book, we will also use the notation $p_{\boldsymbol{\theta}}$ instead of $p_{\boldsymbol{\lambda}}$ when $\boldsymbol{\theta}$ are the canonical parameters of an exponential family distribution (Section 3.4).

3.3.2   Inference

The main advantage of this probabilistic approach is that our prediction model is much richer than if we just learned a function from $\mathcal{X}$ to $\mathcal{Y}$.

We now have access to the whole distribution over possible outcomes in $\mathcal{Y}$ and can compute various statistics:

- Probability: $\mathbb{P}(Y = \boldsymbol{y}|X = \boldsymbol{x})$ or $\mathbb{P}(Y \in \mathcal{A}|X = \boldsymbol{x})$,

- Expectation: $\mathbb{E}[\phi(Y)|X = \boldsymbol{x}]$ for some function ϕ,

- Variance: $\mathbb{V}[\phi(Y)|X = \boldsymbol{x}]$,

- Mode: $\arg\max_{\boldsymbol{y} \in \mathcal{Y}} p_\lambda(\boldsymbol{y})$.

We now review probability distributions useful for binary classification, multiclass classification, regression, multivariate regression, and integer regression. In the following, to make the notation more lightweight, we omit the dependence on $\boldsymbol{x}$.

3.3.3   Binary classification

For **binary outcomes**, where $\mathcal{Y} = \{0, 1\}$, we can use a **Bernouilli distribution** with parameter

$$\lambda := \pi \in [0, 1].$$

When a random variable Y is distributed according to a Bernouilli distribution with parameter π, we write

$$Y \sim \text{Bernouilli}(\pi).$$

The PMF of this distribution is

$$p_\lambda(y) := \begin{cases} \pi & \text{if } y = 1 \\ 1 - \pi & \text{if } y = 0 \end{cases}.$$

The Bernouilli distribution is a **binomial distribution** with a single trial. Since $y \in \{0, 1\}$, the PMF can be rewritten as

$$p_\lambda(y) = \pi^y (1 - \pi)^{1-y}.$$

The mean is

$$\mathbb{E}[Y] = \pi = \mathbb{P}(Y = 1)$$

and the variance is

$$\mathbb{V}[Y] = \pi(1 - \pi) = \mathbb{P}(Y = 1)\mathbb{P}(Y = 0).$$

Parameterization using a sigmoid

Since the parameter π of a Bernouilli distribution needs to belong to $[0, 1]$, we typically use a **sigmoid function**, such as a **logistic function** as the output layer:

$$\pi := f(\boldsymbol{x}, \boldsymbol{w}) := \text{logistic}(g(\boldsymbol{x}, \boldsymbol{w})),$$

where $g \colon \mathcal{X} \times \mathcal{W} \to \mathbb{R}$ is for example a neural network and

$$\text{logistic}(a) := \frac{1}{1 + \exp(-a)} \in (0, 1).$$

See also Section 4.4.3 for more details. When g is linear in $\boldsymbol{w}$, this is known as **binary logistic regression**.

Remark 3.1 (Link with the logistic distribution). The logistic distribution with mean and scale parameters μ and σ is a **continuous** probability distribution with PDF

$$p_{\mu,\sigma}(u) := p_{0,1}\left(\frac{u - \mu}{\sigma}\right)$$

where

$$p_{0,1}(z) := \frac{\exp(-z)}{(1 + \exp(-z))^2}.$$

The corresponding CDF is

$$\mathbb{P}(U \leq u) = \int_{-\infty}^{u} p_{\mu,\sigma}(u) du = \text{logistic}\left(\frac{u - \mu}{\sigma}\right).$$

Therefore, if

$$U \sim \text{Logistic}(\mu, \sigma)$$

and

$$Y \sim \text{Bernouilli}\left(\text{logistic}\left(\frac{u - \mu}{\sigma}\right)\right),$$

then

$$\mathbb{P}(Y = 1) = \mathbb{P}(U \leq u).$$

Here, U can be interpreted as a latent continuous variable and u as a threshold.

3.3.4 Multiclass classification

For **categorical outcomes** with M possible choices, where $\mathcal{Y} = [M]$, we can use a **categorical distribution** with parameters

$$\boldsymbol{\lambda} \coloneqq \boldsymbol{\pi} \in \triangle^M,$$

where we define the probability simplex

$$\triangle^M \coloneqq \{\boldsymbol{\pi} \in \mathbb{R}_+^M : \langle \boldsymbol{\pi}, \mathbf{1} \rangle = 1\},$$

i.e., the set of valid discrete probability distributions. When Y follows a categorical distribution with parameter $\boldsymbol{\pi}$, we write

$$Y \sim \text{Categorical}(\boldsymbol{\pi}).$$

The PMF of the categorical distribution is

$$p_{\boldsymbol{\lambda}}(y) \coloneqq \langle \boldsymbol{\pi}, \phi(y) \rangle = \pi_y,$$

where

$$\phi(y) \coloneqq \boldsymbol{e}_y$$

is the standard basis vector for the coordinate $y \in [M]$.

Since Y is a categorical variable, it does not make sense to compute the expectation of Y but we can compute that of $\phi(Y) = \boldsymbol{e}_Y$,

$$\mathbb{E}_{Y \sim p_{\boldsymbol{\lambda}}}[\phi(Y)] = \boldsymbol{\pi}.$$

That is, the mean and the probability distribution (represented by the vector $\boldsymbol{\pi}$) are the same in this case.

Parameterization using a softargmax

Since the parameter vector $\boldsymbol{\pi}$ of a categorical distribution needs to belong to $\triangle^M$, we typically use a softargmax as the output layer:

$$\boldsymbol{\pi} \coloneqq f(\boldsymbol{x}, \boldsymbol{w}) \coloneqq \text{softargmax}(g(\boldsymbol{x}, \boldsymbol{w})),$$

where $g \colon \mathcal{X} \times \mathcal{W} \to \mathbb{R}^M$ is for example a neural network and

$$\text{softargmax}(\boldsymbol{u}) \coloneqq \frac{\exp(\boldsymbol{u})}{\sum_j \exp(u_j)} \in \text{relint}(\triangle^M).$$

The output of the softargmax is in the relative interior of $\triangle^M$, $\text{relint}(\triangle^M) = \triangle^M \cap \mathbb{R}^M_{>0}$. That is, the produced probabilities are always strictly positive. The categorical distribution is a **multinomial distribution** with a single trial. When g is linear in $\boldsymbol{w}$, this is therefore known as **multiclass** or **multinomial logistic regression**, though strictly speaking a multinomial distribution could use more than one trial.

3.3.5 Regression

For **real outcomes**, where $\mathcal{Y} = \mathbb{R}$, we can use, among other choices, a **normal distribution** with parameters

$$\boldsymbol{\lambda} := (\mu, \sigma),$$

where $\mu \in \mathbb{R}$ is the mean parameter and $\sigma \in \mathbb{R}_+$ is the standard deviation parameter. The PDF is

$$p_\lambda(y) := \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\frac{(y-\mu)^2}{\sigma^2}\right).$$

The expectation is

$$\mathbb{E}_{Y \sim p_\lambda}[Y] = \mu.$$

One advantage of the probabilistic perspective, however, is that we are not limited to predicting the mean. We can also compute the CDF

$$\mathbb{P}(Y \leq y) = \frac{1}{2}\left[1 + \text{erf}\left(\frac{y-\mu}{\sigma\sqrt{2}}\right)\right], \tag{3.1}$$

where we used the **error function**

$$\text{erf}(z) := \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} \, dt.$$

This function is available in most scientific computing libraries, such as SciPy. From the CDF, we also easily obtain

$$\mathbb{P}(a < Y \leq b) = \frac{1}{2}\left[\text{erf}\left(\frac{b-\mu}{\sigma\sqrt{2}}\right) - \text{erf}\left(\frac{a-\mu}{\sigma\sqrt{2}}\right)\right].$$

Parameterization

Typically, in regression, the mean is output by a model, while the standard deviation σ is kept fixed (typically set to 1). Since μ is unconstrained, we can simply set

$$\mu := f(\boldsymbol{x}, \boldsymbol{w}) \in \mathbb{R},$$

where $f\colon \mathcal{X} \times \mathcal{W} \to \mathbb{R}$ is for example a neural network. That is, the output of f is the mean of the distribution,

$$\mathbb{E}_{Y \sim p_{\boldsymbol{\lambda}}}[Y] = \mu = f(\boldsymbol{x}, \boldsymbol{w}).$$

We can also use μ to predict $\mathbb{P}(Y \le y)$ or $\mathbb{P}(a < Y \le b)$, as shown above.

3.3.6 Multivariate regression

More generally, for **multivariate outcomes**, where $\mathcal{Y} = \mathbb{R}^M$, we can use a **multivariate normal distribution** with parameters

$$\boldsymbol{\lambda} := (\boldsymbol{\mu}, \boldsymbol{\Sigma}),$$

where $\boldsymbol{\mu} \in \mathbb{R}^M$ is the mean and $\boldsymbol{\Sigma} \in \mathbb{R}^{M \times M}$ is the covariance matrix. The PDF is

$$p_{\boldsymbol{\lambda}}(\boldsymbol{y}) := \frac{1}{\sqrt{2\pi^M |\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}\langle \boldsymbol{y} - \boldsymbol{\mu}, \boldsymbol{\Sigma}^{-1}(\boldsymbol{y} - \boldsymbol{\mu})\rangle \right).$$

Using a diagonal covariance matrix is equivalent to using M independent normal distributions for each Y_j, for $j \in [M]$. The expectation is

$$\mathbb{E}_{Y \sim p_{\boldsymbol{\lambda}}}[Y] = \boldsymbol{\mu}.$$

Parameterization

Typically, in multivariate regression, the mean is output by a model, while the covariance matrix is kept fixed (typically set to the identity matrix). Since $\boldsymbol{\mu}$ is again unconstrained, we can simply set

$$\boldsymbol{\mu} := f(\boldsymbol{x}, \boldsymbol{w}) \in \mathbb{R}^M.$$

More generally, we can parametrize the function f so as to output both the mean $\boldsymbol{\mu}$ and the covariance matrix $\boldsymbol{\Sigma}$, i.e.,

$$(\boldsymbol{\mu}, \boldsymbol{\Sigma}) := f(\boldsymbol{x}, \boldsymbol{w}) \in \mathbb{R}^M \times \mathbb{R}^{M \times M}.$$

The function f must be designed such that $\boldsymbol{\Sigma}$ is symmetric and positive semi-definite. This is easy to achieve for instance by parametrizing $\boldsymbol{\Sigma} = \boldsymbol{S}\boldsymbol{S}^\top$ for some matrix $\boldsymbol{S}$.

3.3.7 Integer regression

For **integer outcomes**, where $\mathcal{Y} = \mathbb{N}$, we can use, among other choices, a **Poisson distribution** with mean parameter $\lambda > 0$. The PMF is

$$p_\lambda(y) := \frac{\lambda^y \exp(-\lambda)}{y!}.$$

The Poisson distribution implies that the **index of dispersion** (the ratio between variance and mean) is 1, since

$$\mathbb{E}[Y] = \mathbb{V}[Y] = \lambda.$$

When this assumption is inappropriate, one can use generalized Poisson distributions (Satterthwaite, 1942).

Parameterization using an exponential

Since the parameter λ of a Poisson distribution needs to be strictly positive, we typically use an exponential function as output layer:

$$\lambda := f(\boldsymbol{x}, \boldsymbol{w}) := \exp(g(\boldsymbol{x}, \boldsymbol{w})) > 0,$$

where $g \colon \mathcal{X} \times \mathcal{W} \to \mathbb{R}$.

3.3.8 Loss functions

In the conditional setting, we can now use maximum likelihood estimation (MLE) to estimate the model parameters $\boldsymbol{w} \in \mathcal{W}$ of f. Given a set of input-output pairs $(\boldsymbol{x}_1, \boldsymbol{y}_1), \ldots, (\boldsymbol{x}_N, \boldsymbol{y}_N)$, we choose the model parameters that maximize the **likelihood** of the data,

$$\widehat{\boldsymbol{w}}_N := \operatorname*{arg\,max}_{\boldsymbol{w} \in \mathcal{W}} \prod_{i=1}^N p_{\boldsymbol{\lambda}_i}(\boldsymbol{y}_i),$$

where
$$\boldsymbol{\lambda}_i := f(\boldsymbol{x}_i, \boldsymbol{w}).$$

Again, this is equivalent to minimizing the **negative log-likelihood**,

$$\widehat{\boldsymbol{w}} = \operatorname*{arg\,min}_{\boldsymbol{w} \in \mathcal{W}} - \sum_{i=1}^{N} \log p_{\boldsymbol{\lambda}_i}(\boldsymbol{y}_i).$$

Interestingly, MLE allows us to recover several popular loss functions.

- For the Bernouilli distribution with parameter $\lambda_i = \pi_i = \text{logistic}(g(\boldsymbol{x}_i, \boldsymbol{w}))$, we have

$$- \log p_{\lambda_i}(y_i) = - \left[y_i \log \pi_i + (1 - y_i) \log(1 - \pi_i) \right],$$

  which is the **binary logistic loss** function.

- For the categorical distribution with parameters $\boldsymbol{\lambda}_i = \boldsymbol{\pi}_i = \text{softargmax}(g(\boldsymbol{x}_i, \boldsymbol{w}))$, we have

$$- \log p_{\boldsymbol{\lambda}_i}(y_i) = \log \sum_{j=1}^{M} \exp(\pi_{i,j}) - \pi_{i,y_i}$$
$$= \text{logsumexp}(\boldsymbol{\pi}_i) - \langle \boldsymbol{\pi}_i, \boldsymbol{e}_{y_i} \rangle,$$

  which is the **multiclass logistic loss** function, also known as **cross-entropy loss**.

- For the normal distribution with mean $\lambda_i = \mu_i = f(\boldsymbol{x}_i, \boldsymbol{w})$ and fixed variance σ_i^2, we have

$$- \log p_{\lambda_i}(\boldsymbol{y}_i) = \frac{1}{\sigma_i^2}(y_i - \mu_i)^2 + \frac{1}{2} \log \sigma_i^2 + \frac{1}{2} \log(2\pi),$$

  which is, up to constant and with unit variance, the **squared loss** function.

- For the Poisson distribution with mean $\lambda_i \exp(g(\boldsymbol{x}_i, \boldsymbol{w}))$, we have

$$- \log p_{\lambda_i}(\boldsymbol{y}_i) = -(y_i \mu_i - \exp(\mu_i) - \log(y_i!)),$$

  which is the **Poisson loss** function.

3.4 Exponential family distributions

3.4.1 Definition

The exponential family is a class of probability distributions, whose PMF or PDF can be written in the form

$$p_{\boldsymbol{\theta}}(\boldsymbol{y}) = \frac{h(\boldsymbol{y}) \exp\left[\langle \boldsymbol{\theta}, \phi(\boldsymbol{y})\rangle\right]}{\exp(A(\boldsymbol{\theta}))}$$
$$= h(\boldsymbol{y}) \exp\left[\langle \boldsymbol{\theta}, \phi(\boldsymbol{y})\rangle - A(\boldsymbol{\theta})\right],$$

where $\boldsymbol{\theta}$ are the **natural** or **canonical parameters** of the distribution. The function h is known as the base measure. The function ϕ is the **sufficient statistic**: it holds all the information about $\boldsymbol{y}$ and is used to embed $\boldsymbol{y}$ in a vector space. The function A is the **log-partition** or **log-normalizer** (see below for a details). All the distributions we reviewed in Section 3.3 belong to the exponential family. With some abuse of notation, we use $p_{\boldsymbol{\lambda}}$ for the distribution in **original form** and $p_{\boldsymbol{\theta}}$ for the distribution in **exponential family form**. As we will see, we can go from $\boldsymbol{\theta}$ to $\boldsymbol{\lambda}$ and vice-versa. We illustrate how to rewrite a distribution in exponential family form below.

> **Example 3.2** (Bernouilli distribution). The PMF of the Bernouilli distribution with parameter $\lambda = \pi$ equals
>
> $$p_{\lambda}(y) := \pi^y (1-\pi)^{1-y}$$
> $$= \exp(\log(\pi^y (1-\pi)^{1-y}))$$
> $$= \exp(y \log(\pi) + (1-y) \log(1-\pi))$$
> $$= \exp(\log(\pi/(1-\pi))y + \log(1-\pi))$$
> $$= \exp(\theta y - \log(1 + \exp(\theta)))$$
> $$= \exp(\theta y - \text{softplus}(\theta))$$
> $$=: p_{\theta}(y).$$
>
> Therefore, Bernouilli distributions belong to the exponential family, with natural parameter $\theta = \text{logit}(\pi) := \log(\pi/(1+\pi))$.

We rewrite the previously-described distributions in exponential family form in Table 3.1. This list is non-exhaustive: there are many more distributions in the exponential family!

Table 3.1: Examples of distributions in the exponential family.

	Bernouilli	Categorical
$\mathcal{Y}$	$\{0,1\}$	$[M]$
$\boldsymbol{\lambda}$	$\pi = \text{logistic}(\theta)$	$\boldsymbol{\pi} = \text{softmax}(\boldsymbol{\theta})$
$\boldsymbol{\theta}$	$\text{logit}(\pi)$	$\log \boldsymbol{\pi} + \exp(A(\boldsymbol{\theta}))$
$\phi(y)$	y	$\boldsymbol{e}_y$
$A(\boldsymbol{\theta})$	$\text{softplus}(\theta) = -\log(1-\pi)$	$\text{logsumexp}(\boldsymbol{\theta})$
$h(y)$	1	1

	Normal (location only)	Normal (location-scale)
$\mathcal{Y}$	$\mathbb{R}$	$\mathbb{R}$
$\boldsymbol{\lambda}$	$\mu = \theta\sigma$	$(\mu, \sigma^2) = (\frac{-\theta_1}{2\theta_2}, \frac{-1}{2\theta_2})$
$\boldsymbol{\theta}$	$\frac{\mu}{\sigma}$	$(\frac{\mu}{\sigma^2}, \frac{-1}{2\sigma^2})$
$\phi(y)$	$\frac{y}{\sigma}$	(y, y^2)
$A(\boldsymbol{\theta})$	$\frac{\theta^2}{2} = \frac{\mu^2}{2\sigma^2}$	$\frac{-\theta_1^2}{4\theta_2} - \frac{1}{2}\log(-2\theta_2) = \frac{\mu^2}{\sigma^2} + \log\sigma$
$h(y)$	$\frac{\exp(\frac{-y^2}{2\sigma^2})}{\sqrt{2\pi}\sigma}$	$\frac{1}{\sqrt{2\pi}}$

	Multivariate normal	Poisson
$\mathcal{Y}$	$\mathbb{R}^M$	$\mathbb{N}$
$\boldsymbol{\lambda}$	$(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (-\frac{1}{2}\boldsymbol{\theta}_2^{-1}\boldsymbol{\theta}_1, -\frac{1}{2}\boldsymbol{\theta}_2^{-1})$	$\lambda = \exp(\theta)$
$\boldsymbol{\theta}$	$(\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}, -\frac{1}{2}\boldsymbol{\Sigma}^{-1})$	$\log\lambda$
$\phi(\boldsymbol{y})$	$(\boldsymbol{y}, \boldsymbol{y}\boldsymbol{y}^\top)$	y
$A(\boldsymbol{\theta})$	$-\frac{1}{4}\boldsymbol{\theta}_1^\top\boldsymbol{\theta}_2^{-1} - \frac{1}{2}\log|-2\boldsymbol{\theta}_2|$ $= \frac{1}{2}\boldsymbol{\mu}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \frac{1}{2}\log|\boldsymbol{\Sigma}|$	$\exp(\theta)$
$h(y)$	$(2\pi)^{-M/2}$	$1/y!$

3.4.2 The log-partition function

The log-partition function A is the logarithm of the distribution's normalization factor. That is,

$$A(\boldsymbol{\theta}) := \log \sum_{\boldsymbol{y} \in \mathcal{Y}} h(\boldsymbol{y}) \exp\left[\langle \boldsymbol{\theta}, \phi(\boldsymbol{y}) \rangle\right]$$

for discrete random variables and

$$A(\boldsymbol{\theta}) := \log \int_{\mathcal{Y}} h(y) \exp\left[\langle \boldsymbol{\theta}, \phi(y) \rangle\right] dy$$

for continuous random variables. We denote the set of valid parameters

$$\Theta := \{\boldsymbol{\theta} \in \mathbb{R}^M : A(\boldsymbol{\theta}) < +\infty\} \subseteq \mathbb{R}^M.$$

We can conveniently rewrite $A(\boldsymbol{\theta})$ for discrete random variables as

$$A(\boldsymbol{\theta}) = \text{logsumexp}(B(\boldsymbol{\theta})) := \log \sum_{\boldsymbol{y} \in \mathcal{Y}} [B(\boldsymbol{\theta})]_{\boldsymbol{y}},$$

and similarly for continuous variables. Here, we defined the **linear map**

$$B(\boldsymbol{\theta}) := (\langle \boldsymbol{\theta}, \phi(\boldsymbol{y}) \rangle + \log h(y))_{\boldsymbol{y} \in \mathcal{Y}}.$$

Since $A(\boldsymbol{\theta})$ is the composition of logsumexp, a convex function, and of B, a linear map, we immediately obtain the following proposition.

> **Proposition 3.1** (Convexity of the log-partition). $A(\boldsymbol{\theta})$ is a convex function.

A major property of the log-partition function is that its gradient coincides with the expectation of $\phi(Y)$ according to $p_{\boldsymbol{\theta}}$.

> **Proposition 3.2** (Gradient of the log-partition).
>
> $$\boldsymbol{\mu}(\boldsymbol{\theta}) := \nabla A(\boldsymbol{\theta}) = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\phi(Y)] \in \mathcal{M}.$$

Proof. The result follows directly from

$$\nabla A(\boldsymbol{\theta}) = \partial B(\boldsymbol{\theta})^* \nabla \text{logsumexp}(B(\boldsymbol{\theta})) = (\phi(\boldsymbol{y}))_{\boldsymbol{y} \in \mathcal{Y}} \, \text{softmax}(B(\boldsymbol{\theta})).$$

$\square$

The gradient $\nabla A(\boldsymbol{\theta})$ is therefore often called the **mean function**. The set of achievable means $\boldsymbol{\mu}(\boldsymbol{\theta})$ is defined by

$$\mathcal{M} \coloneqq \operatorname{conv}(\phi(\mathcal{Y})) \coloneqq \{\mathbb{E}_p[\phi(Y)] \colon p \in \mathcal{P}(\mathcal{Y})\},$$

where $\operatorname{conv}(\mathcal{S})$ is the convex hull of $\mathcal{S}$ and $\mathcal{P}(\mathcal{Y})$ is the set of valid probability distributions over $\mathcal{Y}$.

Similarly, the Hessian $\nabla^2 A(\boldsymbol{\theta})$ coincides with the covariance matrix of $\phi(Y)$ according to $p_{\boldsymbol{\theta}}$ (Wainwright and Jordan, 2008, Chapter 3).

When the exponential family is **minimal**, which means that the parameters $\boldsymbol{\theta}$ uniquely identify the distribution, it is known that ∇A is a one-to-one mapping from Θ to $\mathcal{M}$. That is, $\boldsymbol{\mu}(\boldsymbol{\theta}) = \nabla A(\boldsymbol{\theta})$ and $\boldsymbol{\theta} = (\nabla A)^{-1}(\boldsymbol{\mu}(\boldsymbol{\theta}))$.

3.4.3   Maximum entropy principle

Suppose we observe the empirical mean $\widehat{\boldsymbol{\mu}} = \frac{1}{N} \sum_{i=1}^n \phi(\boldsymbol{y}_i) \in \mathcal{M}$ of some observations $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N$. How do we find a probability distribution achieving this mean? Clearly, such a distribution may not be unique. One way to choose among all possible distributions is by using the **maximum entropy principle**. Let us define the Shannon entropy by

$$H(p) \coloneqq -\sum_{\boldsymbol{y} \in \mathcal{Y}} p(\boldsymbol{y}) \log p(\boldsymbol{y})$$

for discrete variables and by

$$H(p) \coloneqq -\int_{\mathcal{Y}} p(y) \log p(y) dy$$

for continuous variables. This captures the level of "uncertainty" in p, i.e., it is maximized when the distribution is uniform. Then, the **maximum entropy distribution** satisfying the first-order moment condition (i.e., whose expectation matches the empirical mean) is

$$p^\star \coloneqq \operatorname*{arg\,max}_{p \in \mathcal{P}(\mathcal{Y})} H(p) \quad \text{s.t.} \quad \mathbb{E}_{Y \sim p}[\phi(Y)] = \widehat{\boldsymbol{\mu}}.$$

It can be shown that the maximum entropy distribution is necessarily in the exponential family with sufficient statistics defined by ϕ and its canonical parameters $\boldsymbol{\theta}$ coincide with the **Lagrange multipliers** of the above constraint (Wainwright and Jordan, 2008, Section 3.1).

3.4.4 Maximum likelihood estimation

Similarly as in Section 3.2, to fit the parameters $\boldsymbol{\theta} \in \Theta$ of an exponential family distribution to some observations $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N$, we can use the MLE principle, i.e.,

$$\widehat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta} \in \Theta} \prod_{i=1}^{N} p_{\boldsymbol{\theta}}(\boldsymbol{y}_i) = \arg\min_{\boldsymbol{\theta} \in \Theta} -\sum_{i=1}^{N} \log p_{\boldsymbol{\theta}}(\boldsymbol{y}_i).$$

Fortunately, for exponential family distributions, the log probability/density enjoys a particularly simple form.

> **Proposition 3.3** (Negative log-likelihood). The negative log-likelihood of an exponential family distribution is
>
> $$-\log p_{\boldsymbol{\theta}}(\boldsymbol{y}) = A(\boldsymbol{\theta}) - \langle \boldsymbol{\theta}, \phi(\boldsymbol{y}) \rangle - \log h(\boldsymbol{y}).$$
>
> Its gradient is
>
> $$-\nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\boldsymbol{y}) = \nabla A(\boldsymbol{\theta}) - \phi(\boldsymbol{y}) = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\phi(Y)] - \phi(\boldsymbol{y})$$
>
> and its Hessian is
>
> $$-\nabla_{\boldsymbol{\theta}}^2 \log p_{\boldsymbol{\theta}}(\boldsymbol{y}) = \nabla^2 A(\boldsymbol{\theta}),$$
>
> which is **independent** of $\boldsymbol{y}$.

It follows from Proposition 3.1 that $\boldsymbol{\theta} \mapsto -\log p_{\boldsymbol{\theta}}(\boldsymbol{y})$ is **convex**. Interestingly, we see that the gradient is the **residual** between the expectation according to the model and the observation.

3.4.5 Probabilistic learning with exponential families

In the supervised probabilistic learning setting, we wish to estimate a conditional distribution of the form $p_{\boldsymbol{w}}(\boldsymbol{y} \mid \boldsymbol{x})$. Given a model function f, such as a neural network, a common approach for defining such a conditional distribution is by reduction to the unconditional setting,

$$p_{\boldsymbol{w}}(\boldsymbol{y} \mid \boldsymbol{x}) \coloneqq p_{\boldsymbol{\theta}}(\boldsymbol{y}) \quad \text{where} \quad \boldsymbol{\theta} \coloneqq f(\boldsymbol{x}, \boldsymbol{w}).$$

In other words, the role of f is to produce the parameters of $p_{\boldsymbol{\theta}}$ given some input $\boldsymbol{x}$. It is a function from $\mathcal{X} \times \mathcal{W}$ to Θ. Note that f must be

designed such that it produces an output in

$$\Theta := \{\boldsymbol{\theta} \in \mathbb{R}^M : A(\boldsymbol{\theta}) < +\infty\}.$$

For instance, as we previously discussed, for a multivariate normal distribution, where $\boldsymbol{\theta}_i = (\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) = f(\boldsymbol{x}_i, \boldsymbol{w})$, we need to ensure that $\boldsymbol{\Sigma}_i$ is a positive semidefinite matrix.

Given input-output pairs $\{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^N$, we then seek to find the parameters $\boldsymbol{w}$ of $f(\boldsymbol{x}, \boldsymbol{w})$ by minimizing

$$\underset{\boldsymbol{w} \in \mathcal{W}}{\arg\min} - \sum_{i=1}^N \log \boldsymbol{p}_{\boldsymbol{\theta}_i}(\boldsymbol{y}_i) = \underset{\boldsymbol{w} \in \mathcal{W}}{\arg\min} \sum_{i=1}^N A(\boldsymbol{\theta}_i) - \langle \boldsymbol{\theta}_i, \phi(\boldsymbol{y}_i) \rangle$$

where $\boldsymbol{\theta}_i := f(\boldsymbol{x}_i, \boldsymbol{w})$. While $-\log p_{\boldsymbol{\theta}}(\boldsymbol{y})$ is a convex function of $\boldsymbol{\theta}$ for exponential family distributions, we emphasize that $-\log p_{f(\boldsymbol{x},\boldsymbol{w})}(\boldsymbol{y})$ is typically a nonconvex function of $\boldsymbol{w}$, when f is a **nonlinear** function, such as a neural network.

Inference

Once we found $\boldsymbol{w}$ by minimizing the objective function above, there are several possible strategies to perform inference for a new input $\boldsymbol{x}$.

- **Expectation.** When the goal is to compute the expectation of $\phi(Y)$, we can use $\nabla A(f(\boldsymbol{x}, \boldsymbol{w}))$. That is, we compute the distribution parameters associated with $\boldsymbol{x}$ by $\boldsymbol{\theta} = f(\boldsymbol{x}, \boldsymbol{w})$ and then we compute the mean by $\boldsymbol{\mu} = \nabla A(\boldsymbol{\theta})$. When f is linear in $\boldsymbol{w}$, the composition $\nabla A \circ f$ is called a **generalized linear model**.

- **Probability.** When the goal is to compute the probability of a certain $\boldsymbol{y}$, we can compute the distribution parameters associated with $\boldsymbol{x}$ by $\boldsymbol{\theta} = f(\boldsymbol{x}, \boldsymbol{w})$ and then we can compute $\mathbb{P}(Y = \boldsymbol{y}|X = \boldsymbol{x}) = p_{\boldsymbol{\theta}}(\boldsymbol{y})$. In the particular case of the categorical distribution (of which the Bernouilli distribution is a special case), we point out again that the mean and the probability vector coincide:

$$\boldsymbol{\mu} = \boldsymbol{p} = \nabla A(\boldsymbol{\theta}) = \text{softargmax}(\boldsymbol{\theta}) \in \triangle^M.$$

- **Other statistics.** When the goal is to compute other quantities, such as the variance or the CDF, we can convert the natural parameters $\boldsymbol{\theta}$ to the original distribution parameters $\boldsymbol{\lambda}$ (see Table 3.1

for examples). Then, we can use established formulas for the distribution in original form, to compute the desired quantities.

3.5 Summary

In this chapter, we started by reviewing **discrete** and **continuous** probability distributions. We saw how to fit distribution parameters to data using the **maximum likelihood estimation** (MLE) principle and saw its connection with the **Kullback-Leibler divergence**. Instead of designing a model function from the input space $\mathcal{X}$ to the output space $\mathcal{Y}$, we saw that we can perform **probabilistic supervised learning** by designing a model function from $\mathcal{X}$ to **distribution parameters** Λ. Leveraging the so-obtained parametric **conditional distribution** then allowed us to compute, not only output probabilities, but also various statistics such as the mean and the variance of the outputs. Finally, we reviewed the **exponential family**, a principled generalization of numerous distributions, which we saw is tightly connected with the **maximum entropy principle**. Importantly, the approaches described in this chapter produce perfectly valid **computation graphs**, meaning that we can combine them with neural networks and we can use automatic differentiation, to compute their derivatives.

Part II

Differentiable programs

4

Parameterized programs

Neural networks can be thought as parameterized programs: programs with learnable parameters. In this chapter, we begin by reviewing how to represent programs mathematically. We then review several key neural network architectures and components.

4.1 Representing computer programs

4.1.1 Computation chains

To begin with, we consider simple programs that apply a **sequence** of functions $f_1, \ldots, f_K$ to an input $s_0 \in \mathcal{S}_0$. We call such programs **computation chains**. For example, an image may go through a sequence of transformations such as cropping, rotation, normalization, and so on. In neural networks, the transformations are typically parametrized and the parameters are learned, leading to feedforward networks, presented in Section 4.2. Another example of sequence of functions is a for loop, presented in Section 5.8.
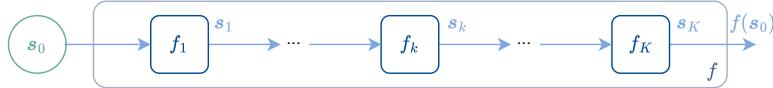
Figure 4.1: A computation chain is a sequence of function compositions. In the graph above, each intermediate node represents a single function. The first node represents the input, the last node the output. Edges represent the dependencies of the functions with respect to previous outputs or to the initial input.

Formally, a computation chain can be written as

$$s_0 \in \mathcal{S}_0$$
$$s_1 := f_1(s_0) \in \mathcal{S}_1$$
$$\vdots$$
$$s_K := f_K(s_{K-1}) \in \mathcal{S}_K$$
$$f(s_0) := s_K. \tag{4.1}$$

Here, s_0 is the **input**, $s_k \in \mathcal{S}_k$ is an intermediate **state** of the program, and $s_K \in \mathcal{S}_K$ is the final **output**. Of course, the domain (input space) of f_k must be compatible with the image (output space) of f_{k-1}. That is, we should have $f_k : \mathcal{S}_{k-1} \to \mathcal{S}_k$. We can write the program equivalently as

$$f(s_0) = (f_K \circ \cdots \circ f_2 \circ f_1)(s_0)$$
$$= f_K(\ldots f_2(f_1(s_0))).$$

A computation chain can be represented by a directed graph, shown in Fig. 4.1. The edges in the chain define a **total order**. The order is total, since two nodes are necessarily linked to each other by a path.

4.1.2   Directed acyclic graphs

In generic programs, intermediate functions may depend, not only on the previous function output, but on the outputs of several different functions. Such dependences are best expressed using graphs.

A **directed graph** $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is defined by a set of **vertices** or **nodes** $\mathcal{V}$ and a set of **edges** $\mathcal{E}$ defining directed dependencies between
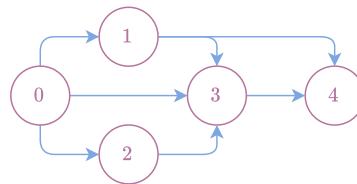
Figure 4.2: Example of a **directed acyclic graph**. Here the nodes are $\mathcal{V} = \{0, 1, 2, 3, 4\}$, the edges are $\mathcal{E} = \{(0, 1), (0, 2), (0, 3), (1, 3), (2, 3), (1, 4), (3, 4)\}$. Parents of the node 3 are parents$(3) = \{0, 1, 2\}$. Children of node 1 are children$(1) = \{3, 4\}$. There is a unique root, 0, and a unique leaf, 4; $0 \to 3 \to 4$ is a path from 0 to 4. This is an acyclic graph since there is no cycle (i.e., a path from a node to itself). We can order nodes 0 and 3 as $0 \leq 3$ since there is no path from 3 to 0. Similarly, we can order 1 and 2 as $1 \leq 2$ since there is no path from 2 to 1. Two possible topological orders of the nodes are $(0, 1, 2, 3, 4)$ and $(0, 2, 1, 3, 4)$.

vertices. An edge $(i, j) \in \mathcal{E}$ is an ordered pair of vertices $i \in \mathcal{V}$ and $j \in \mathcal{V}$. It is also denoted $i \to j$, to indicate that j depends on i. For representing inputs and outputs, it will be convenient to use **incoming half-edges** $\to j$ and **outgoing half-edges** $i \to$.

In a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, the **parents** of a vertex j is the set of nodes pointing to j, denoted parents$(j) := \{i : i \to j\}$. The **children** of a vertex i is the set of nodes i is pointing to, that is, children$(i) := \{j : i \to j\}$. Vertices without parents are called **roots** and vertices without children are called **leaves**.

A **path** from i to j is defined by a sequence of vertices $j_1, \ldots, j_m$, potentially empty, such that $i \to j_1 \to \ldots \to j_m \to j$. An **acyclic** graph is a graph such that there exists no vertex i with a path from i to i. A **directed acyclic graph** (DAG) is a graph that is both directed and acyclic.

The edges of a DAG define a **partial order** of the vertices, denoted $i \preceq j$ if there exists a path from i to j. The order is partial, since two vertices may not necessarily be linked to each other by a path. Nevertheless, we can define a total order called a **topological order**: any order such that $i \leq j$ if and only if there is no path from j to i.
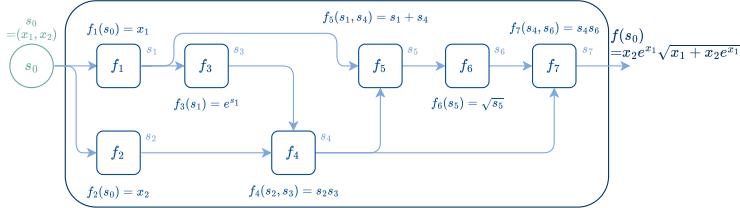
Figure 4.3: Representation of $f(x_1, x_2) = x_2 e^{x_1} \sqrt{x_1 + x_2 e^{x_1}}$ as a DAG, with functions as nodes and variables as edges. The function is decomposed as 8 functions in topological order.

4.1.3 Computer programs as DAGs

We assume that a program defines a mathematically valid function (a.k.a. pure function): the program should return identical values for identical arguments and should not have any side effects. We also assume that the program halts, i.e., that it terminates in a **finite** number of steps. As such a program is made of a finite number of intermediate functions and intermediate variables, the dependencies between functions and variables can be expressed using a directed acyclic graph (DAG). Without loss of generality, we make the following simplifying assumptions:

1. There is a single input $s_0 \in \mathcal{S}_0$.

2. There is a single output $s_K \in \mathcal{S}_K$.

3. Each intermediate function f_k in the program outputs a single variable $s_k \in \mathcal{S}_k$.

We number the nodes as $\mathcal{V} := \{0, 1, \ldots, K\}$. Node 0 is the root, corresponding to the input $s_0 \in \mathcal{S}_0$. Node K is the leaf, corresponding to the final output $s_K \in \mathcal{S}_K$. Because of the third assumption above, apart from s_0, each variable s_k is in **bijection** with a function f_k. Therefore, node 0 represents the input s_0, and nodes $1, \ldots, K$ represent both a function f_k and an output variable s_k.

Edges in the DAG represent dependences. The parents $i_1, \ldots, i_{p_k} :=$ parents(k) of node k, where $p_k := |\text{parents}(k)|$, indicate the variables $s_{\text{parents}}(k) := s_{i_1}, \ldots, s_{i_{p_k}}$ that the function f_k needs to perform its computation. Put differently, the parents $i_1, \ldots, i_{p_k}$ indicate the functions $f_{i_1}, \ldots, f_{i_{p_k}}$ that need to be evaluated, prior to evaluating f_k.

Algorithm 4.1 Executing a program

Functions: $f_1, \ldots, f_K$ in topological order
Input: input $s_0 \in \mathcal{S}_0$
1: **for** $k := 1, \ldots, K$ **do**
2:       Retrieve parent nodes $i_1, \ldots, i_{p_k} := \text{parents}(k)$
3:       Compute $s_k := f_k(s_{\text{parents}(k)}) := f_k(s_{i_1}, \ldots, s_{i_{p_k}})$
4: **Output:** $f(s_0) := s_K$

An example of computation graph in our formalism is presented in Fig. 4.3.

Executing a program

To execute a program, we need to ensure that we evaluate the intermediate functions in the correct order. Therefore, we assume that the nodes $0, 1, \ldots, K$ are in a topological order (if this is not the case, we need to perform a topological sort first). We can then execute a program by evaluating for $k \in [K]$

$$s_k := f_k(s_{\text{parents}(k)}) := f_k(s_{i_1}, \ldots, s_{i_{p_k}}) \in \mathcal{S}_k.$$

Note that we can either view f_k as a single-input function of $s_{\text{parents}(k)}$, which is a tuple of elements, or as a multi-input function of $s_{i_1}, \ldots, s_{i_{p_k}}$. The two views are essentially equivalent.

The procedure for executing a program is summarized in Algorithm 4.1.

Dealing with multiple program inputs or outputs

When a program has multiple inputs, we can always group them into $s_0 \in \mathcal{S}_0$ as $s_0 = (s_{0,1}, \ldots, s_{0,N_0})$ with $\mathcal{S}_0 = (\mathcal{S}_{0,1} \times \cdots \times \mathcal{S}_{0,N_0})$, since later functions can always filter out what elements of s_0 they need. Likewise, if an intermediate function f_k has multiple outputs, we can always group them as a single output $s_k = (s_{k,1}, \ldots, s_{k,N_k})$ with $\mathcal{S}_k = (\mathcal{S}_{k,1} \times \cdots \times \mathcal{S}_{k,N_k})$, since later functions can filter out the elements of s_k that they need.

Figure 4.4: Two possible representations of a program. **Left:** Functions and output variables are represented by the same nodes. **Right:** functions and variables are represented by a disjoint set of nodes.

Alternative representation: bipartite graphs

In our formalism, because a function f_k always have a single output s_k, a node k can be seen as representing both the variable s_k and the function f_k. Alternatively, as shown in Fig. 4.4, we can represent variables and functions as separate nodes, that is, using a **bipartite graph**. This formalism is akin to **factor graphs** (Frey *et al.*, 1997; Loeliger, 2004) used in probabilistic modeling, but with directed edges. One advantage of this formalism is that is allows functions to explicitly have multiple outputs. We focus on our formalism for simplicity.

4.1.4 Arithmetic circuits

Arithmetic circuits are one of the simplest examples of computation graph, originating from **computational complexity theory**. Formally, an arithmetic circuit over a field $\mathbb{F}$, such as the reals $\mathbb{R}$, is a directed acyclic graph (DAG) whose root nodes are elements of $\mathbb{F}$ and whose functions f_k are either $+$ or $\times$. The latter are often called **gates**. Contrary to the general computation graph case, because each f_k is either $+$ or $\times$, it is important to allow the graph to have several root nodes. Root nodes can be either variables or constants, and should belong to $\mathbb{F}$.

Arithmetic circuits can be used to compute **polynomials**. There are potentially multiple arithmetic circuits for representing a given polynomial. One important question is then to find the most efficient arithmetic circuit for computing a given polynomial. To compare arithmetic circuits representing the same polynomial, an intuitive notion of complexity is the **circuit size**, as defined below.

> **Definition 4.1** (Circuit and polynomial sizes). The size $S(\mathcal{C})$ of a circuit $\mathcal{C}$ is the number of edges in the directed acyclic graph representing $\mathcal{C}$. The size $S(f)$ a polynomial f is the smallest $S(\mathcal{C})$ among all $\mathcal{C}$ representing f.

For more information on arithmetic circuits, we refer the reader to the excellent book of Chen *et al.* (2011).

4.2 Feedforward networks

A feedforward network can be seen as a computation chain with **parameterized** functions f_k,

$$
\begin{aligned}
s_0 &:= x \\
s_1 &:= f_1(s_0, w_1) \\
s_2 &:= f_2(s_1, w_2) \\
&\vdots \\
s_K &:= f_K(s_{K-1}, w_K),
\end{aligned}
$$

for a given input $x \in \mathcal{X}$ and **learnable parameters** $w_1, \ldots, w_K \in \mathcal{W}_1 \times \cdots \times \mathcal{W}_K$. Each function f_k is called a **layer** and each $s_k \in \mathcal{S}_k$ can be seen as an **intermediate representation** of the input x. The dimensionality of $\mathcal{S}_k$ is known as the **width** (or number of hidden units) of layer k. A feedforward network defines a function $s_K =: f(x, w)$ from $\mathcal{X} \times \mathcal{W}$ to $\mathcal{S}_K$, where $w := (w_1, \ldots, w_K) \in \mathcal{W} := \mathcal{W}_1 \times \ldots \times \mathcal{W}_K$.

Given such a parameterized program, we can learn the parameters by adjusting w to fit some data. For instance, given a dataset of (x_i, y_i) pairs, we may minimize the squared loss $\|y_i - f(x_i, w)\|_2^2$ on average over the data, w.r.t. w. The minimization of such a loss requires accessing its gradients with respect to w.

4.3 Multilayer perceptrons

4.3.1 Combining affine layers and activations

In the previous section, we did not specify how to parametrize the feedforward network. A typical parametrization, called the multilayer

perceptron (MLP), uses **fully-connected** (also called **dense**) layers of the form

$$s_k = f_k(s_{k-1}, w_k) \coloneqq a_k(W_k s_{k-1} + b_k),$$

where we defined the tuple $w_k \coloneqq (W_k, b_k)$ and where we assumed that W_k and b_k are a matrix and vector of appropriate size. We can further decompose the layer into two functions. The function $s \mapsto W_k s + b_k$ is called an affine layer. The function $v \mapsto a_k(v)$ is a parameter-free **nonlinearity**, often called an **activation function** (see Section 4.4).

More generally, we may replace the matrix-vector product $W_k s_{k-1}$ by any parametrized linear function of s_{k-1}. For example, **convolutional layers** use the convolution of an input s_{k-1} with some filters W_k.

> **Remark 4.1** (Dealing with multiple inputs). Sometimes, it is necessary to deal with networks of multiple inputs. For example, suppose we want to design a function $g(x_1, x_2, w_g)$, where $x_1 \in \mathcal{X}_1$ and $x_2 \in \mathcal{X}_2$. A simple way to do so is to use the concatenation $x \coloneqq x_1 \oplus x_2 \in \mathcal{X}_2 \oplus \mathcal{X}_2$ as input to a network $f(x, w_f)$. Alternatively, instead of concatenating x_1 and x_2 at the input layer, they can be concatenated after having been through one or more hidden layers.

4.3.2 Link with generalized linear models

When the depth is $K = 1$ (only one layer), the output of an MLP is

$$s_1 = a_1(W_1 x + b_1).$$

This is called a **generalized linear model** (GLM); see Section 3.4. Therefore, MLPs include GLMs as a special case. In particular, when a_1 is the softargmax (see Section 4.4), we obtain (multiclass) logistic regression. For general depth K, the output of an MLP is

$$s_K = a_K(W_K s_{K-1} + b_K).$$

This can be seen as a GLM on top of **learned representation** s_{K-1} of the input x. This is the main appeal of MLPs: they learn the feature representation and the output model at the same time! We will see that MLPs can also be used as subcomponents in other architectures.

4.4 Activation functions

As we saw in Section 4.3, feedforward networks typically use an activation function a_k at each layer. In this section, we describe various nonlinearities from scalar to scalar or from vector to scalar. We also present probability mappings that can be used as such activations.

4.4.1 Scalar-to-scalar nonlinearities

The **ReLU** (rectified linear unit) is a popular nonlinearity defined as the **non-negative part** of its input

$$\text{relu}(u) := \max(u, 0) = \begin{cases} u, & u \geq 0 \\ 0, & u < 0 \end{cases}.$$

It is a piecewise linear function and includes a kink at $u = 0$. A multilayer perceptron with ReLU activations is called a **rectifier neural network**. The layers take the form

$$\boldsymbol{s}_k = \text{relu}(\boldsymbol{A}_k \boldsymbol{s}_{k-1} + \boldsymbol{b}_k),$$

where the ReLU is applied element-wise. The ReLU can be replaced with a smooth approximation (i.e., without kinks), called the **softplus**

$$\text{softplus}(u) := \log(1 + e^u).$$

Unlike the ReLU, it is always strictly positive. Other smoothed variants of the ReLU are possible, see Section 12.4.1.

4.4.2 Vector-to-scalar nonlinearities

It is often useful to **reduce** vectors to a scalar value. This scalar value can be seen as a "statistic", summarizing the vector. A simple way to do so is to use the maximum value, also known as **max pooling**. Given a vector $\boldsymbol{u} \in \mathbb{R}^M$, it is defined as

$$\boldsymbol{u} \mapsto \max_{j \in [M]} u_j.$$

As a smooth approximation of it, we can use the **log-sum-exp** function, which is known to behave like a "soft" maximum

$$\text{logsumexp}(\boldsymbol{u}) := \text{softmax}(\boldsymbol{u}) := \log \sum_{j=1}^{M} e^{u_j}.$$

The log-sum-exp can be seen as a generalization of the softplus, as we have for all $u \in \mathbb{R}$

$$\mathrm{logsumexp}((u,0)) = \mathrm{softplus}(u).$$

A numerically stable implementation of the log-sum-exp is given by

$$\mathrm{logsumexp}(\boldsymbol{u}) = \mathrm{logsumexp}(\boldsymbol{u} - c\,\boldsymbol{1}) + c,$$

where $c := \max_{j \in [M]} u_j$.

4.4.3   Scalar-to-scalar probability mappings

Oftentimes we want to map some real value to a number between 0 and 1, that can represent the probability of an event. For that purpose, we generally use **sigmoids**. A sigmoid is a function with a characteristic "S"-shaped curve. These functions are used to squash real values to some interval. An example is the binary step function, also known as **Heaviside step function**,

$$\mathrm{step}(u) := \begin{cases} 1, & u \geq 0 \\ 0, & u < 0 \end{cases}.$$

It is a mapping from $\mathbb{R}$ to $\{0, 1\}$. Unfortunately, it has a discontinuity: a jump in its graph at $u = 0$. Moreover, because the function is constant at all other points, it has zero derivative at these points, which makes it difficult to use as part of a neural network trained with backpropagation.

A better sigmoid is the **logistic function**, which is a mapping from $\mathbb{R}$ to $(0, 1)$ and is defined as

$$\begin{aligned}
\mathrm{logistic}(u) &:= \frac{1}{1 + e^{-u}} \\
&= \frac{e^u}{1 + e^u} \\
&= \frac{1}{2} + \frac{1}{2}\tanh\left(\frac{u}{2}\right).
\end{aligned}$$

It maps $(-\infty, 0)$ to $(0, 0.5)$, $[0, +\infty)$ to $[0.5, 1)$ and it satisfies $\mathrm{logistic}(0) = 0.5$. It can therefore be seen as mapping from real values to probability values. The logistic can be seen as a differentiable approximation to the

discontinuous binary step function $\text{step}(u)$. The logistic function can be shown to be the derivative of softplus, i.e., for all $u \in \mathbb{R}$

$$\text{softplus}'(u) = \text{logistic}(u).$$

Two important properties of the logistic function are that for all $u \in \mathbb{R}$

$$\text{logistic}(-u) = 1 - \text{logistic}(u)$$

and

$$\begin{aligned} \text{logistic}'(u) &= \text{logistic}(u) \cdot \text{logistic}(-u) \\ &= \text{logistic}(u) \cdot (1 - \text{logistic}(u)). \end{aligned}$$

Other sigmoids are possible; see Section 12.4.3.

4.4.4 Vector-to-vector probability mappings

It is often useful to transform a real vector into a vector of probabilities. This is a mapping from $\mathbb{R}^M$ to the probability simplex, defined by

$$\triangle^M := \left\{ \boldsymbol{\pi} \in \mathbb{R}^M : \forall j \in [M], \ \pi_j \geq 0, \ \sum_{j=1}^{M} \pi_j = 1 \right\}.$$

One such mapping is the argmax operator, defined by

$$\text{argmax}(\boldsymbol{u}) := \phi \left(\arg\max_{j \in [M]} u_j \right),$$

where $\phi(j)$ denotes the one-hot encoding of an integer $j \in [M]$, that is,

$$\phi(j) := (0, \ldots, 0, \underbrace{1}_{j}, 0, \ldots, 0) = \boldsymbol{e}_j \in \{0, 1\}^M.$$

This mapping puts all the probability mass onto a single coordinate (in case of ties, we pick a single coordinate arbitrarily). Unfortunately, this mapping is a discontinuous function. As a differentiable everywhere relaxation, we can use the **softargmax** defined by

$$\text{softargmax}(\boldsymbol{u}) := \frac{\exp(\boldsymbol{u})}{\sum_{j=1}^{M} \exp(u_j)}.$$

This operator is commonly known in the literature as *softmax* but this is a misnomer: this operator really defines a differentiable relaxation of the argmax. The output of the softargmax belongs to the relative interior of the probability simplex, meaning that it can never reach the borders of the simplex. If we denote $\boldsymbol{\pi} = \text{softargmax}(\boldsymbol{u})$, this means that $\pi_j \in (0, 1)$, that is, π_j can never be exactly 0 or 1. The softargmax is the gradient of log-sum-exp,

$$\nabla \text{logsumexp}(\boldsymbol{u}) = \text{softargmax}(\boldsymbol{u}).$$

The softargmax can be seen as a generalization of the logistic function, as we have for all $u \in \mathbb{R}$

$$[\text{softargmax}((u, 0))]_1 = \text{logistic}(u).$$

Remark 4.2 (Degrees of freedom and invertibility of softargmax). The softargmax operator satisfies the property for all $\boldsymbol{u} \in \mathbb{R}^M$ and $c \in \mathbb{R}$

$$\boldsymbol{\pi} := \text{softargmax}(\boldsymbol{u}) = \text{softargmax}(\boldsymbol{u} + c\,\boldsymbol{1}).$$

This means that the softargmax operator has $M - 1$ degrees of freedom and is a non-invertible function. However, due to the above property, without loss of generality, we can impose $\boldsymbol{u}^\top \boldsymbol{1} = \sum_{i=1}^M u_i = 0$ (if this is not the case, we simply do $u_i \leftarrow u_i - \bar{u}$, where $\bar{u} := \frac{1}{M} \sum_{j=1}^M u_j$). Using this constraint together with

$$\log \pi_i = u_i - \log \sum_{j=1}^M \exp(u_j),$$

we then obtain

$$\sum_{i=1}^M \log \pi_i = -M \log \sum_{j=1}^M \exp(u_j)$$

so that

$$u_i = [\text{softargmax}^{-1}(\boldsymbol{\pi})]_i = \log \pi_i - \frac{1}{M} \sum_{j=1}^M \log \pi_j.$$

4.5   Residual neural networks

We now discuss another feedforward network parametrization: residual neural networks. Consider a feedforward network with $K + 1$ layers $f_1, \ldots, f_K, f_{K+1}$. Surely, as long as f_{K+1} can exactly represent the identity function, the set of functions that this feedforward network can express should be a superset of the functions that $f_1, \ldots, f_K$ can express. In other words, depth should in theory not hurt the expressive power of feedforward networks. Unfortunately, the assumption that each f_k can exactly represent the identity function may not hold in practice. This means that deeper networks can sometimes be more difficult to train than shallower ones, making the accuracy saturate or degrade as a function of depth.

The key idea of residual neural networks (He *et al.*, 2016) is to design layers f_k, called **residual blocks**, that make it easier to represent the identity function. Formally, a residual block takes the form

$$s_k = f_k(s_{k-1}, w_k) \coloneqq s_{k-1} + h_k(s_{k-1}, w_k).$$

The function h_k is called **residual**, since it models the difference $s_k - s_{k-1}$. The addition with s_{k-1} is often called a **skip connection**. As long as it is easy to adjust w_k so that $h_k(s_{k-1}, w_k) = 0$, f_k can freely become the identity function. For instance, if we use

$$h_k(s_{k-1}, w_k) \coloneqq C_t a_k(W_k s_{k-1} + b_k) + d_k,$$

where $w_k = (W_k, b_k, C_k, d_k)$, it suffices to set C_k and d_k to a zero matrix and vector. Residual blocks are known to remedy the so-called vanishing gradient problem.

Many papers and software packages include an additional activation and instead define the residual block as

$$s_k = f_k(s_{k-1}, w_k) \coloneqq a_k(s_{k-1} + h_k(s_{k-1}, w_k)),$$

where a_k is typically chosen to be the ReLU activation. Whether to include this additional activation or not is essentially a modelling choice. In practice, residual blocks may also include additional operations such as batch norm and convolutional layers.

4.6 Recurrent neural networks

Recurrent neural networks (RNNs) are a class of neural networks that operate on sequences of vectors, either as input, output or both. Their actual parametrization depends on the setup but the core idea is to maintain a **state vector** that is updated from step to step by a recursive function that uses **shared parameters** across steps. Unrolling this recursion defines a valid computational graph, as we will see in Chapter 7. We distinguish between the following setups illustrated in Fig. 4.5:

- Vector to sequence: $\boldsymbol{f}^d \colon \mathbb{R}^D \times \mathbb{R}^P \to \mathbb{R}^{L \times M}$

- Sequence to vector: $\boldsymbol{f}^e \colon \mathbb{R}^{L \times D} \times \mathbb{R}^P \to \mathbb{R}^M$

- Sequence to sequence (aligned): $\boldsymbol{f}^a \colon \mathbb{R}^{L \times D} \times \mathbb{R}^P \to \mathbb{R}^{L \times M}$

- Sequence to sequence (unaligned): $\boldsymbol{f}^u \colon \mathbb{R}^{L \times D} \times \mathbb{R}^P \to \mathbb{R}^{L' \times M}$

where L stands for length. Note that we use the same number of parameters P for each setup for notational convenience, but this of course does not need to be the case. Throughout this section, we use the notation $\boldsymbol{p}_{1:L} \coloneqq (\boldsymbol{p}_1, \dots, \boldsymbol{p}_L)$ for a sequence of L vectors.

4.6.1 Vector to sequence

In this setting, we define a **decoder** function $\boldsymbol{p}_{1:L} = \boldsymbol{f}^d(\boldsymbol{x}, \boldsymbol{w})$ from an **input vector** $\boldsymbol{x} \in \mathbb{R}^D$ and parameters $\boldsymbol{w} \in \mathbb{R}^P$ to an **output sequence** $\boldsymbol{p}_{1:L} \in \mathbb{R}^{L \times M}$. This is for instance useful for image caption generation, where a sentence (a sequence of word embeddings) is generated from an image (a vector of pixels). Formally, we may define $\boldsymbol{p}_{1:L} \coloneqq \boldsymbol{f}^d(\boldsymbol{x}, \boldsymbol{w})$ through the recursion

$$\boldsymbol{z}_l \coloneqq \boldsymbol{g}(\boldsymbol{x}, \boldsymbol{z}_{l-1}, \boldsymbol{w}_g) \quad l \in [L]$$
$$\boldsymbol{p}_l \coloneqq \boldsymbol{h}(\boldsymbol{s}_l, \boldsymbol{w}_h) \quad l \in [L].$$

where $\boldsymbol{w} \coloneqq (\boldsymbol{w}_g, \boldsymbol{w}_h, \boldsymbol{s}_0)$. The goal of $\boldsymbol{g}$ is to update the current **decoder state** $\boldsymbol{z}_l$ given the input $\boldsymbol{x}$, and the previous decoder state $\boldsymbol{z}_{l-1}$. The goal of $\boldsymbol{h}$ is to generate the output $\boldsymbol{p}_l$ given the current decoder state $\boldsymbol{z}_l$. Importantly, the parameters of $\boldsymbol{g}$ and $\boldsymbol{h}$ are **shared across steps**.

(a) One to many (decoder)

(b) Many to one (encoder)

(c) Sequence to sequence aligned

(d) Sequence to sequence unaligned
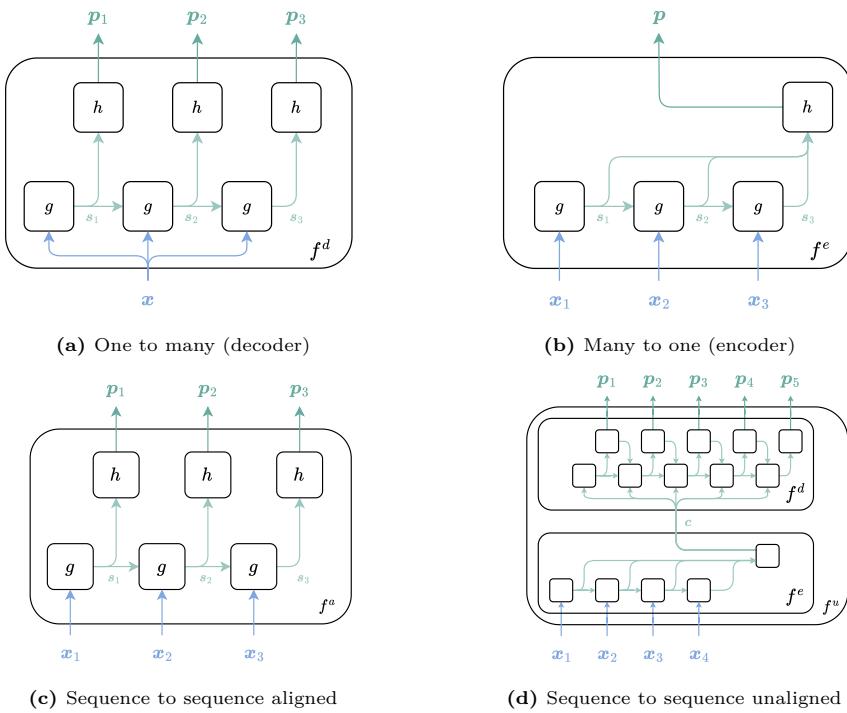
Figure 4.5: Recurrent neural network architectures

Typically, $\boldsymbol{g}$ and $\boldsymbol{h}$ are parametrized using one-hidden-layer MLPs. Note that $\boldsymbol{g}$ has multiple inputs; we discuss how to deal with such cases in Section 4.3.

4.6.2 Sequence to vector

In this setting, we define an **encoder** function $\boldsymbol{p} = \boldsymbol{f}^e(\boldsymbol{x}_{1:L}, \boldsymbol{w})$ from an **input sequence** $\boldsymbol{x}_{1:L} \in \mathbb{R}^{L \times D}$ and parameters $\boldsymbol{w} \in \mathbb{R}^P$ to an **output vector** $\boldsymbol{p} \in \mathbb{R}^M$. This is for instance useful for sequence classification, such as sentiment analysis. Formally, we may define $\boldsymbol{p} := \boldsymbol{f}^e(\boldsymbol{x}_{1:L}, \boldsymbol{w})$ using the recursion

$$\boldsymbol{s}_l := \boldsymbol{\gamma}(\boldsymbol{x}_l, \boldsymbol{s}_{l-1}, \boldsymbol{w}_g) \quad l \in [L]$$
$$\boldsymbol{p} = \text{pooling}(\boldsymbol{s}_{1:L})$$

where $\boldsymbol{w} := (\boldsymbol{w}_g, \boldsymbol{s}_0)$. The goal of $\boldsymbol{\gamma}$ is similar as $\boldsymbol{g}$, except that it updates **encoder states** and does not take previous predictions as input. The **pooling** function is typically parameter-less. Its goal is to reduce a sequence to a vector. Examples include using the last state, the average of states and the coordinate-wise maximum of states.

4.6.3 Sequence to sequence (aligned)

In this setting, we define a function $\boldsymbol{p}_{1:L} = \boldsymbol{f}^a(\boldsymbol{x}_{1:L}, \boldsymbol{w})$ from an **input sequence** $\boldsymbol{x}_{1:L} \in \mathbb{R}^{L \times D}$ and parameters $\boldsymbol{w} \in \mathbb{R}^P$ to an **output sequence** $\boldsymbol{p}_{1:L} \in \mathbb{R}^{L \times M}$, which we know to be of the **same length**. An example of application is part-of-speech tagging, where the goal is to assign each word $\boldsymbol{x}_l$ to a part-of-speech (noun, verb, adjective, etc). Formally, we may define $\boldsymbol{p}_{1:L} = \boldsymbol{f}^a(\boldsymbol{x}_{1:L}, \boldsymbol{w})$ as

$$\boldsymbol{s}_l := \boldsymbol{\gamma}(\boldsymbol{x}_l, \boldsymbol{s}_{l-1}, \boldsymbol{w}_\gamma) \quad l \in [L]$$
$$\boldsymbol{p}_l = \boldsymbol{h}(\boldsymbol{s}_l, \boldsymbol{w}_h) \quad l \in [L]$$

where $\boldsymbol{w} := (\boldsymbol{w}_\gamma, \boldsymbol{w}_h, \boldsymbol{s}_0)$. The function $\boldsymbol{\gamma}$ and $\boldsymbol{h}$ are similar as before.

4.6.4 Sequence to sequence (unaligned)

In this setting, we define a function $\boldsymbol{p}_{1:L'} = \boldsymbol{f}^u(\boldsymbol{x}_{1:L}, \boldsymbol{w})$ from an **input sequence** $\boldsymbol{x}_{1:L} \in \mathbb{R}^{L \times D}$ and parameters $\boldsymbol{w} \in \mathbb{R}^P$ to an output sequence

$\boldsymbol{p}_{1:L'} \in \mathbb{R}^{L' \times M}$, which potentially has a **different length**. An example of application is machine translation, where the sentences in the source and target languages do not necessarily have the same length. Typically, $\boldsymbol{p}_{1:L'} = \boldsymbol{f}^u(\boldsymbol{x}_{1:L}, \boldsymbol{w})$ is defined as the following two steps

$$\boldsymbol{c} := \boldsymbol{f}^e(\boldsymbol{x}_{1:L}, \boldsymbol{w}_e)$$
$$\boldsymbol{p}_{1:L'} := \boldsymbol{f}^d(\boldsymbol{c}, \boldsymbol{w}_d)$$

where $\boldsymbol{w} := (\boldsymbol{w}_e, \boldsymbol{w}_d)$, and where we reused the previously-defined encoder $\boldsymbol{f}_e$ and decoder $\boldsymbol{f}_d$. Putting the two steps together, we obtain

$$\boldsymbol{s}_l := \boldsymbol{\gamma}(\boldsymbol{x}_l, \boldsymbol{s}_{l-1}, \boldsymbol{w}_\gamma) \quad l \in [L]$$
$$\boldsymbol{c} = \text{pooling}(\boldsymbol{s}_{1:L})$$
$$\boldsymbol{z}_l := \boldsymbol{g}(\boldsymbol{c}, \boldsymbol{p}_{l-1}, \boldsymbol{z}_{l-1}, \boldsymbol{w}_g) \quad l \in [L']$$
$$\boldsymbol{p}_l := \boldsymbol{h}(\boldsymbol{z}_l, \boldsymbol{w}_h) \quad l \in [L'].$$

This architecture is aptly named the **encoder-decoder** architecture. Note that we denoted the length of the target sequence as L'. However, in practice, the target length can be input dependent and is often not known ahead of time. To deal with this issue, the vocabulary (of size D is our notation) is typically augmented with an "end of sequence" (EOS) token so that, at inference time, we know when to stop generating the output sequence. One disadvantage of this encoder-decoder architecture, however, is that all the information about the input sequence is contained in the **context vector** $\boldsymbol{c}$, which can therefore become a **bottleneck**. For this reason, this architecture has been largely replaced with attention mechanisms and transformers, which we study in the next sections.

4.7 Summary

In this chapter, we reviewed how to mathematically represent a program as a directed acyclic graph. We then presented various popular neural network architectures, that we view as **parameterized programs**. For instance, the feedfoward network can be seen as a parameterized computation chain. Multilayer perceptrons (MLPs), residual neural networks (ResNets) and convolutional neural network (CNNs) are particular parametrizations of this class of network. Finally, we reviewed recurrent neural networks, for working with sequential data.

5

Control flows

Control flows, such as conditionals or loops, are an essential part of computer programming, as they allow us to express complex programs. It is therefore natural to ask whether these constructs can be included in a differentiable program. This is what we study in this chapter.

5.1 Comparison operators

Control flows rely on **comparison operators**, a.k.a. **relational operators**. Formally, we can define a comparison operator $\pi = \mathrm{op}(u_1, u_2)$ as a function from $u_1 \in \mathbb{R}$ and $u_2 \in \mathbb{R}$ to $\pi \in \{0, 1\}$. The binary (Boolean) output π can then be used within a conditional statement (see Section 5.6, Section 5.7) to decide whether to execute one branch or another. We define the following operators:

- **greater than:**

$$\mathrm{gt}(u_1, u_2) := \begin{cases} 1 & \text{if } u_1 \geq u_2 \\ 0 & \text{otherwise} \end{cases}$$
$$= \mathrm{step}(u_1 - u_2)$$

- **less than:**

$$\mathrm{lt}(u_1, u_2) := \begin{cases} 1 & \text{if } u_1 \leq u_2 \\ 0 & \text{otherwise} \end{cases}$$

$$= 1 - \mathrm{gt}(u_1, u_2)$$

$$= \mathrm{step}(u_2 - u_1)$$

- **equal:**

$$\mathrm{eq}(u_1, u_2) := \begin{cases} 1 & \text{if } |u_1 - u_2| = 0 \\ 0 & \text{otherwise} \end{cases}$$

$$= \mathrm{gt}(u_2, u_1) \cdot \mathrm{gt}(u_1, u_2)$$

$$= \mathrm{step}(u_2 - u_1) \cdot \mathrm{step}(u_1 - u_2)$$

- **not equal:**

$$\mathrm{neq}(u_1, u_2) := \begin{cases} 1 & \text{if } |u_1 - u_2| > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$= 1 - \mathrm{eq}(u_1, u_2)$$

$$= 1 - \mathrm{step}(u_2 - u_2) \cdot \mathrm{step}(u_1 - u_2),$$

where $\mathrm{step} \colon \mathbb{R} \to \{0, 1\}$ is the **Heaviside step function**

$$\mathrm{step}(u) := \begin{cases} 1 & \text{if } u \geq 0 \\ 0 & \text{otherwise} \end{cases}.$$

The Heaviside step function is piecewise constant. At $u = 0$, the function is discontinuous. At $u \neq 0$, it is continuous and has **null derivative**. Since the comparison operators we presented are all expressed in terms of the step function, they are all continuous and differentiable almost everywhere, with null derivative. Therefore, while their derivatives are well-defined almost everywhere, they are **uninformative** and prevent gradient backpropagation.

5.2 Soft inequality operators

5.2.1 Heuristic definition

To obtain a **continuous relaxation** of inequality operators, we can heuristically replace the step function in the expression of *greater than* and *less than* by a sigmoid, such as the logistic function or the Gaussian's CDF. We then obtain

$$\text{gt}(\mu_1, \mu_2) = \text{step}(\mu_1 - \mu_2) \approx \text{sigmoid}(\mu_1 - \mu_2)$$
$$\text{lt}(\mu_1, \mu_2) = \text{step}(\mu_2 - \mu_1) \approx \text{sigmoid}(\mu_2 - \mu_1) = 1 - \text{sigmoid}(\mu_1 - \mu_2).$$

In the limit, we have that $\text{sigmoid}(\mu_1 - \mu_2) \to 1$ when $\mu_1 - \mu_2 \to \infty$. In the limit, a sigmoid therefore outputs a probability of 1 if μ_1 and μ_2 are infinitely apart. Besides the logistic function and the Gaussian's CDF, other sigmoid functions are possible, as discussed in Section 12.4.3. In particular, with sparse sigmoids, there exists a finite value τ such that $\mu_1 - \mu_2 \geq \tau \implies \text{sigmoid}(\mu_1 - \mu_2) = 1$.

5.2.2 Stochastic process perspective

For the logistic function and the Gaussian's CDF, another equivalent approach is to perturb each variable in the inequality operator with a random variable and take the expectation. For example, for the *greater than* operator, this gives the approximation

$$\text{gt}(\mu_1, \mu_2) \approx \mathbb{E}[\text{gt}(\mu_1 + Z_1, \mu_2 + Z_2)],$$

where Z_1 and Z_2 are two independent random variables. At a high level, we replaced the real numbers μ_1 and μ_2 by a **stochastic process** (U_1, U_2), where $U_1 := \mu_1 + Z_1$ and $U_2 := \mu_2 + Z_2$.

Choosing Z_1 and Z_2 distributed as **Gumbel noise**, we get (see Proposition 13.3)

$$\mathbb{E}[\text{gt}(\mu_1 + Z_1, \mu_2 + Z_2)] = \text{logistic}(\mu_1 - \mu_2),$$

where

$$\text{logistic}(u) := \frac{1}{1 + e^{-u}} \in (0, 1).$$

Choosing Z_1 and Z_2 to be distributed as **Gaussian noise**, we get

$$\mathbb{E}[\text{gt}(\mu_1 + Z_1, \mu_2 + Z_2)] = \Phi((\mu_1 - \mu_2)/\sqrt{2}),$$

were Φ the cumulative distribution function (CDF) of the standard normal distribution, defined in Eq. (3.1).

5.3 Soft equality operators

5.3.1 Heuristic definition

The equality operator can be written as

$$\text{eq}(\mu_1, \mu_2) = \delta(\mu_1 - \mu_2)$$

where

$$\delta(u) := \begin{cases} 1 & \text{if } u = 0 \\ 0 & \text{if } u \neq 0 \end{cases}.$$

It equals 1 when $\mu_1 = \mu_2$ and is zero everywhere else. A natural idea to obtain a continuous and smooth relaxation is therefore to replace δ by a bell-shaped function. For this purpose, we can use a kernel, such as the PDF of a distribution centered at 0. Formally, we may define

$$\text{eq}(\mu_1, \mu_2) \approx \frac{\kappa(\mu_1, \mu_2)}{\kappa(0, 0)},$$

where

$$\kappa(\mu_1, \mu_2) := p_{0,1}(\mu_1 - \mu_2),$$

for $p_{0,1}$ the PDF of a zero-mean unit-scale distribution in the location-scale family. The normalization $\kappa(0,0)$ ensures that the soft equality operator is 1 at $\mu_1 = \mu_2$. For instance, we can use the **Gaussian kernel**

$$\kappa(\mu_1, \mu_2) := e^{-(\mu_1 - \mu_2)^2/2}$$

or the **logistic kernel**

$$\kappa(\mu_1, \mu_2) := \frac{\exp(\mu_2 - \mu_1)}{(1 + \exp(\mu_2 - \mu_1))^2}$$

$$= \frac{1}{2 + e^{(\mu_2 - \mu_1)} + e^{(\mu_1 - \mu_2)}}$$

$$= \text{sech}^2((\mu_2 - \mu_1)/2),$$

where we defined the hyperbolic secant $\text{sech}(u) := 2\exp(u)/(\exp(2u)+1)$. The soft equality operators obtained with these kernels are illustrated

in Fig. 5.1. The soft equality operator obtained with the logistic kernel coincides with the expression Petersen *et al.* (2021) arrive at, in a different manner.

5.3.2   Gaussian process perspective

To handle the equality operator from a perturbation perspective, we cannot simply perturb with two independent random noise variables, as we did for the inequality operator, because we would get $\mathbb{E}[\text{eq}(\mu_1 + Z_1, \mu_2 + Z_2] = \mathbb{P}(\mu_1 + Z_1 = \mu_2 + Z_2) = 0$ for any μ_1 and μ_2.

We can nevertheless generalize the previous approach by using a **Gaussian process** (Hida and Hitsuda, 1976). A Gaussian process on $\mathbb{R}$ associates a multivariate Gaussian random variable $(U_1, \ldots, U_K)$ to a collection of real numbers $(\mu_1, \ldots, \mu_K)$. The Gaussian process is characterized by the mean function $\mathbb{E}[U_i] = \mu_i$ and its covariance function, a.k.a. , kernel, that defines the covariance between two points as $\text{Cov}(U_i, U_j) \coloneqq \kappa(\mu_i, \mu_j)$. Equipped with such mapping from real numbers to random variables, we need a measure of equality between random variables. A natural measure for Gaussian random variables is their **correlation**

$$\text{corr}(U_i, U_j) \coloneqq \frac{\text{Cov}(U_i, U_j)}{\sqrt{\text{Var}(U_i)\,\text{Var}(U_j)}} = \frac{\kappa(\mu_i, \mu_j)}{\kappa(0, 0)} \in [0, 1].$$

From a high-level perspective, we can see the covariance as an inner product between random variables and so the correlation is a natural alignment measure, just as $(\boldsymbol{x}, \boldsymbol{y}) \mapsto \langle \boldsymbol{x}, \boldsymbol{y} \rangle / \|\boldsymbol{x}\|_2 \|\boldsymbol{y}\|_2$ between two vectors.

In the case $K = 2$, we recover the previous heuristically-defined soft equality operator,

$$\text{eq}(\mu_1, \mu_2) \approx \text{corr}(U_1, U_2) = \frac{\kappa(\mu_1, \mu_2)}{\kappa(0, 0)}.$$

Both the Gaussian and logistic kernels arise naturally as the density of $\mu_1 + Z_1 - (\mu_2 + Z_2)$ at 0, with Z_1 and Z_2 Gaussian or Gumbel random variables.
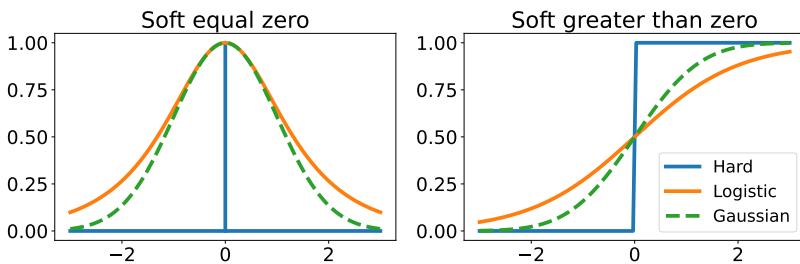
Figure 5.1: Soft equality and soft greater than operators can be defined as normalized kernels (PDF) and as CDF functions, respectively.

5.4 Logical operators

Logical operators can be used to perform Boolean algebra. Formally, we can define them as functions from $\{0, 1\} \times \{0, 1\}$ to $\{0, 1\}$. The **and** (logical conjunction a.k.a. logical product), **or** (logical disjunction a.k.a. logical addition) and **not** (logical negation a.k.a. logical complement) operators, for example, are defined by

$$\text{and}(\pi, \pi') := \begin{cases} 1 & \text{if } \pi = \pi' = 1 \\ 0 & \text{otherwise} \end{cases}$$

$$\text{or}(\pi, \pi') := \begin{cases} 1 & \text{if } 1 \in \{\pi, \pi'\} \\ 0 & \text{otherwise} \end{cases}$$

$$\text{not}(\pi) := \begin{cases} 0 & \text{if } \pi = 1 \\ 1 & \text{if } \pi = 0 \end{cases}.$$

Classical properties of these operators include

- Commutativity:

$$\text{and}(\pi, \pi') = \text{and}(\pi', \pi)$$
$$\text{or}(\pi, \pi') = \text{and}(\pi', \pi)$$

- Associativity:

$$\text{and}(\pi, \text{and}(\pi', \pi'')) = \text{and}(\text{and}(\pi, \pi'), \pi'')$$
$$\text{or}(\pi, \text{or}(\pi', \pi'')) = \text{or}(\text{or}(\pi, \pi'), \pi'')$$

- Distributivity of **and** over **or**:

$$\text{and}(\pi, \text{or}(\pi', \pi'')) = \text{or}(\text{and}(\pi, \pi'), \text{and}(\pi, \pi''))$$

- Neutral element:

$$\text{and}(\pi, 1) = \pi$$
$$\text{or}(\pi, 0) = \pi$$

- De Morgan's laws:

$$\text{not}(\text{or}(\pi, \pi')) = \text{and}(\text{not}(\pi), \text{not}(\pi'))$$
$$\text{not}(\text{and}(\pi, \pi')) = \text{or}(\text{not}(\pi), \text{not}(\pi')).$$

More generally, for a binary vector $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_K) \in \{0, 1\}^K$, we can define **all** (universal quantification, $\forall$) and **any** (existential quantification, $\exists$) operators, which are functions from $\{0, 1\}^K$ to $\{0, 1\}$, as

$$\text{all}(\boldsymbol{\pi}) := \begin{cases} 1 & \text{if } \pi_1 = \cdots = \pi_K = 1 \\ 0 & \text{otherwise} \end{cases}$$

and

$$\text{any}(\boldsymbol{\pi}) := \begin{cases} 1 & \text{if } 1 \in \{\pi_1, \ldots, \pi_K\} \\ 0 & \text{otherwise} \end{cases}.$$

5.5 Continuous extensions of logical operators

5.5.1 Probabilistic continuous extension

We can equivalently write the **and**, **or** and **not** operators as

$$\text{and}(\pi, \pi') = \pi \cdot \pi'$$
$$\text{or}(\pi, \pi') = \pi + \pi' - \pi \cdot \pi'$$
$$\text{not}(\pi) = 1 - \pi.$$

These are **extensions** of the previous definitions: we can use them as functions from $[0, 1] \times [0, 1] \to [0, 1]$, as illustrated in Fig. 5.2. This means that we can use the soft comparison operators defined in Section 5.2 to
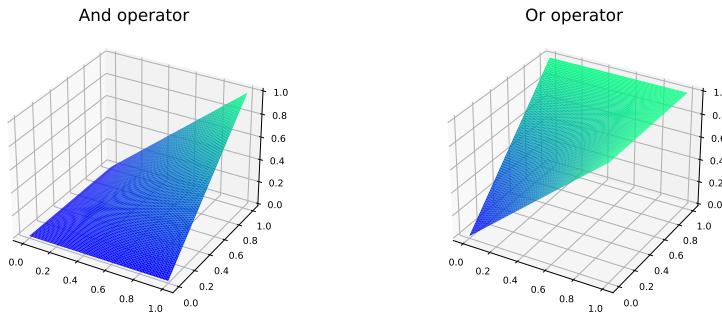
Figure 5.2: The Boolean **and** and **or** operators are functions from $\{0,1\} \times \{0,1\}$ to $\{0,1\}$ but their continuous extensions $\mathrm{and}(\pi, \pi') := \pi \cdot \pi'$ as well as $\mathrm{or}(\pi, \pi') := \pi + \pi' - \pi \cdot \pi'$ define a function from $[0,1] \times [0,1]$ to $[0,1]$.

obtain $\pi, \pi' \in [0,1]$. Likewise, we can define continuous extensions of **all** and **any**, which are functions from $[0,1]^K$ to $[0,1]$, as

$$\mathrm{all}(\boldsymbol{\pi}) = \prod_{i=1}^{K} \pi_i$$

$$\mathrm{any}(\boldsymbol{\pi}) = 1 - \prod_{i=1}^{K} (1 - \pi_i).$$

From a probabilistic perspective, if we let Y and Y' to be two independent random variables distributed according to **Bernoulli distributions** with parameter π and π', then

$$\mathrm{and}(\pi, \pi') = \mathbb{P}(Y = 1 \cap Y' = 1) = \mathbb{P}(Y = 1) \cdot \mathbb{P}(Y' = 1)$$
$$\mathrm{or}(\pi, \pi') = \mathbb{P}(Y = 1 \cup Y' = 1)$$
$$= \mathbb{P}(Y = 1) + \mathbb{P}(Y' = 1) - \mathbb{P}(Y = 1 \cap Y' = 1)$$
$$= \mathbb{P}(Y = 1) + \mathbb{P}(Y' = 1) - \mathbb{P}(Y = 1)\mathbb{P}(Y' = 1)$$
$$\mathrm{not}(\pi) = \mathbb{P}(Y \neq 1) = 1 - \mathbb{P}(Y = 1).$$

In probability theory, these correspond to the product rule of two independent variables, the addition rule, and the complement rule.

Likewise, if we let $Y = (Y_1, \ldots, Y_K) \in \{0,1\}^K$ be a random variable distributed according to a **multivariate Bernoulli distribution** with

parameters $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_K)$, then

$$\text{all}(\boldsymbol{\pi}) = \mathbb{P}(Y_1 = 1 \cap \cdots \cap Y_K = 1) = \prod_{i=1}^{K} \mathbb{P}(Y_i = 1)$$

$$\text{any}(\boldsymbol{\pi}) = \mathbb{P}(Y_1 = 1 \cup \cdots \cup Y_K = 1) = 1 - \prod_{i=1}^{K}(1 - \mathbb{P}(Y_i = 1)).$$

This is the chain rule of probability for K independent variables, and the addition rule for K variables.

5.5.2   Triangular norms and co-norms

More generally, in the **fuzzy logic** literature (Jayaram and Baczynski, 2008), the concepts of triangular norms and co-norms have been introduced to provide continuous relaxations of the **and** and **or** operators, respectively.

> **Definition 5.1** (Triangular norms and conorms). A triangular norm, a.k.a. t-norm, is a function from $[0,1] \times [0,1]$ to $[0,1]$ which is is commutative, associative, neutral w.r.t. 1 and is monotone, meaning that $T(\pi, \pi') \leq T(\tau, \tau')$ for all $\pi \leq \tau$ and $\pi' \leq \tau'$. A triangular conorm, a.k.a. t-conorm, is defined similarly but is neutral w.r.t. 0.

The previously-defined probabilistic extensions of **and** and **or** are examples of triangle norm and conorm. More examples are given in Table 5.1. Thanks to the associative property of these operators, we can generalize them to vectors $\boldsymbol{\pi} \in [0,1]^K$ to define continuous extensions of the **all** and **any** operators, as shown in Table 5.2. For more examples and analysis, see for instance van Krieken (2024, Chapters 2 and 3).

5.6   If-else statements

An if-else statement executes different code depending on a condition. Formally, we can define the ifelse: $\{0,1\} \times \mathcal{V} \times \mathcal{V} \to \mathcal{V}$ function by

$$\text{ifelse}(\pi, \boldsymbol{v}_1, \boldsymbol{v}_0) := \begin{cases} \boldsymbol{v}_1 & \text{if } \pi = 1 \\ \boldsymbol{v}_0 & \text{if } \pi = 0 \end{cases} \tag{5.1}$$

$$= \pi \cdot \boldsymbol{v}_1 + (1 - \pi) \cdot \boldsymbol{v}_0.$$

Table 5.1: Examples of triangular norms and conorms, which are continuous relaxations of the **and** and **or** operators, respectively. More instances can be obtained by smoothing out the min and max operators.

	t-norm	t-conorm
Probabilistic	$\pi \cdot \pi'$	$\pi + \pi' - \pi \cdot \pi'$
Extremum	$\min(\pi, \pi')$	$\max(\pi, \pi')$
Łukasiewicz	$\max(\pi + \pi' - 1, 0)$	$\min(\pi + \pi', 1)$

Table 5.2: Continuous extensions of the **all** and **any** operators.

	All ($\forall$)	Any ($\exists$)
Probabilistic	$\prod_{i=1}^{K} \pi_i$	$1 - \prod_{i=1}^{K}(1 - \pi_i)$
Extremum	$\min(\pi_1, \ldots, \pi_K)$	$\max(\pi_1, \ldots, \pi_K)$
Łukasiewicz	$\max(\sum_{i=1}^{K} \pi_i - (K-1), 0)$	$\min(\sum_{i=1}^{K} \pi_i, 1)$

The π variable is called the **predicate**. It is a **binary** (Boolean) variable, making the function ifelse undefined if $\pi \notin \{0, 1\}$. The function is therefore discontinuous and nondifferentiable w.r.t. $\pi \in \{0, 1\}$. On the other hand, $\boldsymbol{v}_0 \in \mathcal{V}$ and $\boldsymbol{v}_1 \in \mathcal{V}$, which correspond to the false and true **branches**, can be **continuous** variables. If $\pi = 1$, the function is linear w.r.t. $\boldsymbol{v}_1$ and constant w.r.t. $\boldsymbol{v}_0$. Conversely, if $\pi = 0$, the function is linear w.r.t. $\boldsymbol{v}_0$ and constant w.r.t. $\boldsymbol{v}_1$. We now discuss how to differentiate through ifelse.

5.6.1 Differentiating through branch variables

For $\pi \in \{0, 1\}$ fixed, ifelse$(\pi, \boldsymbol{v}_1, \boldsymbol{v}_0)$ is a valid function w.r.t. $\boldsymbol{v}_1 \in \mathcal{V}$ and $\boldsymbol{v}_0 \in \mathcal{V}$, and can therefore be used as a node in a computational graph (Section 7.3). Due to the linearity w.r.t. $\boldsymbol{v}_1$ and $\boldsymbol{v}_0$, we obtain that the Jacobians w.r.t. $\boldsymbol{v}_1$ and $\boldsymbol{v}_0$ are

$$\partial_{\boldsymbol{v}_0}\text{ifelse}(\pi, \boldsymbol{v}_1, \boldsymbol{v}_0) := \begin{cases} 0 & \text{if } \pi = 1 \\ I & \text{if } \pi = 0 \end{cases}$$

$$= (1 - \pi) \cdot I$$

and

$$\partial_{v_1}\text{ifelse}(\pi, \boldsymbol{v}_1, \boldsymbol{v}_0) := \begin{cases} I & \text{if } \pi = 1 \\ 0 & \text{if } \pi = 0 \end{cases}$$
$$= \pi \cdot I,$$

where I is the identity matrix of appropriate size. Most of the time, if-else statements are composed with other functions. Let $g_1 : \mathcal{U}_1 \to \mathcal{V}$ and $g_0 : \mathcal{U}_0 \to \mathcal{V}$ be differentiable functions. We then define $\boldsymbol{v}_1 := g_1(\boldsymbol{u}_1)$ and $\boldsymbol{v}_0 := g_0(\boldsymbol{u}_0)$, where $\boldsymbol{u}_1 \in \mathcal{U}_1$ and $\boldsymbol{u}_0 \in \mathcal{U}_0$. The composition of ifelse, g_1 and g_0 is then the function $f : \{0, 1\} \times \mathcal{U}_1 \times \mathcal{U}_0 \to \mathcal{V}$ defined by

$$f(\pi, \boldsymbol{u}_1, \boldsymbol{u}_0) := \text{ifelse}(\pi, g_1(\boldsymbol{u}_1), g_0(\boldsymbol{u}_0))$$
$$= \pi \cdot g_1(\boldsymbol{u}_1) + (1 - \pi) \cdot g_0(\boldsymbol{u}_0).$$

We obtain that the Jacobians are

$$\partial_{\boldsymbol{u}_1} f(\pi, \boldsymbol{u}_1, \boldsymbol{u}_0) = \pi \cdot \partial g_1(\boldsymbol{u}_1)$$

and

$$\partial_{\boldsymbol{u}_0} f(\pi, \boldsymbol{u}_1, \boldsymbol{u}_0) = (1 - \pi)\partial g_0(\boldsymbol{u}_0).$$

As long as g_1 and g_0 are differentiable functions, we can therefore differentiate through the branch variables $\boldsymbol{u}_1$ and $\boldsymbol{u}_0$ without any issue. More problematic is the predicate variable π, as we now discuss.

5.6.2   Differentiating through predicate variables

The predicate variable π is binary and therefore cannot be differentiated directly. However, π can be the output of a comparison operator. For example, suppose we want to express the function $f : \mathbb{R} \times \mathcal{U}_1 \times \mathcal{U}_0 \to \mathcal{V}$ defined by

$$f_h(p, \boldsymbol{u}_1, \boldsymbol{u}_0) := \begin{cases} g_1(\boldsymbol{u}_1) & \text{if } p \geq 0 \\ g_0(\boldsymbol{u}_0) & \text{otherwise} \end{cases}.$$

Using our notation, this can be rewritten as

$$f_h(p, \boldsymbol{u}_1, \boldsymbol{u}_0) := \text{ifelse}(\text{gt}(p, 0), g_1(\boldsymbol{u}_1), g_0(\boldsymbol{u}_0))$$
$$= \text{ifelse}(\text{step}(p), g_1(\boldsymbol{u}_1), g_0(\boldsymbol{u}_0))$$
$$= \text{step}(p)g_1(\boldsymbol{u}_1) + (1 - \text{step}(p))g_0(\boldsymbol{u}_0).$$

The Heaviside step function has a **discontinuity** at $p = 0$, but it is continuous and differentiable with derivative $\text{step}'(p) = 0$ for all $p \neq 0$. The function f_h therefore has **null derivative** w.r.t. $p \neq 0$,

$$
\begin{aligned}
\partial_p f_h(p, \boldsymbol{u}_1, \boldsymbol{u}_0) &= \partial_1 f_h(p, \boldsymbol{u}_1, \boldsymbol{u}_0) \\
&= \text{step}'(p)(g_1(\boldsymbol{u}_1) - g_0(\boldsymbol{u}_0)) \\
&= \mathbf{0}.
\end{aligned}
$$

In other words, while f_h has **well-defined** derivatives w.r.t. p for $p \neq 0$, the derivatives are **uninformative**. As another example, let us now consider the function

$$
g_h(\boldsymbol{u}_1, \boldsymbol{u}_0) := f_h(t(\boldsymbol{u}_1), \boldsymbol{u}_1, \boldsymbol{u}_0),
$$

for some differentiable function t. This time, $\boldsymbol{u}_1$ influences both the predicate and the true branch. Then, using Proposition 2.8, we obtain

$$
\begin{aligned}
\partial_{\boldsymbol{u}_1} g_h(\boldsymbol{u}_1, \boldsymbol{u}_0) &= \partial t(\boldsymbol{u}_1) \partial_1 f_h(t(\boldsymbol{u}_1), \boldsymbol{u}_1, \boldsymbol{u}_0) + \partial_2 f_h(t(\boldsymbol{u}_1), \boldsymbol{u}_1, \boldsymbol{u}_0) \\
&= \partial_2 f_h(t(\boldsymbol{u}_1), \boldsymbol{u}_1, \boldsymbol{u}_0).
\end{aligned}
$$

In other words, the derivatives of the predicate $t(\boldsymbol{u}_1)$ do not influence the derivatives of g_h.

5.6.3 Continuous relaxations

Fortunately, we recall that

$$
\text{ifelse}(\pi, \boldsymbol{v}_1, \boldsymbol{v}_0) = \pi \cdot \boldsymbol{v}_1 + (1 - \pi) \cdot \boldsymbol{v}_0.
$$

This function is perfectly well-defined, even if $\pi \in [0, 1]$, instead of $\pi \in \{0, 1\}$. That is, this definition is an **extension** of Eq. (5.1) from the discrete set $\{0, 1\}$ to the continuous unit segment $[0, 1]$. We saw that

$$
\text{gt}(a, b) \approx \text{sigmoid}(a - b) \in [0, 1],
$$

where sigmoid is for instance the logistic function or the Gaussian CDF. If we now define

$$
\begin{aligned}
f_s(p, \boldsymbol{u}_1, \boldsymbol{u}_0) &:= \text{ifelse}(\text{sigmoid}(p), g_1(\boldsymbol{u}_1), g_0(\boldsymbol{u}_0)) \\
&= \text{sigmoid}(p) g_1(\boldsymbol{u}_1) + (1 - \text{sigmoid}(p)) g_0(\boldsymbol{u}_0), \quad (5.2)
\end{aligned}
$$

the Jacobian becomes

$$\partial_p f_s(p, \boldsymbol{u}_1, \boldsymbol{u}_0) = \text{sigmoid}'(p)(g_1(\boldsymbol{u}_1) - g_0(\boldsymbol{u}_0)).$$

If sigmoid = logistic, the Jacobian is **non-null everywhere**, allowing gradients to backpropagate through the computational graph. This is an example of smoothing by regularization, as studied in Chapter 12.

Probabilistic perspective

From a probabilistic perspective, we can view Eq. (5.2) as the expectation of $g_i(\boldsymbol{u}_i)$, where $i \in \{0, 1\}$ is a binary random variable distributed according to a **Bernoulli distribution** with parameter $\pi = \text{sigmoid}(p)$:

$$f_s(p, \boldsymbol{u}_1, \boldsymbol{u}_0) = \mathbb{E}_{i \sim \text{Bernoulli}(\text{sigmoid}(p))}\left[g_i(\boldsymbol{u}_i)\right].$$

Taking the expectation over the two possibles branches makes the function differentiable with respect to p. Of course, this comes at the cost of evaluating both branches, instead of a single one. The probabilistic perspective suggests that we can also compute the variance if needed as

$$\mathbb{V}_{i \sim \text{Bernoulli}(\text{sigmoid}(p))}\left[g_i(\boldsymbol{u}_i)\right]$$
$$= \mathbb{E}_{i \sim \text{Bernoulli}(\text{sigmoid}(p))}\left[(f_s(p, \boldsymbol{u}_1, \boldsymbol{u}_0) - g_i(\boldsymbol{u}_i))^2\right].$$

Another perspective (Petersen *et al.*, 2021) is based on the **logistic distribution**. Indeed, if P is a random variable following a logistic distribution with mean p and scale 1, we saw in Remark 3.1 that the CDF is $\mathbb{P}(P \leq 0) = \text{logistic}(-p) = 1 - \text{logistic}(p)$ and therefore

$$f_s(p, \boldsymbol{u}_1, \boldsymbol{u}_0) = \text{ifelse}(\text{logistic}(p), g_1(\boldsymbol{u}_1), g_0(\boldsymbol{u}_0))$$
$$= \text{logistic}(p)g_1(\boldsymbol{u}_1) + (1 - \text{logistic}(p))g_0(\boldsymbol{u}_0)$$
$$= \mathbb{P}(P > 0) \cdot g_1(\boldsymbol{u}_1) + \mathbb{P}(P \leq 0) \cdot g_0(\boldsymbol{u}_0).$$

5.7   Else-if statements

In the previous section, we focused on if-else statements: conditionals with only two branches. We now generalize our study to conditionals including else-if statements, that have K branches.

5.7.1 Encoding K branches

For conditionals with only 2 branches, we encoded the branch that the conditional needs to take using the binary variable $\pi \in \{0, 1\}$. For conditionals with K branches, we need a way to encode which of the K branches the conditional needs to take. To do so, we can use a vector $\boldsymbol{\pi} \in \{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_K\}$, where $\boldsymbol{e}_i$ denotes the standard basis vector (a.k.a. one-hot vector)

$$\boldsymbol{e}_i := (0, \ldots, \underbrace{1}_{i}, \ldots, 0),$$

a vector with a single one in the coordinate i and $K - 1$ zeros. The vector $\boldsymbol{e}_i$ is the encoding of a **categorical variable** $i \in [K]$.

Combining booleans

To form, such a vector $\boldsymbol{\pi} \in \{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_K\}$, we can combine the previously-defined comparison and logical operators to define $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_K)$. However, we need to ensure that only one π_i is non-zero. We give an example in Example 5.1.

Argmax and argmin operators

Another way to form $\boldsymbol{\pi}$ is to use the **argmax** and **argmin** operators

$$\operatorname{argmax}(\boldsymbol{p}) := \underset{\boldsymbol{\pi} \in \{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_K\}}{\arg\max} \langle \boldsymbol{\pi}, \boldsymbol{p} \rangle$$

$$\operatorname{argmin}(\boldsymbol{p}) := \underset{\boldsymbol{\pi} \in \{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_K\}}{\arg\min} \langle \boldsymbol{\pi}, \boldsymbol{p} \rangle = \operatorname{argmax}(-\boldsymbol{p}).$$

They can be seen as a natural generalization of the greater than and less than operators. In case of ties, we break them arbitrarily.

5.7.2   Conditionals

We can now express a conditional statement as the function
$\text{cond} \colon \{e_1, \ldots, e_K\} \times \mathcal{V}^K \to \mathcal{V}$ defined by

$$
\text{cond}(\boldsymbol{\pi}, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_K) := \begin{cases} \boldsymbol{v}_1 & \text{if } \boldsymbol{\pi} = \boldsymbol{e}_1 \\ \vdots \\ \boldsymbol{v}_K & \text{if } \boldsymbol{\pi} = \boldsymbol{e}_K \end{cases} \tag{5.3}
$$

$$
= \sum_{i=1}^{K} \pi_i \boldsymbol{v}_i.
$$

Similarly as for the ifelse function, the cond function is discontinuous
and nondifferentiable w.r.t. $\boldsymbol{\pi} \in \{e_1, \ldots, e_K\}$. However, given $\boldsymbol{\pi} = \boldsymbol{e}_i$
fixed for some i, the function is linear in $\boldsymbol{v}_i$ and constant in $\boldsymbol{v}_j$ for $j \neq i$.
We illustrate how to express a simple example, using this formalism.

Example 5.1 (Soft-thresholding operator). The soft-thresholding op-
erator (see also Section 15.4) is a commonly-used operator to pro-
mote sparsity. It is defined by

$$
\text{SoftThreshold}(u, \lambda) := \begin{cases} 0 & \text{if } |u| \leq \lambda \\ u - \lambda & \text{if } u \geq \lambda \\ u + \lambda & \text{if } u \leq -\lambda \end{cases}.
$$

To express it in our formalism, we can define $\boldsymbol{\pi} \in \{e_1, e_2, e_3\}$ using
comparison operators as

$$
\boldsymbol{\pi} := (\text{lt}(|u|, \lambda), \text{gt}(u, \lambda), \text{lt}(u, -\lambda))
$$
$$
= (\text{step}(\lambda - |u|), \text{step}(u - \lambda), \text{step}(-u - \lambda)).
$$

Equivalently, we can also define $\boldsymbol{\pi}$ using an argmax operator as

$$
\boldsymbol{\pi} := \text{argmax}((\lambda - |u|, u - \lambda, -u - \lambda)).
$$

In case of ties, which happens at $|u| = \lambda$, we keep only one non-zero
coordinate in $\boldsymbol{\pi}$. We can then rewrite the operator as

$$
\text{SoftThreshold}(u, \lambda) = \text{cond}(\boldsymbol{\pi}, 0, u - \lambda, u + \lambda).
$$
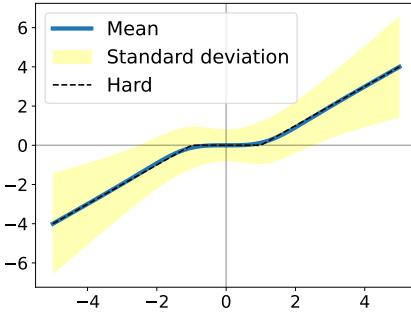
Figure 5.3: Example of conditional with three branches: the soft-thresholding operator. It is a piecewise linear function (dotted black line). Using a softargmax, we can induce a categorical probability distribution over the three branches. The expected value (blue line) can be seen as a smoothed out version of the operator. The induced distribution allows us to also compute the standard deviation.

As we will see, replacing argmax with softargmax induces a categorical distribution over the three possible branches. The mean value can be seen as a smoothed out version of the operator, and we can also compute the standard deviation, as illustrated in Fig. 5.3.

5.7.3   Differentiating through branch variables

For $\boldsymbol{\pi}$ fixed, $\mathrm{cond}(\boldsymbol{\pi}, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_K)$ is a valid function w.r.t. $\boldsymbol{v}_i$, and can therefore again be used as a node in a computational graph. Due to the linearity w.r.t. $\boldsymbol{v}_i$, we obtain that the Jacobian w.r.t. $\boldsymbol{v}_i$ is

$$\partial_{\boldsymbol{v}_i} \mathrm{cond}(\boldsymbol{\pi}, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_K) := \begin{cases} I & \text{if } \boldsymbol{\pi} = \boldsymbol{e}_i \\ \boldsymbol{0} & \text{if } \boldsymbol{\pi} \neq \boldsymbol{e}_i \end{cases}.$$

Let $g_i \colon \mathcal{U}_i \to \mathcal{V}$ be a differentiable function and $\boldsymbol{u}_i \in \mathcal{U}_i$. If we define the composition

$$f(\boldsymbol{\pi}, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_K) := \mathrm{cond}(\boldsymbol{\pi}, g_1(\boldsymbol{u}_1), \ldots, g_K(\boldsymbol{u}_K)),$$

we then obtain that the Jacobian w.r.t. $\boldsymbol{u}_i$ is

$$\partial_{\boldsymbol{u}_i} f(\boldsymbol{\pi}, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_K) := \begin{cases} \partial g_i(\boldsymbol{u}_i) & \text{if } \boldsymbol{\pi} = \boldsymbol{e}_i \\ \boldsymbol{0} & \text{if } \boldsymbol{\pi} \neq \boldsymbol{e}_i \end{cases}.$$

As long as the g_i functions are differentiable, we can therefore differentiate through the branch variables $\boldsymbol{u}_i$ without any issue.

5.7.4 Differentiating through predicate variables

As we saw, $\boldsymbol{\pi}$ can be obtained by combining comparison and logical operators, or it can be obtained by argmax and argmin operators. We illustrate here why these operators are problematic. For example, suppose we want to express the function

$$
f_a(\boldsymbol{p}, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_K) := \begin{cases} \boldsymbol{v}_1 & \text{if } p_1 = \max_j p_j \\ \vdots \\ \boldsymbol{v}_K & \text{if } p_K = \max_j p_j \end{cases}.
$$

In our notation, this can be expressed as

$$
f_a(\boldsymbol{p}, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_K) := \text{cond}(\text{argmax}(\boldsymbol{p}), g_1(\boldsymbol{u}_1), \ldots, g_K(\boldsymbol{u}_K)),
$$

As for the ifelse case, the Jacobian w.r.t. $\boldsymbol{p}$ is null almost everywhere,

$$
\partial_{\boldsymbol{p}} f_a(\boldsymbol{p}, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_K) = \boldsymbol{0}.
$$

5.7.5 Continuous relaxations

Similarly to the Heaviside step function, the argmax and argmin functions are piecewise constant, with discontinuities in case of ties. Their Jacobian are zero almost everywhere, and undefined in case of ties. Therefore, while their Jacobian is well-defined almost everywhere, they are uninformative and prevent gradient backpropagation. We can replace the argmax with a **softargmax**

$$
\text{softargmax}(\boldsymbol{p}) := \frac{\exp(\boldsymbol{p})}{\sum_{i=1}^{K} \exp(p_i)} \in \triangle^K
$$

and similarly

$$
\text{softargmin}(\boldsymbol{p}) := \text{softargmax}(-\boldsymbol{p}) \in \triangle^K.
$$

Other relaxations of the argmax are possible, as discussed in Section 12.4.4. See also Proposition 13.4 for the perturbation perspective.

Fortunately, the definition

$$\text{cond}(\boldsymbol{\pi}, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_K) = \sum_{i=1}^{K} \pi_i \boldsymbol{v}_i$$

is perfectly valid if we use $\boldsymbol{\pi} \in \triangle^K$ instead of $\boldsymbol{\pi} \in \{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_K\}$, and can therefore be seen as an **extension** of Eq. (5.3). If we now define

$$f_s(\boldsymbol{p}, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_K) := \text{cond}(\text{softargmax}(p), g_1(\boldsymbol{u}_1), \ldots, g_K(\boldsymbol{u}_K))$$

$$= \sum_{i=1}^{K} [\text{softargmax}(\boldsymbol{p})]_i \cdot g_i(\boldsymbol{u}_i), \tag{5.4}$$

the Jacobian becomes

$$\partial_p f_s(\boldsymbol{p}, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_K) = \partial \text{softargmax}(\boldsymbol{p})(g_1(\boldsymbol{u}_1), \ldots, g_K(\boldsymbol{u}_K)),$$

which is **non-null everywhere**, allowing gradients to backpropagate through the computational graph.

Probabilistic perspective

From a probabilistic perspective, we can view Eq. (5.4) as the expectation of $g_i(\boldsymbol{u}_i)$, where $i \in [K]$ is a categorical random variable distributed according to a **categorical distribution** with parameter $\boldsymbol{\pi} = \text{softargmax}(\boldsymbol{p})$:

$$f_s(\boldsymbol{p}, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_K) = \mathbb{E}_{i \sim \text{Categorical}(\text{softargmax}(\boldsymbol{p}))} [g_i(\boldsymbol{u}_i)].$$

Taking the expectation over the K possible branches makes the function differentiable with respect to $\boldsymbol{p}$, at the cost of evaluating all branches, instead of a single one. Similarly as for the if-else case, we can compute the variance if needed as

$$\mathbb{V}_{i \sim \text{Categorical}(\text{softargmax}(\boldsymbol{p}))} [g_i(\boldsymbol{u}_i)]$$
$$= \mathbb{E}_{i \sim \text{Categorical}(\text{softargmax}(\boldsymbol{p}))} \left[(f_s(\boldsymbol{p}, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_K) - g_i(\boldsymbol{u}_i))^2 \right].$$

This is illustrated in Fig. 5.3.

5.8   For loops

For loops are a control flow for sequentially calling a fixed number K of functions, reusing the output from the previous iteration. In full generality, a for loop can be written as follows.

Algorithm 5.1 $r = \text{forloop}(s_0)$

---

    for $k := 1, \ldots, K$ **do**

        $s_k := f_k(s_{k-1})$

  $r := s_K$

This defines a computation chain. Assuming the functions f_k are all differentiable, this defines a valid computational graph, we can therefore use automatic differentiation to differentiate forloop w.r.t. its input s_0. Feedforward networks, reviewed in Section 4.2, can be seen as **parameterized for loops**, i.e.,

$$f_k(s_{k-1}) := g_k(s_{k-1}, w_k),$$

for some differentiable function g_k.

Example 5.2 (Unrolled gradient descent). Suppose we want to minimize w.r.t. w the function

$$L(w, \lambda) := \frac{1}{N} \sum_{i=1}^{N} \ell(h(x_i, w), y_i) + \frac{\lambda}{2} \|w\|_2^2.$$

Given an initialization w_0, gradient descent (Section 15.1) performs iterations of the form

$$w_k = f(w_{k-1}, \gamma_k, \lambda) := w_{k-1} - \gamma_k \nabla_1 L(w_{k-1}, \lambda).$$

Gradient descent can therefore be expressed as a for loop with

$$f_k(w_{k-1}) := f(w_{k-1}, \gamma_k, \lambda).$$

This means that we can differentiate through the iterations of gradient descent, as long as f is differentiable, meaning that L is twice differentiable. This is useful for instance to perform gradient-

based optimization of the hyperparameters γ_k or λ. This a special case of bilevel optimization; see also Chapter 10.

Example 5.3 (Bubble sort). Bubble sort is a simple sorting algorithm that works by repeatedly swapping elements if necessary. Mathematically, swapping two elements i and j can be written as a function from $\mathbb{R}^N \times [N] \times [N]$ to $\mathbb{R}^N$ defined by

$$\mathrm{swap}(\boldsymbol{v}, i, j) := \boldsymbol{v} + (v_j - v_i)\boldsymbol{e}_i + (v_i - v_j)\boldsymbol{e}_j.$$

We can then write bubble sort as

$$\begin{aligned} &\textbf{for } i := 1, \ldots, N \textbf{ do} \\ &\quad \textbf{for } j := 1, \ldots, N - i - 1 \textbf{ do} \\ &\quad\quad \boldsymbol{v}' := \mathrm{swap}(\boldsymbol{v}, j, j+1) \\ &\quad\quad \pi := \mathrm{step}(v_j - v_{j+1}) \\ &\quad\quad \boldsymbol{v} \leftarrow \mathrm{ifelse}(\pi, \boldsymbol{v}', \boldsymbol{v}) \end{aligned}$$

Replacing the Heaviside step function with the logistic function gives a smoothed version of the algorithm.

5.9 Scan functions

Scan is a higher-order function (meaning a function of a function) originating from functional programming. It is useful to perform an operation f on individual elements $\boldsymbol{u}_k$ while carrying the result $\boldsymbol{s}_k$ of that operation to the next iteration.

Algorithm 5.2 $\boldsymbol{r} = \mathrm{scan}(\boldsymbol{s}_0, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_K)$

$\quad \textbf{for } k := 1, \ldots, K \textbf{ do}$
$\quad\quad \boldsymbol{s}_k, \boldsymbol{v}_k := f(\boldsymbol{s}_{k-1}, \boldsymbol{u}_k)$
$\quad \boldsymbol{r} := (\boldsymbol{s}_K, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_K)$

Assuming the function f is differentiable, this again defines a valid computational graph and can be differentiated through using autodiff. **Recurrent neural networks** (RNNs), reviewed in Section 4.6, can be

seen as a **parameterized scan**. An advantage of this abstraction is that parallel scan algorithms have been studied extensively in computer science (Blelloch, 1989; Sengupta *et al.*, 2010).

Example 5.4 (Prefix sum). Scan can be seen as a generalization of the **prefix sum** (a.k.a. **cumulated sum**) from the addition to any binary operation. Indeed, a prefix sum amounts to perform

$$\boldsymbol{v}_1 := \boldsymbol{u}_1$$
$$\boldsymbol{v}_2 := \boldsymbol{u}_1 + \boldsymbol{u}_2$$
$$\boldsymbol{v}_3 := \boldsymbol{u}_1 + \boldsymbol{u}_2 + \boldsymbol{u}_3$$
$$\vdots$$

which can be expressed as a scan by defining

$$\boldsymbol{v}_k := \boldsymbol{s}_{k-1} + \boldsymbol{u}_k$$
$$f(\boldsymbol{s}_{k-1}, \boldsymbol{u}_k) := (\boldsymbol{v}_k, \boldsymbol{v}_k)$$

starting from $\boldsymbol{s}_0 = \boldsymbol{0}$ ($\boldsymbol{s}_K$ and $\boldsymbol{v}_K$ are redundant in this case).

5.10 While loops

5.10.1 While loops as cyclic graphs

A while loop is a control flow used to repeatedly perform an operation, reusing the output of the previous iteration, until a certain condition is met. Suppose $f\colon \mathcal{S} \to \{0, 1\}$ is a function to determine whether to stop ($\pi = 1$) or continue ($\pi = 0$) and $g\colon \mathcal{S} \to \mathcal{S}$ is a function for performing an operation. Then, without loss of generality, a while loop can be written as follows.

Algorithm 5.3 $\boldsymbol{r} = \text{whileloop}(\boldsymbol{s})$

$\pi \leftarrow f(\boldsymbol{s})$
while $\pi = 0$ **do**
$\quad \boldsymbol{s} \leftarrow g(\boldsymbol{s})$
$\quad \pi \leftarrow f(\boldsymbol{s})$
$\boldsymbol{r} := \boldsymbol{s}$

This definition is somewhat cyclic, as we used the **while** keyword. However, we can equivalently rewrite the algorithm recursively.

Algorithm 5.4 $r = \mathrm{whileloop}(\boldsymbol{s})$

$\pi := f(\boldsymbol{s})$
if $\pi = 1$ **then**
    $\boldsymbol{r} := \boldsymbol{s}$
else
    $\boldsymbol{r} := \mathrm{whileloop}(g(\boldsymbol{s}))$

Unlike for loops and scan, the number of iterations of while loops is not known ahead of time, and may even be infinite. In this respect, a while loop can be seen as a **cyclic graph**.

Importance of lazy evaluation

We can also implement Algorithm 5.4 in terms of the ifelse function defined in Section 5.6 as

$$\boldsymbol{r} := \mathrm{ifelse}(f(\boldsymbol{s}), \boldsymbol{s}, \mathrm{whileloop}(g(\boldsymbol{s})))$$
$$= f(\boldsymbol{s}) \cdot \boldsymbol{s} + (1 - f(\boldsymbol{s})) \cdot \mathrm{whileloop}(g(\boldsymbol{s})).$$

However, to avoid an infinite recursion, it is crucial that ifelse supports **lazy evaluation**. That is, $\mathrm{whileloop}(g(\boldsymbol{s}))$ in the definition above should be evaluated if and only if $\pi = f(\boldsymbol{s}) = 0$. In other words, the fact that $f(\boldsymbol{s}) \in \{0, 1\}$ is crucial to ensure that the recursion is well-defined.

5.10.2   Unrolled while loops

To avoid the issues with unbounded while loops, we can enforce that a while loop stops after T iterations, i.e., we can truncate the while loop.

Unrolling Algorithm 5.4 gives (here with $T = 3$)

$$\pi_0 := f(s_0)$$
$$\textbf{if } \pi_0 = 1 \textbf{ then}$$
$$\quad r := s_0$$
$$\textbf{else}$$
$$\quad s_1 := g(s_0), \pi_1 := f(s_1)$$
$$\quad \textbf{if } \pi_1 = 1 \textbf{ then}$$
$$\quad\quad r := s_1$$
$$\quad \textbf{else}$$
$$\quad\quad s_2 := g(s_1), \pi_2 := f(s_2)$$
$$\quad\quad \textbf{if } \pi_2 = 1 \textbf{ then}$$
$$\quad\quad\quad r := s_2$$
$$\quad\quad \textbf{else}$$
$$\quad\quad\quad r := s_3 := g(s_2)$$

Using the ifelse function, we can rewrite it as

$$r = \text{ifelse}(\pi_0,$$
$$\qquad s_0,$$
$$\qquad \text{ifelse}(\pi_1,$$
$$\qquad\qquad s_1,$$
$$\qquad\qquad \text{ifelse}(\pi_2,$$
$$\qquad\qquad\qquad s_2,$$
$$\qquad\qquad\qquad s_3))).$$

which is itself equivalent to

$$r = \pi_0 s_0 + (1 - \pi_0)\left[\pi_1 s_1 + (1 - \pi_1)\left[\pi_2 s_2 + (1 - \pi_2)s_3\right]\right]$$
$$= \pi_0 s_0 + (1 - \pi_0)\pi_1 s_1 + (1 - \pi_0)(1 - \pi_1)\pi_2 s_2 + (1 - \pi_0)(1 - \pi_1)(1 - \pi_2)s_3.$$

More generally, for $T \in \mathbb{N}$, the formula is

$$\boldsymbol{r} = \sum_{i=0}^{T} \left((1 - \pi_0) \ldots (1 - \pi_{i-1}) \right) \pi_i \boldsymbol{s}_i$$

$$= \sum_{i=0}^{T} \left(\prod_{j=0}^{i-1} (1 - \pi_j) \right) \pi_i \boldsymbol{s}_i,$$

where we defined

$$\boldsymbol{s}_i := g(\boldsymbol{s}_{i-1}) := g^i(\boldsymbol{s}_0) := \underbrace{g \circ \cdots \circ g}_{i \text{ times}}(\boldsymbol{s}_0) \in \mathcal{S}$$

$$\pi_i := f(\boldsymbol{s}_i) \in \{0, 1\}.$$

Example 5.5 (Computing the square root using Newton's method).
Computing the square root $\sqrt{x}$ of a real number $x > 0$ can be cast
as a root finding problem, which we can solve using Newton's
method. Starting from an initialization s_0, the iterations read

$$s_{i+1} := g(\boldsymbol{s}_i) := \frac{1}{2} \left(s_i + \frac{x}{s_i} \right).$$

To measure the error on iteration i, we can define

$$\varepsilon(s_i) := \frac{1}{2} (s_i^2 - x)^2.$$

As a stopping criterion, we can then use

$$\pi_i := \begin{cases} 1 & \text{if } \varepsilon(s_i) \leq \tau \\ 0 & \text{otherwise} \end{cases}$$

$$= \text{step}(\tau - \varepsilon(s_i)),$$

where $0 < \tau \ll 1$ is an error tolerance and step is the Heaviside
step function.

5.10.3   Markov chain perspective

Given the function $g \colon \mathcal{S} \to \mathcal{S}$ and the initialization $\boldsymbol{s}_0 \in \mathcal{S}$, a while
loop can only go through a discrete set of values $\boldsymbol{s}_0, \boldsymbol{s}_1, \boldsymbol{s}_2, \ldots$ defined

by $s_i = g(s_{i-1})$. This set is potentially countably infinite if the while loop is unbounded, and finite if the while loop is guaranteed to stop. Whether the loop moves from the state s_i to the state s_{i+1}, or stays at s_i, is determined by the stopping criterion $\pi_i \in \{0, 1\}$. To model the state of the while loop, we can then consider a **Markov chain** with a discrete space $\{s_0, s_1, s_2, \dots\}$, which we can always identify with $\{0, 1, 2, \dots\}$, with transition probabilities

$$\mathbb{P}(S_{t+1} = s_i | S_t = s_j) = p_{i,j} := \begin{cases} \pi_i & \text{if } i = j \\ (1 - \pi_i) & \text{if } i = j + 1 \;, \\ 0 & \text{otherwise} \end{cases}$$

and initial state $S_0 = s_0$. Here, S_t is the value at iteration t of the loop. Note that since $\pi_i \in \{0, 1\}$, the values S_t are "degenerate" probabilities. However, this framework lets us generalize to a smooth version of the while loop naturally. To illustrate the framework, if the while loop stops at $T = 3$, the transition probabilities can be cast as a matrix

$$\mathbf{P} := (p_{i,j})_{i,j=0}^T := \begin{array}{c} \\ s_0 \\ s_1 \\ s_2 \\ s_3 \end{array} \begin{array}{cccc} s_0 & s_1 & s_2 & s_3 \\ \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{array}.$$

The output r of the while-loop is determined by the time at which the state stays at the same value

$$I = \min\{i \in \{1, 2, \dots\} \text{ s.t. } S_i = S_{i-1}\}.$$

Note that I itself is a random variable, as it is defined by the S_i variables. It is called a **stopping time**. The output of the chain is then

$$
\begin{aligned}
r &= \mathbb{E}[S_I] \\
&= \sum_{i=1}^{+\infty} \mathbb{P}(I = i)\mathbb{E}[S_i | I = i] \\
&= \sum_{i=1}^{+\infty} \mathbb{P}(I = i)s_{i-1} \\
&= \sum_{i=1}^{+\infty} \prod_{j=0}^{i-2} (1 - \pi_j)\pi_{i-1}s_{i-1} \\
&= \sum_{i=0}^{+\infty} \prod_{j=0}^{i-1} (1 - \pi_j)\pi_i s_i.
\end{aligned}
$$

Because the stopping time is not known ahead of time, the sum over i goes from 0 to ∞. However, if we enforce in the stopping criterion that the while loop run no longer than T iterations, by setting

$$
\pi_i := \text{or}(f(s_i), \text{eq}(i, T)) \in \{0, 1\},
$$

we then naturally recover the expression found by unrolling the while loop before,

$$
r = \mathbb{E}[S_I] = \sum_{i=0}^{T} \prod_{j=0}^{i-1} (1 - \pi_j)\pi_i s_i.
$$

For example, with $T = 3$, the transition probability matrix is

$$
\mathbf{P} = \begin{array}{c} \\ s_0 \\ s_1 \\ s_2 \\ s_3 \end{array} \begin{array}{c} s_0 \quad\quad s_1 \quad\quad s_2 \quad\quad s_3 \\ \left(\begin{array}{cccc} \pi_0 & 1 - \pi_0 & 0 & 0 \\ 0 & \pi_1 & 1 - \pi_1 & 0 \\ 0 & 0 & \pi_2 & 1 - \pi_2 \\ 0 & 0 & 0 & 1 \end{array} \right) \end{array}.
$$

Smoothed while loops

With the help of this framework, we can backpropagate even through the while loop's stopping criterion, provided that we smooth out the predicate. For example, we saw that the stopping criterion in Example 5.5 is

$f(\boldsymbol{s}_i) = \text{step}(\tau - \varepsilon(\boldsymbol{s}_i))$ and therefore

$$\pi_i := \text{or}(f(\boldsymbol{s}_i), \text{eq}(i, T)) \in \{0, 1\}.$$

With step, the derivative of the while loop with respect to τ will always be 0, just like it was the case for if-else statements. If we change the stopping criterion to $f(\boldsymbol{s}_i) = \text{sigmoid}(\tau - \varepsilon(\boldsymbol{s}_i))$, we then have (recall that or is well defined on $[0, 1] \times [0, 1]$)

$$\pi_i := \text{or}(f(\boldsymbol{s}_i), \text{eq}(i, T)) \in [0, 1].$$

With sigmoid, we obtain more informative derivatives. In particular, with sigmoid $=$ logistic, the derivatives w.r.t. τ are always non-zero. The smoothed output is expressed as before as the expectation

$$\boldsymbol{r} = \mathbb{E}[S_I] = \sum_{i=0}^{T} \prod_{j=0}^{i-1} (1 - \pi_j) \pi_i \boldsymbol{s}_i$$

$$= \sum_{i=0}^{T} \prod_{j=0}^{i-1} (1 - \text{sigmoid}(\varepsilon(\boldsymbol{s}_i) - \tau)) \text{sigmoid}(\varepsilon(\boldsymbol{s}_i) - \tau) \boldsymbol{s}_i.$$

5.11   Summary

In this chapter, we studied control flows for differentiable programming.

For conditionals, we saw that differentiating through the branch variables is not problematic. However, for the predicate variable, we saw that a differentiable relaxation is required to avoid null derivatives. To do so, we introduced soft comparison operators in a principled manner, using a stochastic process perspective, as well as the continuous extension of logical operators.

For loops and scan define valid computational graphs, as their number of iterations is fixed ahead of time. Feedforward networks and RNNs can be seen as parameterized for loops and scan, respectively.

Unlike for loops and scan, the number of iterations of while loops is not known ahead of time and may even be infinite. However, unrolled while loops define valid directed acyclic graphs. We defined a principled way to differentiate through the stopping criterion of a while loop, thanks to a Markov chain perspective.

Part III

Differentiating through programs

6

Finite differences

One of the simplest way to numerically compute derivatives is to use finite differences, which approximate the infinitesimal definition of a derivative. Finite differences only require **function evaluations**, and can therefore work with blackbox functions (i.e., they ignore the compositional structure of functions). Without loss of generality, our exposition focuses on computing directional derivatives $\partial f(\boldsymbol{w})[\boldsymbol{v}]$, for a function $f \colon \mathcal{E} \to \mathcal{F}$, evaluated at $\boldsymbol{w} \in \mathcal{E}$, in the direction $\boldsymbol{v} \in \mathcal{E}$.

6.1 Forward differences

From Definition 2.3 and Definition 2.12, the directional derivative and more generally the JVP are defined as a limit,

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] := \lim_{\delta \to 0} \frac{f(\boldsymbol{w} + \delta \boldsymbol{v}) - f(\boldsymbol{w})}{\delta}.$$

This suggests that we can approximate the directional derivative and the JVP using

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] \approx \frac{f(\boldsymbol{w} + \delta \boldsymbol{v}) - f(\boldsymbol{w})}{\delta},$$

for some $0 < \delta \ll 1$. This formula is called a **forward difference**. From the Taylor expansion in Section 2.5.4, we indeed have

$$f(\boldsymbol{w}+\delta\boldsymbol{v})-f(\boldsymbol{w}) = \delta\partial f(\boldsymbol{w})[\boldsymbol{v}]+\frac{\delta^2}{2}\partial^2 f(\boldsymbol{w})[\boldsymbol{v},\boldsymbol{v}]+\frac{\delta^3}{3!}\partial^3 f(\boldsymbol{w})[\boldsymbol{v},\boldsymbol{v},\boldsymbol{v}]+\dots$$

so that

$$
\begin{aligned}
\frac{f(\boldsymbol{w}+\delta\boldsymbol{v})-f(\boldsymbol{w})}{\delta} &= \partial f(\boldsymbol{w})[\boldsymbol{v}] + \frac{\delta}{2}\partial^2 f(\boldsymbol{w})[\boldsymbol{v},\boldsymbol{v}] + \frac{\delta^2}{3!}\partial^3 f(\boldsymbol{w})[\boldsymbol{v},\boldsymbol{v},\boldsymbol{v}] + \dots \\
&= \partial f(\boldsymbol{w})[\boldsymbol{v}] + o(\delta).
\end{aligned}
$$

The error incurred by choosing a finite rather than infinitesimal δ in the forward difference formula is called the **truncation error**. The Taylor approximation above shows that this error is of the order of $o(\delta)$.

However, we cannot choose a too small value of δ, because the evaluation of the function f on a computer rounds the value of f to machine precision. Mathematically, a scalar-valued function f evaluated on a computer becomes a function $\tilde{f}$ such that $\tilde{f}(w) \approx [f(w)/\varepsilon]\varepsilon$, where $[f(w)/\varepsilon]$ denotes the closest integer of $f(w)/\varepsilon \in \mathbb{R}$ and ε is the machine precision, i.e., the smallest non-zero real number encoded by the machine. This means that the difference $f(\boldsymbol{w}+\delta\boldsymbol{v}) - f(\boldsymbol{w})$ evaluated on a computer is prone to **round-off error** of the order of $o(\varepsilon)$. We illustrate the trade-off between truncation and round-off errors in Fig. 6.1.

6.2 Backward differences

As an alternative, we can approximate the directional derivative and the JVP by

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] \approx \frac{f(\boldsymbol{w}) - f(\boldsymbol{w} - \delta\boldsymbol{v})}{\delta},$$

for some $0 < \delta \ll 1$. This formula is called a **backward difference**. From the Taylor expansion in Section 2.5.4, we easily verify that $(f(\boldsymbol{w}) - f(\boldsymbol{w} - \delta\boldsymbol{v}))/\delta = \partial f(\boldsymbol{w})[\boldsymbol{v}] + o(\delta)$, so that the truncation error is the same as for the forward difference.
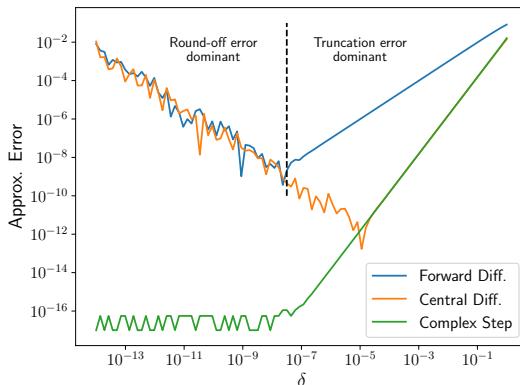
Figure 6.1: The forward or central difference schemes applied to $f(x) := \ln(1 + \exp(-x))$ to approximate $f'(x)$ at $x = 1$ induce both truncation error (for large δ) and round-off error (for small δ).

6.3 Central differences

Rather than using an asymmetric formula to approximate the derivative, we can use

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] \approx \frac{f(\boldsymbol{w} + \delta\boldsymbol{v}) - f(\boldsymbol{w} - \delta\boldsymbol{v})}{2\delta},$$

for some $0 < \delta \ll 1$. This formula is called a **central difference**. From the Taylor expansion in Section 2.5.4, we have

$$f(\boldsymbol{w} + \delta\boldsymbol{v}) - f(\boldsymbol{w} - \delta\boldsymbol{v}) = 2\delta\partial f(\boldsymbol{w})[\boldsymbol{v}] + \frac{2\delta^3}{3!}\partial^3 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}, \boldsymbol{v}]$$
$$+ \frac{2\delta^5}{5!}\partial^5 f(\boldsymbol{w})[\boldsymbol{v}, \dots, \boldsymbol{v}] + \dots$$

so that

$$\frac{f(\boldsymbol{w} + \delta\boldsymbol{v}) - f(\boldsymbol{w} - \delta\boldsymbol{v})}{2\delta} = \partial f(\boldsymbol{w})[\boldsymbol{v}] + \frac{\delta^2}{3!}\partial^3 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}, \boldsymbol{v}] + \dots$$
$$= \partial f(\boldsymbol{w})[\boldsymbol{v}] + o(\delta^2).$$

We see that the terms corresponding to derivatives of **even order** canceled out, allowing the formula to achieve $o(\delta^2)$ truncation error. For any $\delta < 1$, the truncation error of the central difference is much

smaller than the one of the forward or backward differences as confirmed empirically in Fig. 6.1.

6.4 Higher-accuracy finite differences

The truncation error can be further reduced by making use of additional function evaluations. One can generalize the forward difference scheme by a formula of the form

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] \approx \sum_{i=0}^{p} \frac{a_i}{\delta} f(\boldsymbol{w} + i\delta\boldsymbol{v})$$

requiring $p+1$ evaluations. To select the a_i and reach a truncation error of order $o(\delta^p)$, we can use a Taylor expansion on each term of the sum to get

$$\sum_{k=0}^{p} \frac{a_i}{\delta} f(\boldsymbol{w} + i\delta\boldsymbol{v}) = \sum_{k=0}^{p} a_i \sum_{j=0}^{p} \frac{i^j \delta^{j-1}}{j!} \partial^j f(\boldsymbol{w})[\boldsymbol{v}, \ldots, \boldsymbol{v}] + o(\delta^p).$$

By grouping the terms in the sum for each order of derivative, we obtain a set of $p+1$ equations to be satisfied by the $p+1$ coefficients $a_0, \ldots, a_p$, that is,

$$a_0 + a_1 + \ldots + a_p = 0$$
$$a_1 + 2a_2 + \ldots + pa_p = 1$$
$$a_1 + 2^j a_2 + \ldots + p^j a_p = 0 \quad \forall j \in \{2, \ldots, p\}.$$

This system of equations can be solved analytically to derive the coefficients. Backward differences can be generalized similarly by using $\partial f(\boldsymbol{w})[\boldsymbol{v}] \approx \sum_{i=0}^{p} \frac{a_i}{\delta} f(\boldsymbol{w} - i\delta\boldsymbol{v})$. Similarly, the central difference scheme can be generalized by using

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] \approx \sum_{i=-p}^{p} \frac{a_i}{\delta} f(\boldsymbol{w} + i\delta\boldsymbol{v}),$$

to reach a truncation error of order $o(\delta^{2p})$. Solving for the coefficients $a_{-p}, \ldots, a_p$ as above reveals that $a_0 = 0$. Therefore, only $2p$ evaluations are necessary.

6.5   Higher-order finite differences

To approximate higher order derivatives, we can follow a similar reasoning. Namely, we can generalize the forward difference scheme to approximate the derivative of order k by

$$\partial^k f(\boldsymbol{w})[\boldsymbol{v}, \ldots, \boldsymbol{v}] \approx \sum_{i=0}^{p} \frac{a_i}{\delta^k} f(\boldsymbol{w} + i\delta\boldsymbol{v}).$$

As before, we can expand the terms in the sum. For the approximation to capture only the kth derivative, we now require the coefficients a_i to satisfy

$$
\begin{aligned}
0^j a_0 + 1^j a_1 + 2^j a_2 + \ldots + p^j a_p &= 0 \quad \forall j \in \{0, \ldots, k-1\}. \\
0^k a_0 + 1^k a_1 + 2^k a_2 + \ldots + p^k a_p &= k! \\
0^j a_0 + 1^j a_1 + 2^j a_2 + \ldots + p^j a_p &= 0 \quad \forall j \in \{k+1, \ldots, p\}.
\end{aligned}
$$

With the resulting coefficients, we obtain a truncation error of order $o(\delta^{p-k+1})$, while making $p+1$ evaluations. For example, for $p = k = 2$, we can approximate the second-order derivative as

$$\partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}] \approx \frac{-(3/2)f(\boldsymbol{x}) + 2f(\boldsymbol{x} + \delta\boldsymbol{v}) - (1/2)f(\boldsymbol{x} + 2\delta\boldsymbol{v})}{\delta^2},$$

with a truncation error of order $o(\delta)$.

The central difference scheme can be generalized similarly by

$$\partial^k f(\boldsymbol{w})[\boldsymbol{v}, \ldots, \boldsymbol{v}] \approx \sum_{i=-p}^{p} \frac{a_i}{\delta^k} f(\boldsymbol{w} + i\delta\boldsymbol{v}),$$

to reach truncation errors of order $o(\delta^{2p+2-2\lceil(k+1)/2\rceil})$. For example, for $k = 2$, $p = 1$, we obtain the second-order central difference

$$\partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}] \approx \frac{f(\boldsymbol{w} + \delta\boldsymbol{v}) + f(\boldsymbol{w} - \delta\boldsymbol{v}) - 2f(\boldsymbol{w})}{\delta^2}.$$

By using a Taylor expansion we see that, this time, the terms corresponding to derivatives of **odd order** cancel out and the truncation error is $o(\delta^2)$ while requiring 3 evaluations.

6.6 Complex-step derivatives

Suppose f is well defined on $\mathbb{C}^P$, the space of P-dimensional complex numbers. Let us denote the imaginary unit by $i = \sqrt{-1}$. Then, the Taylor expansion of f reads

$$
\begin{aligned}
f(\boldsymbol{w} + (i\delta)\boldsymbol{v}) =& f(\boldsymbol{w}) + (i\delta)\partial f(\boldsymbol{w})[\boldsymbol{v}] + \frac{(i\delta)^2}{2}\partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}] \\
& + \frac{(i\delta)^3}{3!}\partial^3 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}, \boldsymbol{v}] + \dots \\
=& f(\boldsymbol{w}) + (i\delta)\partial f(\boldsymbol{w})[\boldsymbol{v}] - \frac{\delta^2}{2}\partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}] \\
& - \frac{i(\delta)^3}{3!}\partial^3 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{v}, \boldsymbol{v}] + \dots \quad .
\end{aligned}
$$

We see that the real part corresponds to even-degree terms and the imaginary part corresponds to odd-degree terms. We therefore obtain

$$
\mathrm{Re}(f(\boldsymbol{w} + (i\delta)\boldsymbol{v})) = f(\boldsymbol{w}) + o(\delta^2)
$$

and

$$
\mathrm{Im}\left(\frac{f(\boldsymbol{w} + (i\delta)\boldsymbol{v})}{\delta}\right) = \partial f(\boldsymbol{w})[\boldsymbol{v}] + o(\delta^2).
$$

This suggests that we can compute directional derivatives using the approximation

$$
\partial f(\boldsymbol{w})[\boldsymbol{v}] \approx \mathrm{Im}\left(\frac{f(\boldsymbol{w} + (i\delta)\boldsymbol{v})}{\delta}\right),
$$

for $0 < \delta \ll 1$. This is called the **complex-step derivative** approximation (Squire and Trapp, 1998; Martins *et al.*, 2003).

Contrary to forward, backward and central differences, we see that only a **single function call** is necessary. A function call on complex numbers may take roughly twice the cost of a function call on real numbers. However, thanks to the fact that a difference of functions is no longer needed, the complex-step derivative approximation usually enjoys smaller round-off error as illustrated in Fig. 6.1. That said, one drawback of the method is that all elementary operations within the program implementing the function f must be well-defined on complex numbers, e.g., using overloading.

Table 6.1: Computational complexity in number of function evaluations for computing the directional derivative and the gradient of a function $f\colon \mathbb{R}^P \to \mathbb{R}$ by finite differences and complex step derivatives.

	Directional derivative	Gradient
Forward difference	2	$P+1$
Backward difference	2	$P+1$
Central difference	2	$2P$
Complex step	1	P

6.7   Complexity

We now discuss the computational complexity in terms of function evaluations of finite differences and complex-step derivatives. For concreteness, as this is the most common use case in machine learning, we discuss the case of a single $M = 1$ output, i.e., we want to differentiate a function $f\colon \mathbb{R}^P \to \mathbb{R}$. Whether we use forward, backward or central differences, the computational complexity of computing the directional derivative $\partial f(\boldsymbol{w})[\boldsymbol{v}]$ in any direction $\boldsymbol{v}$ amounts to two calls to f. For computing the gradient $\nabla f(\boldsymbol{w})$, we can use (see Definition 2.6) that

$$[\nabla f(\boldsymbol{w})]_j = \langle \nabla f(\boldsymbol{w}), \boldsymbol{e}_j \rangle = \partial f(\boldsymbol{w})[\boldsymbol{e}_j],$$

for $j \in [P]$. For forward and backward differences, we therefore need $P+1$ function calls to compute the gradient, while we need $2P$ function calls for central differences. For the complex step approximation, we need P complex function calls. We summarize the complexities in Table 6.1.

6.8   Summary

We reviewed finite differences, a simple way to numerically compute derivatives using only **function evaluations**. Central differences achieve smaller **truncation error** than forward and backward differences. We saw that it is possible to achieve smaller truncation error, at the cost of more function evaluations. Complex-step derivatives achieve smaller

round-off error than central differences but require the function and the program implementing it to be well-defined on complex numbers. However, whatever the method used, finite differences require a number of function calls that is proportional to the number of dimensions. They are therefore seldom used in machine learning, where there can be millions or billions of dimensions. The main use cases of finite differences are therefore i) for blackbox functions of low dimension and ii) for test purposes (e.g., checking that a gradient function is correctly implemented). For modern machine learning, the main workhorse is automatic differentiation, as it leverages the compositional structure of functions. This is what we study in the next chapter.

7

Automatic differentiation

In Chapter 2, we reviewed the fundamentals of differentiation and stressed the importance of two linear maps: the Jacobian-vector product (JVP) and its adjoint, the vector-Jacobian product (VJP). In this chapter, we review **forward-mode** and **reverse-mode** autodiff using these two linear maps. We start with **computation chains** and then generalize to feedforward networks and general **computation graphs**. We also review checkpointing, reversible layers and randomized estimators.

7.1   Computation chains

To begin with, consider a **computation chain** (Section 4.1.1) representing a function $f \colon \mathcal{S}_0 \to \mathcal{S}_K$ expressed as a sequence of compositions $f := f_K \circ \cdots \circ f_1$, where $f_k \colon \mathcal{S}_{k-1} \to \mathcal{S}_k$. The computation of f can be

unrolled into a sequence of operations

$$
\begin{aligned}
\boldsymbol{s}_0 &\in \mathcal{S}_0 \\
\boldsymbol{s}_1 &\coloneqq f_1(\boldsymbol{s}_0) \in \mathcal{S}_1 \\
&\;\;\vdots \\
\boldsymbol{s}_K &\coloneqq f_K(\boldsymbol{s}_{K-1}) \in \mathcal{S}_K \\
f(\boldsymbol{x}) &\coloneqq \boldsymbol{s}_K.
\end{aligned}
\tag{7.1}
$$

Our goal is to compute the variations of f around a given input $\boldsymbol{s}_0$. In a feedforward network, this amounts to estimating the influence of a given input $\boldsymbol{s}_0$ for fixed parameters (we will see how to estimate the variations w.r.t. parameters $\boldsymbol{w}$ in the sequel).

Jacobian matrix. We first consider the computation of the full Jacobian $\boldsymbol{\partial} f(\boldsymbol{s}_0)$, seen as a **matrix**, as the notation $\boldsymbol{\partial}$ indicates. Following Proposition 2.2, we have

$$
\boldsymbol{\partial} f(\boldsymbol{s}_0) = \boldsymbol{\partial} f_K(\boldsymbol{s}_{K-1}) \boldsymbol{\partial} f_{K-1}(\boldsymbol{s}_{K-2}) \dots \boldsymbol{\partial} f_2(\boldsymbol{s}_1), \boldsymbol{\partial} f_1(\boldsymbol{s}_0),
\tag{7.2}
$$

where $\boldsymbol{\partial} f_k(\boldsymbol{s}_{k-1})$ are the Jacobians of the intermediate functions computed at $\boldsymbol{s}_0, \dots, \boldsymbol{s}_K$, as defined in Eq. (7.1). The main drawback of this approach is computational: computing the full $\boldsymbol{\partial} f(\boldsymbol{s}_0)$ requires to materialize the intermediate Jacobians in memory and to perform matrix-matrix multiplications. However, in practice, computing the full Jacobian is rarely needed. Indeed, oftentimes, we only need to right-multiply or left-multiply with $\boldsymbol{\partial} f(\boldsymbol{s}_0)$. This gives rise to forward-mode and reverse-mode autodiff, respectively.

7.1.1 Forward-mode

We now interpret the Jacobian $\partial f(\boldsymbol{s}_0)$ as a **linear map**, as the non-bold ∂ indicates. Following Proposition 2.6, $\partial f(\boldsymbol{s}_0)$ is the composition of the intermediate linear maps,

$$
\partial f(\boldsymbol{s}_0) = \partial f_K(\boldsymbol{s}_{K-1}) \circ \partial f_{K-1}(\boldsymbol{s}_{K-2}) \circ \dots \circ \partial f_2(\boldsymbol{s}_1) \circ \partial f_1(\boldsymbol{s}_0).
$$
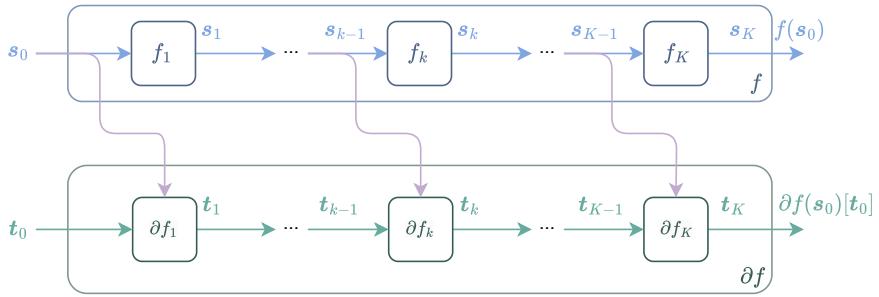
Figure 7.1: Forward-mode autodiff for a chain of computations. For readability, we denoted the intermediate JVP as a function of two variables $\partial f_k : \boldsymbol{s}_{k-1}, \boldsymbol{t}_{k-1} \mapsto \partial f_k(\boldsymbol{s}_{k-1})[\boldsymbol{t}_{k-1}]$ with $\partial f_k(\boldsymbol{s}_{k-1})[\boldsymbol{t}_{k-1}] = \boldsymbol{t}_k$.

Evaluating $\partial f(\boldsymbol{s}_0)$ on an **input direction** $\boldsymbol{v} \in \mathcal{S}_0$ can be decomposed, like the function Eq. (7.1) itself, into intermediate computations

$$\boldsymbol{t}_0 := \boldsymbol{v}$$
$$\boldsymbol{t}_1 := \partial f_1(\boldsymbol{s}_0)[\boldsymbol{t}_1]$$
$$\vdots$$
$$\boldsymbol{t}_K := \partial f_K(\boldsymbol{s}_{K-1})[\boldsymbol{t}_{K-1}]$$
$$\partial f(\boldsymbol{s}_0)[\boldsymbol{v}] := \boldsymbol{t}_K.$$

Each intermediate linear map $\partial f_k(\boldsymbol{s}_{k-1})$ amounts to a Jacobian-vector product (JVP) and can be performed in a **forward** manner, along the computation of the intermediate states $\boldsymbol{s}_k$. This can also be seen as multiplying the matrix defined in Eq. (7.2) with a vector, from **right to left**. This is illustrated in Fig. 7.1 and the procedure is summarized in Algorithm 7.1.

Computational complexity. The JVP follows exactly the computations of f, with an additional variable $\boldsymbol{t}_k$ being propagated. If we consider that computing ∂f_k is roughly as costly as computing f_k, then computing a JVP has roughly twice the computational cost of f. See Section 7.3.3 for a more general and more formal statement.

Algorithm 7.1 Forward-mode autodiff for chains of computations

---

Functions: $f \coloneqq f_K \circ \ldots \circ f_1$
Inputs: input $\boldsymbol{s}_0 \in \mathcal{S}_0$, input direction $\boldsymbol{v} \in \mathcal{S}_0$
1: Initialize $\boldsymbol{t}_0 \coloneqq \boldsymbol{v}$
2: **for** $k \coloneqq 1, \ldots, K$ **do**
3:     Compute $\boldsymbol{s}_k \coloneqq f_k(\boldsymbol{s}_{k-1}) \in \mathcal{S}_k$
4:     Compute $\boldsymbol{t}_k \coloneqq \partial f_k(\boldsymbol{s}_{k-1})[\boldsymbol{t}_{k-1}] \in \mathcal{S}_k$
Outputs: $f(\boldsymbol{s}_0) \coloneqq \boldsymbol{s}_K$, $\partial f(\boldsymbol{s}_0)[\boldsymbol{v}] = \boldsymbol{t}_K$

Memory usage. The memory usage of a program at a given evaluation step is the number of variables that need to be stored in memory to ensure the execution of all remaining steps. The memory cost of a program is then the maximal memory usage over all evaluation steps. For our purposes, we analyze the memory usage and memory cost by examining the given program. Formal definitions of operations on memory such as read, write, delete and associated memory costs are presented by Griewank and Walther (2008, Chapter 4).

For example, to execute the chain $f = f_K \circ \cdots \circ f_1$, at each step k, we only need to have access to $\boldsymbol{s}_{k-1}$ to execute the rest of the program. As we compute $\boldsymbol{s}_k$, we can delete $\boldsymbol{s}_{k-1}$ from memory and replace it by $\boldsymbol{s}_k$. Therefore, the memory cost associated to the evaluation of f is just the maximal dimension of the $\boldsymbol{s}_k$ variables.

For forward mode autodiff, as we follow the computations of f, at each step k, we only need to have access to $\boldsymbol{s}_{k-1}$ and $\boldsymbol{t}_{k-1}$ to execute the rest of the program. The memory used by $\boldsymbol{s}_{k-1}$ and $\boldsymbol{t}_{k-1}$ can directly be used for $\boldsymbol{s}_k, \boldsymbol{t}_k$ once they are computed. The memory usage associated to the JVP is summarized in Fig. 7.2. Overall the memory cost of the JVP is then exactly twice the memory cost of the function itself.

7.1.2 Reverse-mode

In machine learning, most functions whose gradient we need to compute take the form $\ell \circ f$, where ℓ is a scalar-valued loss function and f is a network. As seen in Proposition 2.3, the gradient takes the form

$$\nabla(\ell \circ f)(\boldsymbol{s}_0) = \partial f(\boldsymbol{s}_0)^*[\nabla \ell(f(\boldsymbol{s}_0))].$$
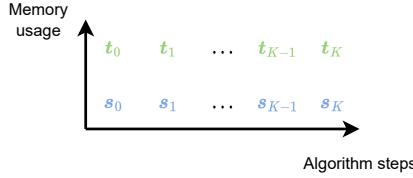
Figure 7.2: Memory usage of forward-mode autodiff for a computation chain. Here $t_0 = v$, $s_K = f(s_0)$, $t_K = \partial f(s_0)[v]$.

This motivates the need for applying the **adjoint** $\partial f(s_0)^*$ to $\nabla \ell(f(s_0)) \in \mathcal{S}_K$ and more generally to any **output direction** $u \in \mathcal{S}_K$. From Proposition 2.7, we have

$$\partial f(s_0)^* = \partial f_1(s_0)^* \circ \ldots \circ \partial f_K(s_{K-1})^*.$$

Evaluating $\partial f(s_0)^*$ on an output direction $u \in \mathcal{S}_K$ is decomposed as

$$
\begin{aligned}
r_K &= u \\
r_{K-1} &= \partial f_K(s_{K-1})^*[r_K] \\
&\vdots \\
r_0 &= \partial f_1(s_0)^*[r_1] \\
\partial f(s_0)^*[u] &= r_0.
\end{aligned}
$$

Each intermediate adjoint $\partial f_k(s_{k-1})^*$ amounts to a vector-Jacobian product (VJP). The key difference with the forward mode is that the procedure runs **backward** through the chain, hence the name **reverse mode** autodiff. This can also be seen as multiplying Eq. (7.2) from **left to right**. The procedure is illustrated in Fig. 7.3 and summarized in Algorithm 7.2.

Computational complexity.   In terms of number of operations, the VJP simply passes two times through the chain, once forward, then backward. If we consider the intermediate VJPs to be roughly as costly as the intermediate functions themselves, the VJP amounts just to twice the cost of the original function, just as the JVP. See Section 7.3.3 for a more generic and formal statement.
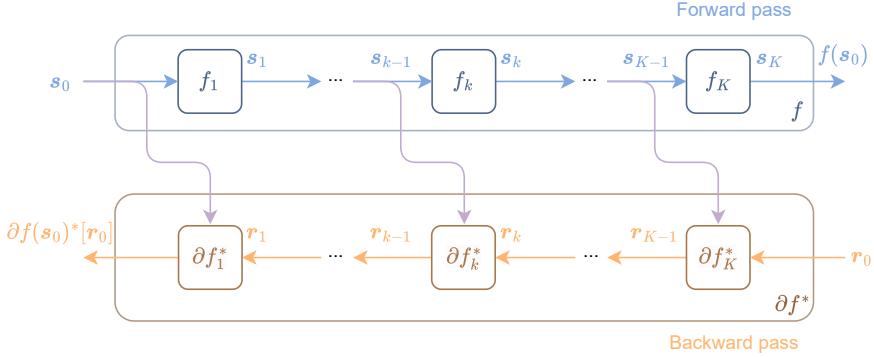
Figure 7.3: Reverse mode of automatic differentiation for a chain of computations. For readability, we denoted the intermediate VJP as a function of two variables $\partial f_k^* : (s_{k-1}, r_k) \mapsto \partial f_k(s_{k-1})^*[r_k]$ with $\partial f_k(s_{k-1})^*[r_k] = r_{k-1}$.

Algorithm 7.2 Reverse-mode autodiff for chains of computations

---

Functions: $f := f_K \circ \ldots \circ f_1$,
Inputs: input $s_0 \in \mathcal{S}_0$, output direction $u \in \mathcal{S}_K$
1: **for** $k := 1, \ldots, K$ **do**   ▷ Forward pass
2:     Compute $s_k := f_k(s_{k-1}) \in \mathcal{S}_k$

3: Initialize $r_K := u$.
4: **for** $k := K, \ldots, 1$ **do**   ▷ Backward pass
5:     Compute $r_{k-1} := \partial f_k(s_{k-1})^*[r_k] \in \mathcal{S}_{k-1}$
Outputs: $f(s_0) := s_K$, $\partial f(s_0)^*[u] = r_0$
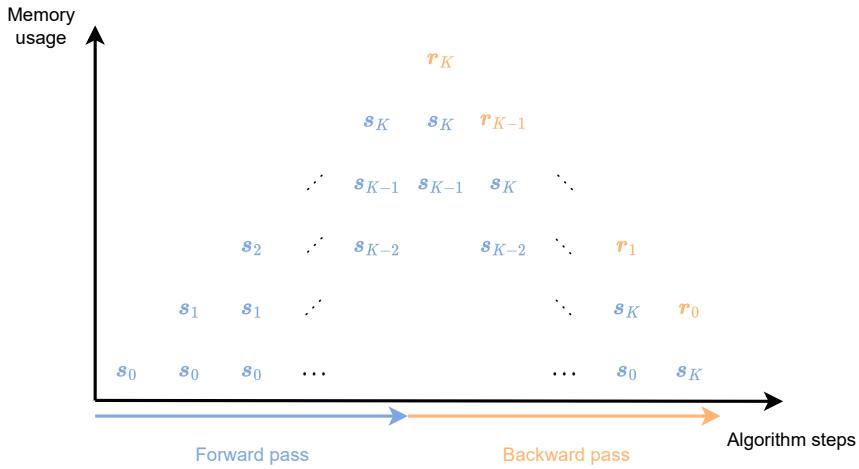
Figure 7.4: Memory usage of reverse mode autodiff for a computation chain.

Memory usage.   Recall that the memory usage of a program at a given evaluation step is the number of variables that need to be stored in memory to ensure the execution of the remaining steps. If we inspect Algorithm 7.3, to execute all backward steps, that is the loop in line 4, we need to have access to all the intermediate inputs $s_0, \ldots, s_{K-1}$. Therefore, the memory cost of reverse-mode autodiff is proportional to the length of the chain K. Fig. 7.4 illustrates the memory usage during reverse mode autodiff. It grows linearly until the end of the forward pass and then progressively decreases until it outputs the value of the function and the VJP. The memory cost can be mitigated by means of checkpointing techniques presented in Section 7.5.

Decoupled function and VJP evaluations.   The additional memory cost of reverse mode autodiff comes with some advantages. If we need to compute $\partial f(s_0)^*[u_i]$ for n different output directions u_i, we only need to compute and store once the intermediate computations s_k and then make n calls to the backward pass. In other words, by storing in memory the intermediate computations s_k, we may instantiate a **VJP operator**, which we may apply to any u through the backward pass.

Formally, the forward and backward passes can be decoupled as

$$\text{forward}(f, \boldsymbol{s}_0) := (f(\boldsymbol{s}_0), \partial f(\boldsymbol{s}_0)^*)$$

where

$$\partial f(\boldsymbol{s}_0)^*[\boldsymbol{u}] := \text{backward}(\boldsymbol{u}; \boldsymbol{s}_0, \dots, \boldsymbol{s}_{K-1}).$$

In functional programming terminology, the VJP $\partial f(\boldsymbol{s}_0)^*$ is a **closure**, as it contains the intermediate computations $\boldsymbol{s}_0, \dots \boldsymbol{s}_K$. The same can be done for the JVP $\partial f(\boldsymbol{s}_0)$ if we want to apply to multiple directions $\boldsymbol{v}_i$.

Example 7.1 (Multilayer perceptron with fixed parameters). As a running example, consider a multilayer perceptron (MLP) with one hidden layer and (for now) given fixed weights. As presented in Chapter 4, an MLP can be decomposed as

$$\begin{aligned}
\boldsymbol{s}_0 &= \boldsymbol{x} \\
\boldsymbol{s}_1 &= f_1(\boldsymbol{s}_0) = \sigma(\boldsymbol{A}_1 \boldsymbol{s}_0 + \boldsymbol{b}_1) \\
\boldsymbol{s}_2 &= f_2(\boldsymbol{s}_1) = \boldsymbol{A}_2 \boldsymbol{s}_1 + \boldsymbol{b}_2 \\
f(\boldsymbol{x}) &= \boldsymbol{s}_2,
\end{aligned}$$

for $\boldsymbol{A}_1, \boldsymbol{A}_2, \boldsymbol{b}_1, \boldsymbol{b}_2$ some fixed parameters and σ an activation function such as the softplus activation function $\sigma(x) = \log(1 + e^x)$ with derivative $\sigma'(x) = e^x/(1 + e^x)$.

Evaluating the JVP of f on an input $\boldsymbol{x}$ along a direction $\boldsymbol{v}$ can then be decomposed as

$$\begin{aligned}
\boldsymbol{t}_0 &= \boldsymbol{v} \\
\boldsymbol{t}_1 &= \sigma'(\boldsymbol{A}_1 \boldsymbol{s}_0 + \boldsymbol{b}_1) \odot (\boldsymbol{A}_1 \boldsymbol{t}_0) \\
\boldsymbol{t}_2 &= \boldsymbol{A}_2 \boldsymbol{t}_1 \\
\partial f(\boldsymbol{x})[\boldsymbol{v}] &= \boldsymbol{t}_2,
\end{aligned}$$

where we used in the second line the JVP of element-wise function as in Example 7.3.

Evaluating the VJP of f at $\boldsymbol{x}$ requires to evaluate the interme-

diate VJPs at the stored activations

$$
\begin{aligned}
\boldsymbol{r}_2 &= \boldsymbol{u} \\
\boldsymbol{r}_1 &= \partial f_2(\boldsymbol{s}_1)^*[\boldsymbol{r}_2] = \boldsymbol{A}_2^\top \boldsymbol{r}_2 \\
\boldsymbol{r}_0 &= \partial f_1(\boldsymbol{s}_0)^*[\boldsymbol{r}_1] = \boldsymbol{A}_1^\top (\sigma'(\boldsymbol{A}_1 \boldsymbol{s}_0 + \boldsymbol{b}_1) \odot \boldsymbol{r}_1)
\end{aligned}
$$
$$
\partial f(\boldsymbol{x})^*[\boldsymbol{u}] = \boldsymbol{r}_0.
$$

7.1.3 Complexity of entire Jacobians

In this section, we analyze the time and space complexities of forward-mode and reverse-mode autodiff for computing the **entire** Jacobian matrix $\partial f(\boldsymbol{s}_0)$ of a computain chain $f = f_K \circ \cdots \circ f_1$. We assume $\mathcal{S}_k \subseteq \mathbb{R}^{D_k}$, $D_K = M$ and $D_0 = D$.

Complexity of forward-mode autodiff

Using Definition 2.8, we find that we can extract each **column** $\partial_j f(\boldsymbol{s}_0) \in \mathbb{R}^M$ of the Jacobian matrix, for $j \in [D]$, by multiplying with the standard basis vector $\boldsymbol{e}_j \in \mathbb{R}^D$:

$$
\partial_1 f(\boldsymbol{s}_0) = \partial f(\boldsymbol{s}_0)\boldsymbol{e}_1
$$
$$
\vdots
$$
$$
\partial_D f(\boldsymbol{s}_0) = \partial f(\boldsymbol{s}_0)\boldsymbol{e}_D.
$$

Computing the full Jacobian matrix therefore requires D JVPs with vectors in $\mathbb{R}^D$. Assuming each f_k in the chain composition has the form $f_k : \mathbb{R}^{D_{k-1}} \to \mathbb{R}^{D_k}$, seen as a matrix, $\partial f_k(\boldsymbol{s}_{k-1})$ has size $D_k \times D_{k-1}$. Therefore, the computational cost of D JVPs is $O\left(D \sum_{k=1}^K D_k D_{k-1}\right)$. The memory cost is $O(\max_{k \in [K]} D_k)$, since we can release intermediate computations after each layer is processed. Setting $D_1 = \cdots = D_{K-1} = D$ for simplicity and using $D_K = M$, we obtain that the computational cost of computing D JVPs and therefore of computing the full Jacobian matrix by forward-mode autodiff is $O(MD^2 + KD^3)$. The memory cost is $O(\max\{D, M\})$. If a function is single-input $D = 1$, then the forward mode computes at once all the Jacobian, which reduces to a single directional derivative.

	Forward-mode	Reverse-mode
Time	$O(MD^2 + KD^3)$	$O(M^2D + KMD^2)$
Space	$O(\max\{M, D\})$	$O(KD + M)$

Table 7.1: Time and space complexities of forward-mode and reverse-mode autodiff for computing the full Jacobian of a chain of functions $f = f_K \circ \cdots \circ f_1$, where $f_k \colon \mathbb{R}^D \to \mathbb{R}^D$ if $k = 1, \ldots, K - 1$ and $f_K \colon \mathbb{R}^D \to \mathbb{R}^M$. We assume ∂f_k is a dense linear operator. Forward mode requires D JVPs. Reverse mode requires M VJPs.

Complexity of reverse-mode autodiff

Using Definition 2.8, we find that we can extract each **row** of the Jacobian matrix, which corresponds to the transposed gradients $\nabla f_i(\boldsymbol{s}_0) \in \mathbb{R}^D$, for $i \in [M]$, by multiplying with the standard basis vector $\boldsymbol{e}_i \in \mathbb{R}^M$:

$$\nabla f_1(\boldsymbol{s}_0) = \partial f(\boldsymbol{s}_0)^* \boldsymbol{e}_1$$

$$\vdots$$

$$\nabla f_M(\boldsymbol{s}_0) = \partial f(\boldsymbol{s}_0)^* \boldsymbol{e}_M.$$

Computing the full Jacobian matrix therefore requires M VJPs with vectors in $\mathbb{R}^M$. Assuming as before that each f_k in the chain composition has the form $f_k : \mathbb{R}^{D_{k-1}} \to \mathbb{R}^{D_k}$, the computational cost of M VJPs is $O\left(M \sum_{k=1}^{K} D_k D_{k-1}\right)$. However, the memory cost is $O(\sum_{k=1}^{K} D_k)$, as we need to store the intermediate computations for each of the K layers. Setting $D_0 = \cdots = D_{K-1} = D$ for simplicity and using $D_K = M$, we obtain that the computational cost of computing M VJPs and therefore of computing the full Jacobian matrix by reverse-mode autodiff is $O(M^2D + KMD^2)$. The memory cost is $O(KD + M)$. If the function is single-output $M = 1$, reverse-mode autodiff computes at once the Jacobian, which reduces to the gradient.

When to use forward-mode vs. reverse-mode autodiff?

We summarize the time and space complexities in Table 7.1. Generally, if $M < D$, reverse-mode is more advantageous at the price of some memory cost. If $M \geq D$, forward mode is more advantageous.

7.2   Feedforward networks

In the previous section, we derived forward-mode autodiff and reverse-mode autodiff for computation chains with an input $s_0 \in \mathcal{S}_0$. In this section, we now derive reverse-mode autodiff for feedforward networks, in which each layer f_k is now allowed to depend explicitly on some additional parameters $\boldsymbol{w}_k \in \mathcal{W}_k$. The recursion is

$$s_0 := \boldsymbol{x} \in \mathcal{S}_0$$
$$s_1 := f_1(\boldsymbol{s}_0, \boldsymbol{w}_1) \in \mathcal{S}_1$$
$$\vdots$$
$$s_K := f_K(\boldsymbol{s}_{K-1}, \boldsymbol{w}_K) \in \mathcal{S}_K$$
$$f(\boldsymbol{x}, \boldsymbol{w}) := \boldsymbol{s}_K,$$

where $\mathcal{S}_0 = \mathcal{X}$ and $\boldsymbol{w} = (\boldsymbol{w}_1, \ldots, \boldsymbol{w}_K) \in \mathcal{W}_1 \times \cdots \times \mathcal{W}_K$. Each f_k is now a function of two arguments. The first argument depends on the previous layer, but the second argument does not. This is illustrated in Fig. 7.5. We now explain how to differentiate a feedforward network.

7.2.1   Computing the adjoint

The function has the form $f \colon \mathcal{E} \to \mathcal{F}$, where $\mathcal{E} := \mathcal{X} \times (\mathcal{W}_1 \times \cdots \times \mathcal{W}_K)$ and $\mathcal{F} := \mathcal{S}_K$. From Section 2.3, we know that the VJP has the form $\partial f(\boldsymbol{x}, \boldsymbol{w})^* \colon \mathcal{F} \to \mathcal{E}$. Therefore, we want to be able to compute $\partial f(\boldsymbol{x}, \boldsymbol{w})^*[\boldsymbol{u}] \in \mathcal{E}$ for any $\boldsymbol{u} \in \mathcal{F}$.

  Fortunately, the backward recursion is only a slight modification of the computation chain case. Indeed, since $f_k \colon \mathcal{E}_k \to \mathcal{F}_k$, where $\mathcal{E}_k := \mathcal{S}_{k-1} \times \mathcal{W}_k$ and $\mathcal{F}_k := \mathcal{S}_k$, the intermediate VJPs have the form $\partial f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k)^* \colon \mathcal{F}_k \to \mathcal{E}_k$. We therefore arrive at the recursion

$$\boldsymbol{r}_K = \boldsymbol{u} \in \mathcal{S}_K$$
$$(\boldsymbol{r}_{K-1}, \boldsymbol{g}_K) = \partial f_K(\boldsymbol{s}_{K-1}, \boldsymbol{w}_K)^*[\boldsymbol{r}_K] \in \mathcal{S}_{K-1} \times \mathcal{W}_K$$
$$\vdots$$
$$(\boldsymbol{r}_0, \boldsymbol{g}_1) = \partial f_1(\boldsymbol{s}_0, \boldsymbol{w}_1)^*[\boldsymbol{r}_1] \in \mathcal{S}_0 \times \mathcal{W}_1.$$

The final output is

$$\partial f(\boldsymbol{x}, \boldsymbol{w})^*[\boldsymbol{u}] = (\boldsymbol{r}_0, (\boldsymbol{g}_1, \ldots, \boldsymbol{g}_K)).$$
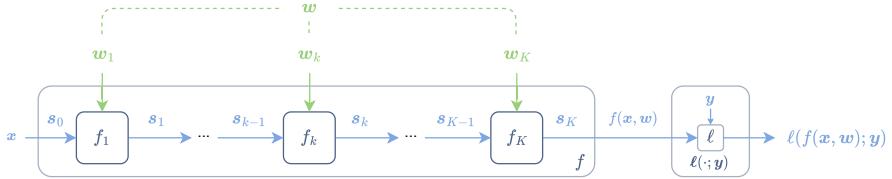
Figure 7.5: Computation graph of an MLP as a function of its parameters.

7.2.2 Computing the gradient

We often compose a network with a loss function

$$L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}) := \ell(f(\boldsymbol{x}, \boldsymbol{w}); \boldsymbol{y}) \in \mathbb{R}.$$

From Proposition 2.7, the gradient is given by

$$\nabla L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}) = (\boldsymbol{g}_1, \ldots, \boldsymbol{g}_K) \in \mathcal{W}_1 \times \cdots \times \mathcal{W}_K$$

where

$$\partial f(\boldsymbol{x}, \boldsymbol{w})^*[\boldsymbol{u}] = (\boldsymbol{r}_0, (\boldsymbol{g}_1, \ldots, \boldsymbol{g}_K)),$$

with $\boldsymbol{u} = \nabla\ell(f(\boldsymbol{x}, \boldsymbol{w}); \boldsymbol{y}) \in \mathcal{S}_K$. The output $\boldsymbol{r}_0 \in \mathcal{S}_0$, where $\mathcal{S}_0 = \mathcal{X}$, corresponds to the gradient w.r.t. $\boldsymbol{x} \in \mathcal{X}$ and is typically not needed, except in generative modelling settings. The full procedure is summarized in Algorithm 7.3.
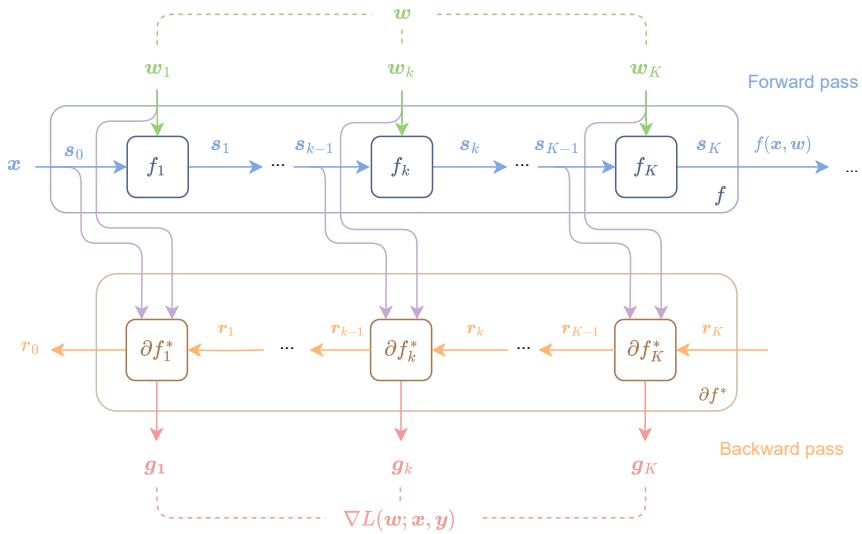
Figure 7.6: Reverse mode of automatic differentiation, a.k.a., gradient back-propagation to compute the gradient of the loss of an MLP on an input label pair. For readability, we denoted the intermediate VJPs as $\partial f_k^* : (\boldsymbol{s}_{k-1}, \boldsymbol{w}_{k-1}, \boldsymbol{r}_k) \mapsto \partial f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k)[\boldsymbol{r}_k]$ with $\partial f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k)[\boldsymbol{r}_k] = (\boldsymbol{r}_{k-1}, \boldsymbol{g}_k)$.

Algorithm 7.3 Gradient back-propagation for feedforward networks

---

    Functions: $f_1, \ldots, f_K$ in sequential order
    Inputs: data point $(\boldsymbol{x}, \boldsymbol{y}) \in \mathcal{X} \times \mathcal{Y}$
                 parameters $\boldsymbol{w} = (\boldsymbol{w}_1, \ldots \boldsymbol{w}_K) \in \mathcal{W}_1 \times \cdots \times \mathcal{W}_K$

1: Initialize $\boldsymbol{s}_0 := \boldsymbol{x}$ ▷ Forward pass
2: **for** $k := 1, \ldots, K$ **do**
3:        Compute and store $\boldsymbol{s}_k := f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k) \in \mathcal{S}_k$
4: Compute $\ell(\boldsymbol{s}_K; \boldsymbol{y})$ and $\boldsymbol{u} := \nabla\ell(\boldsymbol{s}_K; \boldsymbol{y}) \in \mathcal{S}_K$
5: Initialize $\boldsymbol{r}_K := \boldsymbol{u} \in \mathcal{S}_K$ ▷ Backward pass
6: **for** $k := K, \ldots, 1$ **do**
7:        Compute $(\boldsymbol{r}_{k-1}, \boldsymbol{g}_k) := \partial f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k)^*[\boldsymbol{r}_k] \in \mathcal{S}_{k-1} \times \mathcal{W}_k$
8: **Outputs:** $L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}) := \ell(\boldsymbol{s}_K; \boldsymbol{y}), \nabla L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}) = (\boldsymbol{g}_1, \ldots, \boldsymbol{g}_K)$

Algorithm 7.4 Forward-mode autodiff for computation graphs

    Functions: $f_1, \ldots, f_K$ in topological order
    Inputs: input $\boldsymbol{s}_0 \in \mathcal{S}_0$, input direction $\boldsymbol{v} \in \mathcal{S}_0$
1: Initialize $\boldsymbol{t}_0 := \boldsymbol{v}$
2: **for** $k := 1, \ldots, K$ **do** $\triangleright$ Forward pass
3:     Retrieve parent nodes $i_1, \ldots, i_{p_k} := \text{parents}(k)$
4:     Compute $\boldsymbol{s}_k := f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})$
5:     Compute

$$\boldsymbol{t}_k := \partial f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})[\boldsymbol{t}_{i_1}, \ldots, \boldsymbol{t}_{i_{p_k}}]$$
$$= \sum_{j=1}^{p_k} \partial_j f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})[\boldsymbol{t}_{i_j}].$$

6: **Outputs:** $f(\boldsymbol{s}_0) := \boldsymbol{s}_K, \; \partial f(\boldsymbol{s}_0)[\boldsymbol{v}] = \boldsymbol{t}_K$

7.3 Computation graphs

In the previous sections, we reviewed autodiff for computation chains and its extension to feedforward networks. In this section, we generalize autodiff to computation graphs introduced in Section 4.1.3.

7.3.1 Forward-mode

The forward mode corresponds to computing a JVP in an input direction $\boldsymbol{v} \in \mathcal{S}_0$. The algorithm consists in computing intermediate JVPs along the forward pass. We initialize $\boldsymbol{t}_0 := \boldsymbol{v} \in \mathcal{S}_0$. Using Proposition 2.8, the derivatives on iteration $k \in [K]$ are propagated as

$$\boldsymbol{t}_k := \partial f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})[\boldsymbol{t}_{i_1}, \ldots, \boldsymbol{t}_{i_{p_k}}]$$
$$= \sum_{j=1}^{p_k} \partial_j f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})[\boldsymbol{t}_{i_j}],$$

where $i_1, \ldots, i_{p_k} = \text{parents}(k)$. The final output is $\partial f(\boldsymbol{s}_0)[\boldsymbol{v}] = \boldsymbol{t}_K$. The resulting generic forward-mode autodiff is summarized in Algorithm 7.4. Although not explicitly mentioned, we can release $\boldsymbol{s}_k$ and $\boldsymbol{t}_k$ from memory when no child node depends on node k.

7.3.2   Reverse-mode

The reverse mode corresponds to computing a VJP in an output direction $\boldsymbol{u} \in \mathcal{S}_K$. We first perform a forward pass to compute the intermediate values and store the corresponding VJP as a pointer, since the VJP shares some computations with the function itself. From Proposition 2.8, the VJP returns a tuple with the same length as the number of inputs to the function:

$$\boldsymbol{\delta}_{i_1,k}, \ldots, \boldsymbol{\delta}_{i_{p_k},k} = \partial f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})^*[\boldsymbol{r}_k].$$

After the forward pass, we traverse the graph in reverse topological order as illustrated in Fig. 7.7. If an intermediate value $\boldsymbol{s}_k$ is used by later functions $f_{j_1}, \ldots, f_{j_{c_k}}$ for $j_1, \ldots, j_{c_k} = \text{children}(k)$, the derivatives with respect to $\boldsymbol{s}_k$ need to sum all the variations through the f_j functions in a variable $\boldsymbol{r}_k$,

$$\boldsymbol{r}_k := \sum_{j \in \{j_1, \ldots, j_{c_k}\}} \boldsymbol{\delta}_{k,j}.$$

In practice, as we go backward through the computation graph, we can accumulate the VJPs corresponding to node k by doing in-place updates of the $\boldsymbol{r}_k$ values. The topological ordering ensures that $\boldsymbol{r}_k$ has been fully computed when we reach node k. The resulting generic reverse-mode autodiff is presented in Algorithm 7.5.

7.3.3   Complexity, the Baur-Strassen theorem

For computing the gradient of a function $f \colon \mathcal{E} \to \mathbb{R}$ represented by a computation graph, we saw that the reverse mode is more efficient than the forward mode. As we previously stated, assuming that the elementary functions f_k in the DAG and their VJP have roughly the same computational complexity, then f and ∇f have roughly the same computational complexity. This fact is crucial and is the pillar on which modern machine learning relies: it allows us to optimize high-dimensional functions by gradient descent.

For arithmetic circuits, reviewed in Section 4.1.4, this crucial fact is made more precise in the celebrated Baur-Strassen theorem (Baur and Strassen, 1983). If f is a polynomial, then so is its gradient ∇f.

Algorithm 7.5 Reverse-mode autodiff for computation graphs

    Functions: $f_1, \ldots, f_K$ in topological order
    Inputs: input $\boldsymbol{s}_0 \in \mathcal{S}_0$, output direction $\boldsymbol{u} \in \mathcal{S}_K$
1: **for** $k := 1, \ldots, K$ **do**   ▷ Forward pass
2:      Retrieve parent nodes $i_1, \ldots, i_{p_k} := \text{parents}(k)$
3:      Compute $\boldsymbol{s}_k := f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})$
4:      Instantiate VJP $\boldsymbol{l}_k := \partial f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})^*$
5: Initialize $\boldsymbol{r}_K := \boldsymbol{u}$, $\boldsymbol{r}_k := 0 \ \forall k \in \{0, \ldots, K-1\}$ ▷ Backward pass
6: **for** $k := K, \ldots, 1$ **do**
7:      Retrieve parent nodes $i_1, \ldots, i_{p_k} = \text{parents}(k)$
8:      Compute $\boldsymbol{\delta}_{i_1,k}, \ldots, \boldsymbol{\delta}_{i_{p_k},k} := \boldsymbol{l}_k[\boldsymbol{r}_k]$
9:      Compute $\boldsymbol{r}_{i_j} \leftarrow \boldsymbol{r}_{i_j} + \boldsymbol{\delta}_{i_j,k} \ \forall j \in \{1, \ldots, p_k\}$
10: **Outputs:** $f(\boldsymbol{s}_0) := \boldsymbol{s}_K$, $\partial f(\boldsymbol{s}_0)^*[\boldsymbol{u}] = \boldsymbol{r}_0$

The theorem gives a lower bound on the size of the best circuit for computing ∇f from the size of the best circuit for computing f.

> **Proposition 7.1** (Baur-Strassen's theorem). For any polynomial $f \colon \mathcal{E} \to \mathbb{R}$, we have
> $$S(\nabla f) \leq 5 \cdot S(f),$$
> where $S(f)$ is defined in Definition 4.1.

A simpler proof by backward induction was given by Morgenstern (1985). See also the proof of Theorem 9.10 in Chen *et al.* (2011). For general computation graphs, that have more primitive functions than just $+$ and $\times$, a similar result can be obtained; see, e.g., (Bolte *et al.*, 2022, Theorem 2).

7.4 Implementation

7.4.1 Primitive functions

An autodiff system implements a set $\mathcal{A}$ of primitive or elementary functions, which serve as building blocks for creating other functions, by function composition. For instance, we saw that in arithmetic circuits
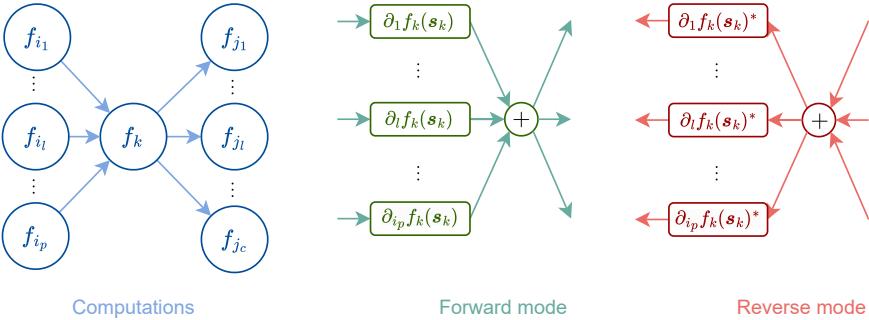
Figure 7.7: Left: Assuming a topological order, the computation of f_k on iteration k involves p_k inputs computed by $f_{i_1}, \ldots, f_{i_{p_k}}$, where $\{i_1, \ldots, i_{p_k}\} = \text{parents}(k)$, and is used in c_k functions $f_{j_1}, \ldots, f_{j_{c_k}}$, where $\{j_1, \ldots, j_{c_k}\} = \text{children}(k)$. **Middle:** Forward-mode autodiff on iteration k, denoting the shorthand $\boldsymbol{s}_k^p \coloneqq (\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})$. This computes $\partial_i f_k(\boldsymbol{s}_k^p)[\boldsymbol{t}_{i_j}]$ for incoming $\boldsymbol{t}_{i_j}$, $j = 1, \ldots, p_k$, then sum these results to pass $\boldsymbol{t}_k$ to the next iterations. **Right:** Reverse-mode autodiff on iteration k. As we traverse the graph backward, we first sum the contributions coming from each child computation $f_{j_1}, \ldots, f_{j_{c_k}}$ for $\{j_1, \ldots, j_{c_k}\} = \text{children}(k)$ to get $\boldsymbol{r}_k$. We then feed this $\boldsymbol{r}_k$ to each $\partial_i f_k(\boldsymbol{s}_k^p)$ and continue the procedure in reverse topological order.

(Section 4.1.4), $\mathcal{A} = \{+, \times\}$. More generally, $\mathcal{A}$ may contain all the necessary functions for expressing programs. We emphasize, however, that $\mathcal{A}$ is not necessarily restricted to low-level functions such as log and exp, but may also contain higher-level functions. For instance, even though the log-sum-exp can be expressed as the composition of elementary operations (log, sum, exp), it is usually included as a primitive on its own, both because it is a very commonly-used building block, but also for numerical stability reasons.

7.4.2   Closure under function composition

Each function f_k in a computation graph belongs to a set $\mathcal{F}$, the class of functions supported by the system. A desirable property of an autodiff implementation is that the set $\mathcal{F}$ is **closed** under function composition, meaning that if $f \in \mathcal{F}$ and $g \in \mathcal{F}$, then $f \circ g \in \mathcal{F}$. This means that composed functions can themselves be used for composing new functions. This property is also crucial for supporting higher-order differentiation (Chapter 8) and automatic linear transposition (Section 7.4.4). When

f_k is a composition of elementary functions in $\mathcal{A}$, then f_k itself is a **nested** DAG. However, we can always **inline** each composite function, such that all functions in the DAG belong to $\mathcal{A}$.

7.4.3 Examples of JVPs and VJPs

An autodiff system must implement for each $f \in \mathcal{A}$ its JVP for supporting the forward mode, and its VJP for supporting the reverse mode. We give a couple of examples. We start with the JVP and VJP of linear functions.

Example 7.2 (JVP and VJP of linear functions). Consider the matrix-vector product $f(\boldsymbol{W}) = \boldsymbol{W}\boldsymbol{x} \in \mathbb{R}^M$, where $\boldsymbol{x} \in \mathbb{R}^D$ is fixed and $\boldsymbol{W} \in \mathbb{R}^{M \times D}$. As already mentioned, the JVP of f at $\boldsymbol{W} \in \mathbb{R}^{M \times D}$ along an input direction $\boldsymbol{V} \in \mathbb{R}^{M \times D}$ is simply

$$\partial f(\boldsymbol{W})[\boldsymbol{V}] = f(\boldsymbol{V}) = \boldsymbol{V}\boldsymbol{x} \in \mathbb{R}^M.$$

To find the associated VJP, we note that for any $\boldsymbol{u} \in \mathbb{R}^M$ and $\boldsymbol{V} \in \mathbb{R}^{M \times D}$, we must have $\langle \partial f(\boldsymbol{W})[\boldsymbol{V}], \boldsymbol{u} \rangle = \langle \boldsymbol{V}, \partial f(\boldsymbol{W})^*[\boldsymbol{u}] \rangle$. Using the properties of the trace, we have

$$\langle \partial f(\boldsymbol{W})[\boldsymbol{V}], \boldsymbol{u} \rangle = \langle \boldsymbol{V}\boldsymbol{x}, \boldsymbol{u} \rangle = \mathrm{tr}(\boldsymbol{x}^\top \boldsymbol{V}^\top \boldsymbol{u}) = \langle \boldsymbol{V}, \boldsymbol{u}\boldsymbol{x}^\top \rangle.$$

Therefore, we find that the VJP is given by

$$\partial f(\boldsymbol{W})^*[\boldsymbol{u}] = \boldsymbol{u}\boldsymbol{x}^\top \in \mathbb{R}^{M \times D}.$$

Similarly, consider now a matrix-matrix product $f(\boldsymbol{W}) = \boldsymbol{W}\boldsymbol{X}$, where $\boldsymbol{W} \in \mathbb{R}^{M \times D}$ and where $\boldsymbol{X} \in \mathbb{R}^{D \times N}$ is fixed. The JVP at $\boldsymbol{W} \in \mathbb{R}^{M \times D}$ along an input direction $\boldsymbol{V} \in \mathbb{R}^{M \times D}$ is simply

$$\partial f(\boldsymbol{W})[\boldsymbol{V}] = f(\boldsymbol{V}) = \boldsymbol{V}\boldsymbol{X} \in \mathbb{R}^{M \times N}.$$

The VJP along the output direction $\boldsymbol{U} \in \mathbb{R}^{M \times N}$ is

$$\partial f(\boldsymbol{W})^*[\boldsymbol{U}] = \boldsymbol{U}\boldsymbol{X}^\top \in \mathbb{R}^{M \times D}.$$

Another simple example are element-wise separable functions.

Example 7.3 (JVP and VJP of separable function). Consider the function $f(\boldsymbol{w}) \coloneqq (g_1(w_1), \ldots, g_P(w_P))$, where each $g_i \colon \mathbb{R} \to \mathbb{R}$ has a derivative g_i'. The Jacobian matrix is then a diagonal matrix

$$\partial f(\boldsymbol{w}) = \mathbf{diag}(g_1'(w_1), \ldots, g_P'(w_P)) \in \mathbb{R}^{P \times P}.$$

In this case, the JVP and VJP are actually the same

$$\partial f(\boldsymbol{w})[\boldsymbol{v}] = \partial f(\boldsymbol{w})^*[\boldsymbol{v}] = (g_1'(w_1), \ldots, g_P'(w_P)) \odot \boldsymbol{v},$$

where $\odot$ indicates element-wise multiplication.

7.4.4   Automatic linear transposition

On first sight, if we want to support both forward ans reverse modes, it appears like we need to implement both the JVP and the VJP for each primitive operation $f \in \mathcal{A}$. Fortunately, there exists a way to recover VJPs from JVPs, and vice-versa.

We saw in Section 2.3 that if $l(\boldsymbol{w})$ is a linear map, then its JVP is $\partial l(\boldsymbol{w})[\boldsymbol{v}] = l(\boldsymbol{v})$ (independent of $\boldsymbol{w}$). Conversely, the VJP is $\partial l(\boldsymbol{w})^*[\boldsymbol{u}] = l^*(\boldsymbol{u})$, where l^* is the adjoint operator of l (again, independent of $\boldsymbol{w}$).

Let us define $l(\boldsymbol{u}; \boldsymbol{w}) \coloneqq \partial f(\boldsymbol{w})^*[\boldsymbol{u}]$, i.e., the VJP of f in the output direction $\boldsymbol{u}$. Since $l(\boldsymbol{u}; \boldsymbol{w})$ is linear in $\boldsymbol{u}$, we can apply the reasoning above to compute its VJP

$$\partial l(\boldsymbol{u}; \boldsymbol{w})^*[\boldsymbol{v}] = l^*(\boldsymbol{v}; \boldsymbol{w}) = \partial f(\boldsymbol{w})^{**}[\boldsymbol{v}] = \partial f(\boldsymbol{w})[\boldsymbol{v}],$$

which is independent of $\boldsymbol{u}$. In words, the VJP of a VJP is the corresponding JVP! This means that we can implement forward-mode autodiff even if we only have access to VJPs. As an illustration and sanity check, we give the following example.

Example 7.4 (Automatic transpose of "dot"). If we define $f(\boldsymbol{x}, \boldsymbol{W}) \coloneqq \boldsymbol{W}\boldsymbol{x}$, from Example 7.2, we know that

$$\begin{aligned}
\partial f(\boldsymbol{x}, \boldsymbol{W})^*[\boldsymbol{u}] &= (\boldsymbol{W}^\top \boldsymbol{u}, \boldsymbol{u}\boldsymbol{x}^\top) \\
&= (f(\boldsymbol{u}, \boldsymbol{W}^\top), f(\boldsymbol{x}^\top, \boldsymbol{u})) \\
&\eqqcolon l(\boldsymbol{u}; \boldsymbol{x}, \boldsymbol{W}).
\end{aligned}$$

Using Proposition 2.9, we obtain

$$
\begin{aligned}
\partial l(\boldsymbol{u}; \boldsymbol{x}, \boldsymbol{W})^*[\boldsymbol{v}, \boldsymbol{V}] &= f(\boldsymbol{v}, \boldsymbol{W}) + f(\boldsymbol{x}, \boldsymbol{V}) \\
&= \boldsymbol{W}\boldsymbol{v} + \boldsymbol{V}\boldsymbol{x} \\
&= \partial f(\boldsymbol{x}, \boldsymbol{W})[\boldsymbol{v}, \boldsymbol{V}].
\end{aligned}
$$

The other direction, automatically creating a VJP from a JVP, is also possible but is more technical and relies on the notion of **partial evaluation** (Frostig *et al.*, 2021; Radul *et al.*, 2022).

7.5 Checkpointing

We saw that forward-mode autodiff can release intermediate computations from memory along the way, while reverse-mode autodiff needs to cache all of them. This means that the memory complexity of reverse-mode autodiff, in its standard form, grows linearly with the number of nodes in the computation graph. A commonly-used technique to circumvent this issue is checkpointing, which trades-off computation time for better memory usage. Checkpointing works by selectively storing only a subset of the intermediate nodes, called **checkpoints**, and by computing others on-the-fly. The specific choice of the checkpoint locations in the computation graph determines the memory-computation trade-off. While it is possible to heuristically set checkpoints at user-specified locations, it is also possible to perform a checkpointing strategy algorithmically, as studied in-depth by Griewank (1992) and Griewank and Walther (2008). In this section, we review two such algorithms: recursive halving and dynamic programming (divide-and-conquer). Our exposition focuses on computation chains $f = f_K \circ \ldots \circ f_1$ with $f_i : \mathbb{R}^D \to \mathbb{R}^D$ for simplicity.

Computational and memory complexities at two extremes. Let $\mathcal{C}(K)$ be the number of calls to the individual functions f_i (we ignore the cost of computing the intermediate VJPs) and $\mathcal{M}(K)$ be the number of function inputs cached, when performing reverse-mode autodiff on a chain $f = f_K \circ \ldots \circ f_1$. On one extreme, if we store all intermediate computations, as done in Algorithm 7.1, to compute only the VJP

Algorithm 7.6 Reverse-mode autodiff with constant memory
`vjp_full_recompute`$(f_K \circ \ldots \circ f_1, s_0, u) := \partial(f_K \circ \ldots \circ f_1)(s_0)^*[u]$

Inputs: Chain $f_K \circ \ldots \circ f_1$, input $s_0 \in \mathcal{S}_0$, output direction $u \in \mathcal{S}_K$

1: **if** $K = 1$ **then**
2:     **return** $\partial f_1(s_0)^*[u]$
3: **else**
4:     Set $r_K = u$
5:     **for** $k := K, \ldots, 1$ **do**
6:         Compute $s_{k-1} = (f_{k-1} \circ \ldots \circ f_1)(s_0)$
7:         Compute $r_{k-1} = \partial f_k(s_{k-1})^*[r_k]$
8:     **return:** r_0

$\partial f(s_0)^*[u]$, we have

$$\mathcal{C}(K) = K - 1 \quad \text{and} \quad \mathcal{M}(K) = K.$$

This is optimal w.r.t. computational complexity, but suboptimal w.r.t. memory. On the other extreme, if we only store the initial input, as done in Algorithm 7.6, then we have

$$\mathcal{C}(K) = K(K-1)/2 \quad \text{and} \quad \mathcal{M}(K) = 1.$$

This is optimal w.r.t. memory but leads to a computational complexity that is quadratic in K.

7.5.1 Recursive halving

As a first step towards obtaining a better computation-memory trade-off, we may split the chain $s_K = f_K \circ \cdots \circ f_1(s_0)$ as

$$s_{K/2} = f_{K/2} \circ \ldots \circ f_1(s_0)$$
$$s_K = f_K \circ \ldots \circ f_{K/2+1}(s_{K/2}),$$

for K even. Then, rather than recomputing all intermediate computations s_k from the input s_0 as in Algorithm 7.6, we can store $s_{K/2}$ and recompute s_k for $k > K/2$ starting from $s_{K/2}$. Formally, this strategy amounts to the follwoing steps.

1. Compute $s_{K/2} = f_{K/2} \circ \ldots \circ f_1(s_0)$

Algorithm 7.7 Reverse-mode autodiff with recursive halving

$\mathtt{vjp\_halving}(f_K \circ \ldots \circ f_1, \boldsymbol{s}_0, \boldsymbol{u}) := \partial(f_K \circ \ldots \circ f_1)(\boldsymbol{s}_0)^*[\boldsymbol{u}]$

    Functions: Chain $f_K \circ \ldots \circ f_1$

    Inputs: input $\boldsymbol{s}_0 \in \mathcal{S}_0$, output direction $\boldsymbol{u} \in \mathcal{S}_K$

1: **if** $K = 1$ **then**

2:     **return** $\partial f_1(\boldsymbol{s}_0)^*[\boldsymbol{u}]$

3: **else**

4:     Compute $\boldsymbol{s}_{K/2} = f_{K/2} \circ \ldots \circ f_1(\boldsymbol{s}_0)$

5:     Compute $\boldsymbol{r}_{K/2} = \mathtt{vjp\_halving}(f_K \circ \ldots \circ f_{K/2+1}, \boldsymbol{s}_{K/2}, \boldsymbol{u})$

6:     Compute $\boldsymbol{r}_0 = \mathtt{vjp\_halving}(f_{K/2} \circ \ldots \circ f_1, \boldsymbol{s}_0, \boldsymbol{r}_{K/2})$

7:     **return:** $\boldsymbol{r}_0$

---

  2. Compute $\boldsymbol{r}_{K/2} = \mathtt{vjp\_full\_recompute}(f_K \circ \ldots \circ f_{K/2+1}, \boldsymbol{s}_{K/2}, \boldsymbol{u})$

  3. Compute $\boldsymbol{r}_0 = \mathtt{vjp\_full\_recompute}(f_{K/2} \circ \ldots \circ f_1, \boldsymbol{s}_0, \boldsymbol{r}_{K/2})$

At the expense of having to store the additional checkpoint $\boldsymbol{s}_{K/2}$, this already roughly halves the computational complexity compared to Algorithm 7.6.

We can then apply this reasoning recursively, as formalized in Algorithm 7.7. The algorithm is known as **recursive binary schedule** (Griewank, 2003) and illustrated in Fig. 7.8. In terms of number of function evaluations $\mathcal{C}(K)$, for K even, we make $K/2$ function calls, and we call the procedure recursively twice, that is,

$$\mathcal{C}(K) = 2\mathcal{C}(K/2) + K/2.$$

If the chain is of length 1, we directly use the VJP, so $\mathcal{C}(1) = 0$. Hence, the numbers of function calls, if K is a power of 2, is

$$\mathcal{C}(K) = \frac{K}{2} \log_2 K.$$

In terms of memory usage, Algorithm 7.7 uses $\boldsymbol{s}_0$ not only at line 4 but also at line 6. So when the algorithm is called recursively on the second half of the chain at line 5, one memory slot is taken by $\boldsymbol{s}_0$. This line is called recursively until the chain is reduced to a single function. At that point, the total number of memory slots used is equal to the
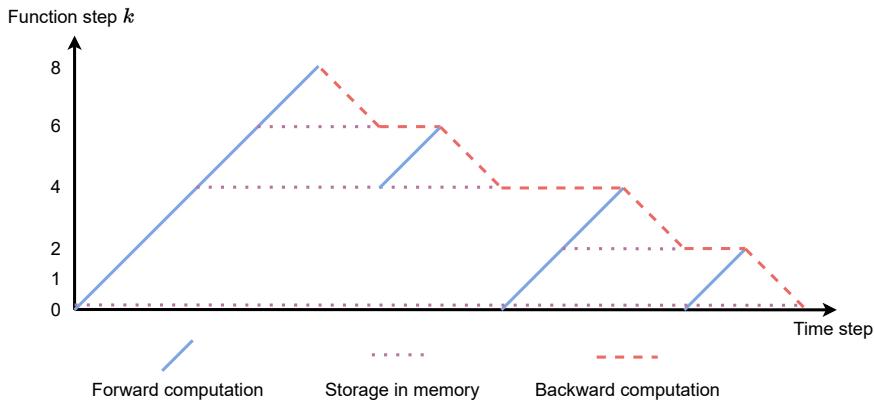
Figure 7.8: Illustration of checkpointing with recursive halving, for a chain of 8 functions. The chain is first fully evaluated while storing some computations as checkpoints in memory. Then, during the backward pass, we recompute some intermediate values from the latest checkpoint available. In contrast, vanilla reverse-mode autodiff (with full caching of the intermediate computations) would lead to a simple triangle shape.

number of times we split the function in half, that is $\log_2 K$ for K a power of 2. On the other hand, the input s_0 is no longer used after line 6 of Algorithm 7.7. At that line, the memory slot taken by s_0 can be consumed by the recursive call on the first-half. In other words, calling the algorithm recursively on the first half does not incur extra memory cost. So if K is a power of 2, the memory cost of Algorithm 7.7 is

$$\mathcal{M}(K) = \log_2 K.$$

7.5.2 Dynamic programming

Recursive halving requires $\log_2 K$ memory slots for a chain of length K. However, as illustrated in Fig. 7.8, at a given time step, all memory slots may not be exploited.

To optimize the approach, we observe that recursive halving is just one instance of a program that splits the chain and calls itself recursively on each part. In other words, it is a form of **divide-and-conquer** algorithm. Rather than splitting the chain in half, we may consider splitting the chain at some index l. One split is used to reverse

the computations from $l+1$ to K by a recursive call that consumes one memory slot. The other split is used on a recursive call that reverses the computations from 0 to l. That second call does not require an additional memory slot, as it can use directly the memory slot used by the original input s_0. To split the chain in such two parts, we need l intermediate computations to go from s_0 to s_l. The computational complexity $\mathcal{C}(k, s)$, counted as the number of function evaluations, for a chain of length k with s memory slots then satisfies the recurrence

$$\mathcal{C}(k, s) = \mathcal{C}(k - l, s - 1) + \mathcal{C}(l, s) + l,$$

for all $l \in \{1, \ldots, k - 1\}$. By simply taking $l = k/2$, we recover exactly the computational complexity of recursive halving. To refine the latter, we may split the chain by selecting l to minimize the complexity. An optimal scheme must satisfy the recursive equation,

$$\mathcal{C}^*(k, s) \coloneqq \min_{1 \leq l \leq K-1} \{\mathcal{C}^*(k - l, s - 1) + \mathcal{C}^*(l, s) + l\}. \qquad (7.3)$$

Note that $\mathcal{C}^*(K, S)$ can be computed from $\mathcal{C}^*(k, s)$ for $k = 1, \ldots, K - 1$, $s = 1, \ldots, S - 1$. This suggests a **dynamic programming** approach to find an optimal scheme algorithmically. For a chain of length $k = 1$, the cost is null as we directly reverse the computation, so $\mathcal{C}^*(1, s) \coloneqq 0$. On the other hand for a memory $s = 1$, there is only one possible scheme that saves only the initial input as in Algorithm 7.6, so $\mathcal{C}^*(k, 1) \coloneqq (k(k - 1))/2$. The values $\mathcal{C}^*(k, s)$ can then be computed incrementally from $k = 1$ to K and $s = 1$ to S using Eq. (7.3). The optimal splits can be recorded along the way as

$$l^*(k, s) \coloneqq \arg\min_{1 \leq l \leq k-1} \{\mathcal{C}^*(k - l, s - 1) + \mathcal{C}^*(l, s) + l\}.$$

The optimal split for K, S can then be found by **backtracking** the optimal splits along both branches corresponding to $\mathcal{C}^*(k - l, s - 1)$ and $\mathcal{C}^*(l, s)$. As the final output consists in traversing a binary tree, it was called **treeverse** (Griewank, 1992). Note that the dynamic programming procedure is generic and could a priori incorporate varying computational costs for the intermediate functions f_k.

Analytical formula

It turns out that we can also find an optimal scheme *analytically*. This scheme was found by Griewank (1992), following the analysis of optimal inversions of sequential programs by divide-and-conquer algorithms done by Grimm *et al.* (1996); see also Griewank (2003, Section 6) for a simple proof. The main idea consists in considering the number of times an evaluation step f_k is repeated. As we split the chain at l, all steps from 1 to l will be repeated at least once. In other words, treating the second half of the chain incurs one memory cost, while treating the first half of the chain incurs one repetition cost. Griewank (1992) shows that for fixed K, S, we can find the minimal number of repetitions analytically and build the corresponding scheme with simple formulas for the optimal splits.

Compared to the dynamic programming approach, it means that we do not need to compute the pointers $l^*(k, s)$, and we can use a simple formula to set $l^*(k, s)$. We still need to traverse the corresponding binary tree given K, S and the $l^*(k, s)$ to obtain the schedules. Note that such optimal scheme does not take into account varying computational costs for the functions f_k.

7.5.3 Online checkpointing

The optimal scheme presented above requires knowing the total number of nodes in the computation graph ahead of time. However, when differentiating through for example a while loop (Section 5.10), this is not the case. To circumvent this issue, online checkpointing schemes have been developed and proven to be nearly optimal (Stumm and Walther, 2010; Wang *et al.*, 2009). These schemes start by defining a set of S checkpoints with the first S computations, then these checkpoints are rewritten dynamically as the computations keep going. Once the computations terminate, the optimal approach presented above for a fixed length is applied on the set of checkpoints recorded.

Algorithm 7.8 Reverse-mode autodiff for reversible chains.

Functions: $f := f_K \circ \ldots \circ f_1$, with each f_k invertible

Inputs: input $\boldsymbol{s}_0 \in \mathcal{S}_0$, output direction $\boldsymbol{u} \in \mathcal{S}_K$

1: Compute $\boldsymbol{s}_K = f_K \circ \ldots \circ f_1(\boldsymbol{s}_0)$
2: **for** $k := K, \ldots, 1$ **do**
3:     Compute $\boldsymbol{s}_{k-1} = f_k^{-1}(\boldsymbol{s}_k)$
4:     Compute $\boldsymbol{r}_{k-1} = \partial f_k(\boldsymbol{s}_{k-1})^*[\boldsymbol{r}_k]$

Outputs: $f(\boldsymbol{s}_0) := \boldsymbol{s}_K$, $\partial f(\boldsymbol{s}_0)^*[\boldsymbol{u}] = \boldsymbol{r}_0$

7.6 Reversible layers

7.6.1 General case

The memory requirements of reverse-mode autodiff can be completely alleviated when the functions f_k are invertible (meaning that f_k^{-1} exists) and when f_k^{-1} is easily accessible. In that case, rather than storing the intermediate computations $\boldsymbol{s}_{k-1}$, necessary to compute the VJP $\boldsymbol{r}_k \mapsto \partial f_k(\boldsymbol{s}_{k-1})^*[\boldsymbol{r}_k]$, one can compute them on the fly during the backward pass from $\boldsymbol{s}_k$ using $\boldsymbol{s}_{k-1} = f_k^{-1}(\boldsymbol{s}_k)$. We summarize the procedure for the case of computation chains in Algorithm 7.8. Compared to vanilla reverse-mode autodiff in Algorithm 7.2, the algorithm has optimal memory complexity, as we can release $\boldsymbol{s}_k$ and $\boldsymbol{r}_k$ as we go.

In practice, f_k^{-1} often does not exist or may not be easily accessible. However, network architectures can be constructed to be easily invertible by design. Examples include reversible residual networks (Gomez *et al.*, 2017), orthonormal RNNs (Helfrich *et al.*, 2018), neural ODEs (Section 11.6), and momentum residual neural networks (Sander *et al.*, 2021a); see also references therein.

7.6.2 Case of orthonormal JVPs

When the JVP of each f_k is an orthonormal linear mapping, i.e.,

$$\partial f_k(\boldsymbol{s}_{k-1})^{-1} = \partial f_k(\boldsymbol{s}_{k-1})^*,$$

it is easy to check that the VJP of $f = f_K \circ \ldots \circ f_1$ is equal to the JVP of $f^{-1} = f_1^{-1} \circ \ldots \circ f_K^{-1}$, that is

$$\partial f(s_0)^*[u] = \partial f^{-1}(s_K)[u].$$

In other words, in the case of orthormal JVPs, reverse-mode autodiff of f coincides with forward-mode autodiff of f^{-1}.

7.7   Randomized forward-mode estimator

Forward-mode autodiff does not require to store intermediate activations. However, for a function $f \colon \mathbb{R}^P \to \mathbb{R}$, computing the gradient ∇f using forward-mode autodiff requires P JVPs, which is intractable if P is large. Can we approximate ∇f with fewer JVPs? The following proposition gives an **unbiased estimator** of ∇f that only involves JVPs.

> **Proposition 7.2** (Unbiased forward-mode estimator of the gradient).
> Let $f \colon \mathbb{R}^P \to \mathbb{R}$ be a differentiable function. Then,
>
> $$\begin{aligned} \nabla f(\boldsymbol{\mu}) &= \mathbb{E}_{Z \sim p}\left[\partial f(\boldsymbol{\mu})[Z]Z\right] \\ &= \mathbb{E}_{Z \sim p}\left[\langle \nabla f(\boldsymbol{\mu}), Z \rangle Z\right]. \end{aligned}$$
>
> where $p \coloneqq \mathrm{Normal}(0,1)^P$ is the isotropic Gaussian distribution.

This estimator is for instance used by Baydin *et al.* (2022). It can be seen as the **zero-temperature limit** of the gradient of a perturbed function, estimated by the score-function estimator (SFE); see Section 13.4.6.

In practice, the expectation above can be approximated by drawing M noise vectors $z_1, \ldots, z_M$, and averaging $\langle \nabla f(\boldsymbol{\mu}), z_i \rangle$ over $i \in [M]$.

A word of caution: while this estimator can be useful for example when we do not want to store the intermediate activations for memory reasons, this of course comes at the cost of increasing the variance, which influences the convergence rate of SGD, as seen in Section 15.2.

7.8   Summary

Computer programs can be seen as **directed acyclic graphs**, where nodes correspond to the output of intermediate operations in the pro-

gram, and edges represent the dependences of current operations on past operations.

Automatic differentiation (autodiff) for a function $f \colon \mathbb{R}^P \to \mathbb{R}^M$ has two main modes: **forward mode** and **reverse mode**. The forward mode: i) uses JVPs, ii) builds the Jacobian one column at a time, iii) is efficient for tall Jacobians ($M \geq P$), iv) need not store intermediate computations. The reverse mode: i) uses VJPs, builds the Jacobian one row at a time, iii) is efficient for wide Jacobians ($P \geq M$), iv) needs to store intermediate computations, in order to be computationally optimal. To trade computational efficiency for better memory efficiency, we can use **checkpointing** techniques.

We saw that the complexity of computing the gradient of a function $f \colon \mathbb{R}^P \to \mathbb{R}$ using the reverse mode is at most a constant time bigger than that of evaluating the function itself. This is the **Baur-Strassen theorem**, in arithmetic circuits. This astonishing result is one of the pillars of modern machine learning.

8

Second-order automatic differentiation

We review in this chapter how to perform automatic differentiation for second-order derivatives.

8.1 Hessian-vector products

We consider in this section a function $f \colon \mathcal{E} \to \mathbb{R}$. Similarly to the Jacobian, for most purposes, we do not need access to the full Hessian but rather to the Hessian-vector product (HVP) $\nabla^2 f(\boldsymbol{w})[\boldsymbol{v}]$ at $\boldsymbol{w} \in \mathcal{E}$, in a direction $\boldsymbol{v} \in \mathcal{E}$, as defined in Definition 2.18. The latter can be computed in four different ways, depending on how we combine the two main modes of autodiff.

8.1.1 Four possible methods

An HVP can be computed in four different ways.

1. **Reverse on reverse:** The Hessian can be seen as the transposed Jacobian of the gradient, hence the HVP can be computed as the **VJP of the gradient**,

$$\nabla^2 f(\boldsymbol{w})[\boldsymbol{v}] = \partial(\nabla f)(\boldsymbol{w})^*[\boldsymbol{v}].$$

2. **Forward on reverse:** Owing to its symmetry (see Proposition 2.10), the Hessian can also be seen as the Jacobian of the gradient, hence the HVP can be computed as the **JVP of the gradient**,

$$\nabla^2 f(\boldsymbol{w})[\boldsymbol{v}] = \partial(\nabla f)(\boldsymbol{w})[\boldsymbol{v}].$$

3. **Reverse on forward:** Recall that for any function $g\colon \mathcal{E} \to \mathcal{E}$, the VJP can equivalently be defined as the gradient along an output direction $\boldsymbol{v} \in \mathcal{E}$, that is,

$$\partial g(\boldsymbol{w})^*[\boldsymbol{v}] = \nabla\langle g, \boldsymbol{v}\rangle(\boldsymbol{w}),$$

where we recall the shorthand $\langle g, \boldsymbol{v}\rangle(\boldsymbol{w}) := \langle \boldsymbol{v}, g(\boldsymbol{w})\rangle$, so that $\langle g, \boldsymbol{v}\rangle$ is a function of $\boldsymbol{w}$. In our case, we can therefore rewrite the reverse-on-reverse approach as

$$\partial(\nabla f)(\boldsymbol{w})^*[\boldsymbol{v}] = \nabla\langle \nabla f, \boldsymbol{v}\rangle(\boldsymbol{w}).$$

We know that $\langle \nabla f, \boldsymbol{v}\rangle(\boldsymbol{w}) = \langle \nabla f(\boldsymbol{w}), \boldsymbol{v}\rangle = \partial f(\boldsymbol{w})[\boldsymbol{v}]$ is the JVP of f at $\boldsymbol{w}$ along $\boldsymbol{v}$. Therefore, we can also compute the HVP as the **gradient of the JVP** of f at $\boldsymbol{w}$ along $\boldsymbol{v}$,

$$\nabla^2 f(\boldsymbol{w})[\boldsymbol{v}] = \nabla(\partial f(\cdot)[\boldsymbol{v}])(\boldsymbol{w}),$$

where we use the notation $(\partial f(\cdot)[\boldsymbol{v}])(\boldsymbol{w}) := \partial f(\boldsymbol{w})[\boldsymbol{v}]$ to insist on the fact that it is a function of $\boldsymbol{w}$.

4. **Forward on forward:** Finally, we can use the definition of the HVP in Definition 2.18 as a vector of second partial derivatives along $\boldsymbol{v}$ and each canonical direction. That is, assuming $\mathcal{E} = \mathbb{R}^P$, we can compute the **JVP of the JVP** P times,

$$\nabla^2 f(\boldsymbol{w})[\boldsymbol{v}] = (\partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{e}_i])_{i=1}^P.$$

The four different ways of computing the HVP are summarized in Table 8.1.

8.1.2 Complexity

To get a sense of the computational and memory complexity of the four approaches, we consider a chain of functions $f := f_K \circ \cdots \circ f_1$ as done

Method	Computation
Reverse on reverse (VJP of gradient)	$\partial(\nabla f)(\boldsymbol{w})^*[\boldsymbol{v}]$
Forward on reverse (JVP of gradient)	$\partial(\nabla f)(\boldsymbol{w})[\boldsymbol{v}]$
Reverse on forward (gradient of JVP)	$\nabla(\partial f(\cdot)[\boldsymbol{v}])(\boldsymbol{w})$
Forward on forward (JVPs of JVPs)	$(\partial^2 f(\boldsymbol{w})[\boldsymbol{v}, \boldsymbol{e}_i])_{i=1}^P$

Table 8.1: Four different ways of computing the HVP $\nabla^2 f(\boldsymbol{w})[\boldsymbol{v}]$.
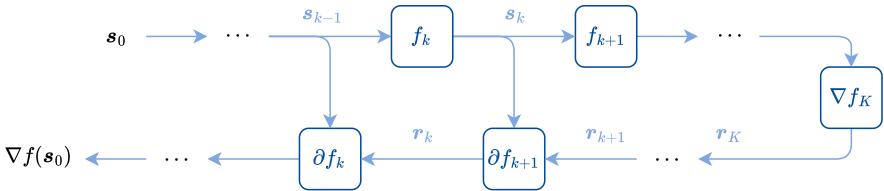
Figure 8.1: Computation graph corresponding to reverse mode autodiff for evaluating the gradient of $f = f_K \circ \ldots f_1$. While f is a simple chain, ∇f is a DAG.

in Section 7.1. To simplify our analysis, we assume $f_k \colon \mathbb{R}^P \to \mathbb{R}^P$ for $k \in \{1, \ldots, K-1\}$ and $f_K \colon \mathbb{R}^P \to \mathbb{R}$.

The computation graph of the reverse mode is illustrated in Fig. 8.1. While $f = f_K \circ \cdots \circ f_1$ would be represented by a simple chain, the computational graph of ∇f is no longer a chain: it is a DAG. This is due to the computations of $\partial f_k(\boldsymbol{s}_{k-1})[\boldsymbol{r}_k]$, where both $\boldsymbol{s}_{k-1}$ and $\boldsymbol{r}_k$ depend on $\boldsymbol{s}_0$.

We illustrate the computation graphs of reverse-on-reverse and forward-on-reverse in Fig. 8.2 and Fig. 8.3 respectively. By applying reverse mode on reverse mode, at each fan-in operation $\boldsymbol{s}_{k-1}, \boldsymbol{r}_k \mapsto \partial f_k(\boldsymbol{s}_{k-1})[\boldsymbol{r}_k]$, the reverse mode on ∇f branches out in two paths that are later merged by a sum. By applying forward mode on top of reverse mode, the flow of computations simply follows the one of ∇f.

With this in mind, following a similar calculation as for Table 7.1, we obtain the following results. We assume that each $\partial f_k(\boldsymbol{s}_{k-1})$ is a dense linear operator, so that its application has the same cost as a matrix-vector multiplication. For the memory complexity, we consider that the inputs of each operation is saved to compute the required
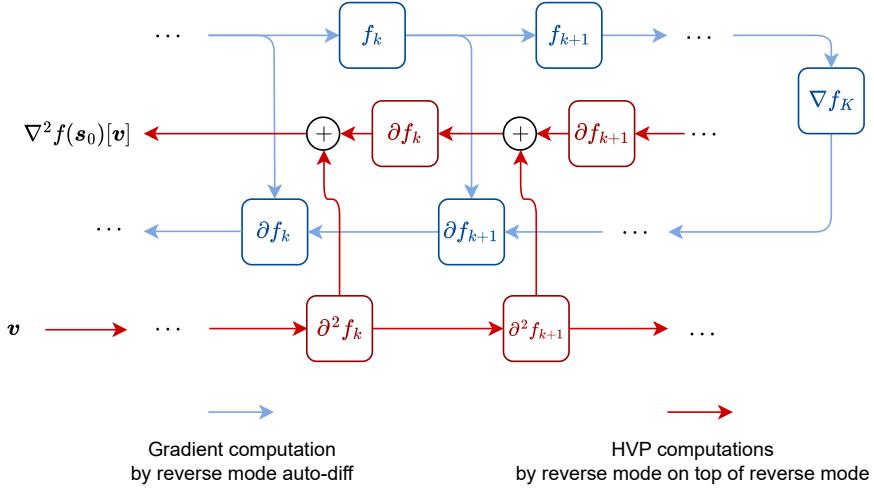
Figure 8.2: Computation graph for computing the HVP $\nabla^2 f(\boldsymbol{x})[\boldsymbol{v}]$ by using reverse mode on top of reverse mode. As the computation graph of ∇f induces fan-in operations $\boldsymbol{s}_{k-1}, \boldsymbol{r}_k \mapsto \partial f_k(\boldsymbol{s}_{k-1})[\boldsymbol{r}_k]$, the reverse mode applied on ∇f induces branching of the computations at each such node.
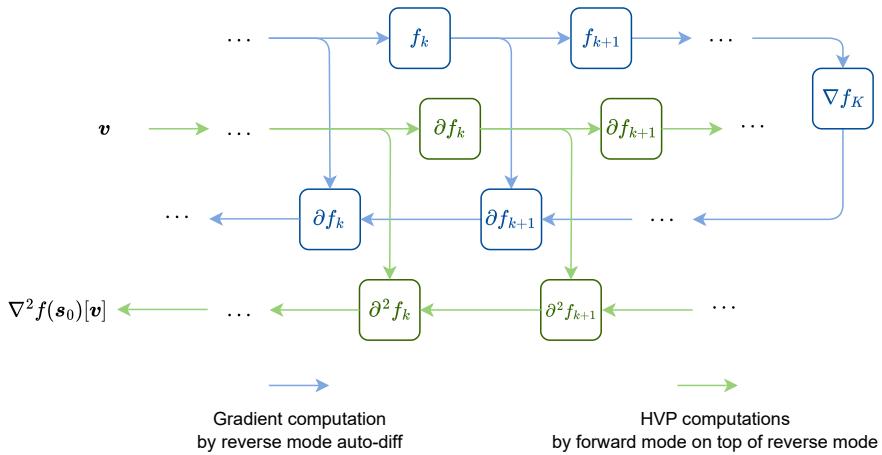
Figure 8.3: Computation graph for computing the HVP $\nabla^2 f(\boldsymbol{x})[\boldsymbol{v}]$ by using forward mode on top of reverse mode. The forward mode naturally follows the computations done for the gradient, except that it passes through the derivatives of the intermediate operations.

derivatives in the backward passes.

1. **Reverse on reverse:** $O(KP^2)$ time and $O(KP)$ space.

2. **Forward on reverse:** $O(KP^2)$ time and $O(KP)$ space.

3. **Reverse on forward:** $O(KP^2)$ time and $O(KP)$ space.

4. **Forward on forward:** $O(KP^3)$ time and $O(3P)$ space for the P JVPs with $e_1, \ldots, e_P$.

We see that, for chains of functions, "reverse on reverse", "forward on reverse" and "reverse on forward" all have similar time complexities up to some constant factors. Using reverse mode on top of reverse mode requires storing the information backpropagated, i.e., the r_k (resp. the information forwarded, i.e., the t_k in Fig. 7.1), to perform the final reverse pass. By using forward mode on top of reverse mode, this additional cost is not incurred, making it slightly less memory expensive. In addition, reverse mode on top of reverse mode induces a few additional summations due to the branching and merge operations depicted in Fig. 8.2. The same holds when using reverse on top of forward as we cannot avoid fan-in operations (this time of the form $s_{k-1}, t_{k-1} \mapsto \partial f_k(s_{k-1})[t_{k-1}]$). Unfortunately, "forward on forward" is prohibitively expensive.

To summarize, among the four approaches presented to compute HVPs, the forward-over-reverse mode is a priori the most preferable in terms of computational and memory complexities. Note, however, that computations of higher derivatives can benefit from dedicated autodiff implementations such as Taylor mode autodiff, that do not merely compose forward and reverse modes. For general functions f, it is reasonable to benchmark the first three methods to determine which method is the best for the function at hand.

8.2 Gauss-Newton matrix

8.2.1 An approximation of the Hessian

The Hessian matrix $\nabla^2 L(\boldsymbol{w})$ of a function $L: \mathcal{W} \to \mathbb{R}$ is often used to construct a quadratic approximation of $L(\boldsymbol{w})$,

$$L(\boldsymbol{w} + \boldsymbol{v}) \approx \langle \nabla L(\boldsymbol{w}), \boldsymbol{v} \rangle + \frac{1}{2} \langle \boldsymbol{v}, \nabla^2 L(\boldsymbol{w}) \boldsymbol{v} \rangle.$$

Unfortunately, when L is nonconvex, $\nabla^2 L(\boldsymbol{w})$ is typically an **indefinite matrix**, which means that the above approximation is a **nonconvex quadratic** w.r.t. $\boldsymbol{v}$. For instance, if $L = \ell \circ f$ with ℓ convex, then L is convex if f is linear, but it is typically nonconvex if f is nonlinear. The (generalized) Gauss-Newton matrix is a principled alternative to the Hessian, which is defined for $L := \ell \circ f$.

Definition 8.1 (Gauss-Newton matrix). Given a differentiable function $f : \mathcal{W} \to \mathcal{M}$ and a twice differentiable function $\ell : \mathcal{M} \to \mathbb{R}$, the (generalized) Gauss-Newton matrix of the composition $L = \ell \circ f$ evaluated at a point $\boldsymbol{w} \in \mathcal{W}$ is defined as

$$\nabla^2_{\mathrm{GN}}(\ell \circ f)(\boldsymbol{w}) := \partial f(\boldsymbol{w})^* \nabla^2 \ell(f(\boldsymbol{w})) \partial f(\boldsymbol{w}).$$

As studied in Section 16.2, the Gauss-Newton matrix is a key ingredient of the Gauss-Newton method. An advantage of the Gauss-Newton matrix is its positive semi-definiteness provided that ℓ is convex.

Proposition 8.1 (Positive semi-definiteness of the GN matrix). If ℓ is convex, then $\nabla^2_{\mathrm{GN}}(\ell \circ f)(\boldsymbol{w})$ is positive semi-definite for all f.

This means that the approximation

$$L(\boldsymbol{w} + \boldsymbol{v}) \approx \langle \nabla L(\boldsymbol{w}), \boldsymbol{v} \rangle + \frac{1}{2} \langle \boldsymbol{v}, \nabla^2_{\mathrm{GN}} L(\boldsymbol{w}) \boldsymbol{v} \rangle$$

is a **convex quadratic** w.r.t. $\boldsymbol{v}$.

Using the chain rule, we find that the Hessian of $L = \ell \circ f$ decomposes into the sum of two terms (see also Proposition 8.7).

> **Proposition 8.2** (Approximation of the Hessian). For f differentiable and ℓ twice differentiable, we have
>
> $$\nabla^2(\ell \circ f)(\boldsymbol{w}) = \partial f(\boldsymbol{w})^* \nabla^2 \ell(f(\boldsymbol{w})) \partial f(\boldsymbol{w}) + \partial^2 f(\boldsymbol{w})^* [\nabla \ell(f(\boldsymbol{w}))]$$
>
> $$= \nabla^2_{\mathrm{GN}}(\ell \circ f)(\boldsymbol{w}) + \sum_{j=1}^{Z} \nabla_j \ell(f(\boldsymbol{w})) \nabla^2 f_j(\boldsymbol{w}).$$
>
> If f is linear, then the Hessian and Gauss-Newton matrices coincide,
>
> $$\nabla^2(\ell \circ f)(\boldsymbol{w}) = \nabla^2_{\mathrm{GN}}(\ell \circ f)(\boldsymbol{w}).$$

The Gauss-Newton operator $\nabla^2_{\mathrm{GN}}(\ell \circ f)$ can therefore be seen as an approximation of the Hessian $\nabla^2(\ell \circ f)$, with equality if f is linear.

8.2.2 Gauss-Newton chain rule

A chain rule for computing the Hessian of a composition of two functions is presented in Proposition 8.7, but the formula is relatively complicated, due to the cross-terms. In contrast, a Gauss-Newton chain rule is straightforward.

> **Proposition 8.3** (Gauss-Newton chain rule).
>
> $$\nabla^2_{\mathrm{GN}}(\ell \circ f \circ g)(\boldsymbol{w}) = \partial g(\boldsymbol{w})^* \nabla^2_{\mathrm{GN}}(\ell \circ f)(g(\boldsymbol{w})) \partial g(\boldsymbol{w}).$$

8.2.3 Gauss-Newton vector product

As for the Hessian, we rarely need to materialize the full Gauss-Newton matrix in memory. Indeed, we can define the Gauss-Newton vector product (GNVP), a linear map for a direction $\boldsymbol{v} \in \mathcal{W}$, as

$$\nabla^2_{\mathrm{GN}}(\ell \circ f)(\boldsymbol{w})[\boldsymbol{v}] := \partial f(\boldsymbol{w})^* \nabla^2 \ell(f(\boldsymbol{w})) \partial f(\boldsymbol{w}) \boldsymbol{v}, \qquad (8.1)$$

where $\nabla^2 \ell(\boldsymbol{\theta}) \boldsymbol{u}$ is the HVP of ℓ, a linear map from $\mathcal{M}$ to $\mathcal{M}$. The GNVP can be computed using the JVP of f, the HVP of ℓ and the VJP of f. Instantiating the VJP requires 1 forward pass through f, from which we get both the value $f(\boldsymbol{w})$ and the adjoint linear map $\boldsymbol{u} \mapsto (\partial f(\boldsymbol{w})^* \boldsymbol{u})$. Evaluating the VJP requires 1 backward pass through

f. Evaluating the JVP requires 1 forward pass through f. In total, evaluating $\boldsymbol{v} \mapsto \nabla^2_{\mathrm{GN}}(\ell \circ f)(\boldsymbol{w})\boldsymbol{v}$ therefore requires 2 forward passes and 1 backward pass through f.

8.2.4 Gauss-Newton matrix factorization

In this section, we assume $\mathcal{W} \subseteq \mathbb{R}^P$ and $\mathcal{M} \subseteq \mathbb{R}^M$. When ℓ is convex, we know that the Gauss-Newton matrix is positive semi-definite and therefore it can be factorized into $\nabla^2_{\mathrm{GN}}(\ell \circ f)(\boldsymbol{w}) = VV^\top$ for some $V \in \mathbb{R}^{P \times R}$, where $R \leq \min\{P, M\}$ is the rank of the matrix. Such a decomposition can actually be computed easily from a factorization of the Hessian of ℓ. For instance, suppose we know the eigendecomposition of the Hessian of ℓ, $\nabla^2 \ell(f(\boldsymbol{w})) = \sum_{j=1}^M \lambda_i \boldsymbol{u}_i \boldsymbol{u}_i^\top$, where the $\boldsymbol{u}_i$ are the eigenvectors and the $\lambda_i \geq 0$ are the eigenvalues (which we know are non-negative due to positive semidefinitess). Then, the Gauss-Newton matrix can be decomposed as

$$
\begin{aligned}
\nabla^2_{\mathrm{GN}}(\ell \circ f) &= \sum_{j=1}^M \lambda_i \partial f(\boldsymbol{w})^* \boldsymbol{u}_i \boldsymbol{u}_i^\top \partial f(\boldsymbol{w})^* \\
&= \sum_{j=1}^M \left(\sqrt{\lambda_i} \partial f(\boldsymbol{w})^* \boldsymbol{u}_i \right) \left(\sqrt{\lambda_i} \partial f(\boldsymbol{w})^* \boldsymbol{u}_i \right)^\top \\
&= \sum_{j=1}^M \boldsymbol{v}_i \boldsymbol{v}_i^\top \quad \text{where } \boldsymbol{v}_i := \sqrt{\lambda_i} \partial f(\boldsymbol{w})^* \boldsymbol{u}_i.
\end{aligned}
$$

Stacking the vectors $\boldsymbol{v}_i$ into a matrix $V = (\boldsymbol{v}_1, \dots, \boldsymbol{v}_M)$, we recover the factorization $\nabla^2_{\mathrm{GN}}(\ell \circ f)(\boldsymbol{w}) = VV^\top$. To form this decomposition, we need to perform the eigendecomposition of $\nabla^2 \ell(f(\boldsymbol{w})) \in \mathbb{R}^{M \times M}$, which takes $O(M^3)$ time. We also need M calls to the VJP of f at $\boldsymbol{w}$. Compared to the direct implementation in Eq. (8.1), the factorization, once computed, allows us to compute the Gauss-Newton vector product (GNVP) as $\nabla^2_{\mathrm{GN}}(\ell \circ f)(\boldsymbol{w})[\boldsymbol{v}] = VV^\top \boldsymbol{v}$. The factorization only requires $P \times M$ memory, while the direct implementation in Eq. (8.1) requires us to maintain the intermediate computations of f. The computation-memory trade-offs therefore depend on the function considered.

8.2.5   Stochastic setting

Suppose the objective function is of the form

$$L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}) := \ell(f(\boldsymbol{w}; \boldsymbol{x}); \boldsymbol{y}).$$

With some slight abuse of notation, we then have that the Gauss-Newton matrix associated with a pair $(\boldsymbol{x}, \boldsymbol{y})$ is

$$\nabla^2_{\mathrm{GN}} L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}) := \partial f(\boldsymbol{w}; \boldsymbol{x})^* \nabla^2 \ell(\boldsymbol{\theta}; \boldsymbol{y}) \partial f(\boldsymbol{w}; \boldsymbol{x}).$$

Given a distribution ρ over $(\boldsymbol{x}, \boldsymbol{y})$ pairs, the Gauss-Newton matrix associated with the averaged loss

$$L(\boldsymbol{w}) := \mathbb{E}_{X,Y \sim \rho} \left[L(\boldsymbol{w}; X, Y) \right]$$

is then

$$\nabla^2_{\mathrm{GN}} L(\boldsymbol{w}) = \mathbb{E}_{X,Y \sim \rho} \left[\nabla^2_{\mathrm{GN}} L(\boldsymbol{w}; X, Y) \right].$$

8.3   Fisher information matrix

8.3.1   Definition using the score function

The Fisher information is a way to measure the amount of information in a random variable S.

> **Definition 8.2** (Fisher information matrix)**.** The **Fisher information matrix**, or Fisher for short, associated with the negative log-likelihood $L(\boldsymbol{w}; S) = -\log q_{\boldsymbol{w}}(S)$ of a probability distribution $q_{\boldsymbol{w}}$ with parameters $\boldsymbol{w}$ is the covariance of the gradients of L at $\boldsymbol{w}$ for S distributed according to $q_{\boldsymbol{w}}$,
>
> $$\nabla^2_{\mathrm{F}} L(\boldsymbol{w}) := \mathbb{E}_{S \sim q_{\boldsymbol{w}}}[\nabla L(\boldsymbol{w}; S) \otimes \nabla L(\boldsymbol{w}; S)]$$
> $$= \mathbb{E}_{S \sim q_{\boldsymbol{w}}}[\nabla_{\boldsymbol{w}} \log q_{\boldsymbol{w}}(S) \otimes \nabla_{\boldsymbol{w}} \log q_{\boldsymbol{w}}(S)].$$
>
> The gradient $\nabla_{\boldsymbol{w}} \log q_{\boldsymbol{w}}(S)$ is known as the **score function**.

As studied in Section 16.3, the Fisher information matrix is a key ingredient of the natural gradient descent method.

8.3.2 Link with the Hessian

Provided that the probability distribution is twice diferentiable w.r.t. $\boldsymbol{w}$ with integrable second derivatives, the Fisher information matrix can also be expressed as the Hessian of the negative log-likelihood (Amari, 1998; Martens, 2020).

Proposition 8.4 (Connection with the Hessian). The Fisher information matrix of the negative log-likelihood $L(\boldsymbol{w}; S) = -\log q_{\boldsymbol{w}}(S)$ satisfies

$$\nabla_{\mathrm{F}}^2 L(\boldsymbol{w}) = \mathbb{E}_{S \sim q_{\boldsymbol{w}}}[\nabla^2 L(\boldsymbol{w}; S)] = \mathbb{E}_{S \sim q_{\boldsymbol{w}}}[-\nabla_{\boldsymbol{w}}^2 \log q_{\boldsymbol{w}}(S)].$$

Remark 8.1 (Empirical Fisher). We emphasize that in the above definitions, S is sampled from the model distribution $q_{\boldsymbol{w}}$, not from the data distribution ρ. That is, we have

$$\nabla_{\mathrm{F}}^2 L(\boldsymbol{w}) = \mathbb{E}_{S \sim q_{\boldsymbol{w}}}[\nabla_{\boldsymbol{w}} \log q_{\boldsymbol{w}}(S) \nabla_{\boldsymbol{w}} \log q_{\boldsymbol{w}}(S)^\top]$$
$$\neq \mathbb{E}_{S \sim \rho}[\nabla_{\boldsymbol{w}} \log q_{\boldsymbol{w}}(S) \nabla_{\boldsymbol{w}} \log q_{\boldsymbol{w}}(S)^\top]$$

The latter is sometimes called ambiguously the "empirical" Fisher, though this name has generated confusion (Kunstner *et al.*, 2019).

8.3.3 Equivalence with the Gauss-Newton matrix

So far, we discussed the Fisher information for a generic random variable $S \sim q_{\boldsymbol{w}}$. We now discuss the supervised probabilistic learning setting where $S = (X, Y)$ and where, using the product rule of probability, we define the PDF $q_{\boldsymbol{w}}(X, Y) \coloneqq \rho_X(X) p_{\boldsymbol{\theta}}(Y)$, with the shorthand $\boldsymbol{\theta} \coloneqq f(\boldsymbol{w}; X)$.

Proposition 8.5 (Fisher matrix in supervised setting). Suppose $(X, Y) \sim q_{\boldsymbol{w}}$ where the PDF of $q_{\boldsymbol{w}}$ is $q_{\boldsymbol{w}}(X, Y) \coloneqq \rho_X(X) p_{\boldsymbol{\theta}}(Y)$. In that case, the Fisher information matrix of the negative log-

likelihood $L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}) = -\log q_{\boldsymbol{w}}(\boldsymbol{x}, \boldsymbol{y})$ decomposes as,

$$
\begin{aligned}
\nabla_{\mathrm{F}}^2 L(\boldsymbol{w}) &= \mathbb{E}_{(X,Y) \sim q_{\boldsymbol{w}}}[\nabla_{\boldsymbol{w}} \log q_{\boldsymbol{w}}(X, Y) \otimes \nabla_{\boldsymbol{w}} \log q_{\boldsymbol{w}}(X, Y)] \\
&= \mathbb{E}_{X \sim \rho_X}[\mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla_{\boldsymbol{w}} \log p_{\boldsymbol{\theta}}(Y) \otimes \nabla_{\boldsymbol{w}} \log p_{\boldsymbol{\theta}}(Y)]] \\
&= \mathbb{E}_{X \sim \rho_X}\left[\partial f(\boldsymbol{w}; X)^* \nabla_{\mathrm{F}}^2 \ell(\boldsymbol{\theta}) \partial f(\boldsymbol{w}; X)\right],
\end{aligned}
$$

where we defined the shorthand $\boldsymbol{\theta} := f(\boldsymbol{w}; X)$ and where we defined the negative log-likelihood loss $\ell(\boldsymbol{\theta}; Y) := -\log p_{\boldsymbol{\theta}}(Y)$.

When $p_{\boldsymbol{\theta}}$ is an exponential family distribution, we can show that the Fisher information matrix and the Gauss-Newton matrix are equivalent.

Proposition 8.6 (Equivalence between Fisher and Gauss-Newton)**.** If $p_{\boldsymbol{\theta}}$ is an exponential family distribution, then

$$
\begin{aligned}
\nabla_{\mathrm{F}}^2 L(\boldsymbol{w}) &= \mathbb{E}_{X \sim \rho_X} \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla L(\boldsymbol{w}; X, Y) \otimes \nabla L(\boldsymbol{w}; X, Y)] \\
&= \mathbb{E}_{X \sim \rho_X} \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\partial f(\boldsymbol{w}; X)^* \nabla \ell(\boldsymbol{\theta}; Y) \otimes \nabla \ell(\boldsymbol{\theta}; Y) \partial f(\boldsymbol{w}; X)] \\
&= \mathbb{E}_{X \sim \rho_X} \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\partial f(\boldsymbol{w}; X)^* \nabla^2 \ell(\boldsymbol{\theta}; Y) \partial f(\boldsymbol{w}; X)] \\
&= \mathbb{E}_{X,Y \sim \rho}\left[\nabla_{\mathrm{GN}}^2 L(\boldsymbol{w}; X, Y)\right],
\end{aligned}
$$

where $\rho_X(\boldsymbol{x}) := \int \rho(\boldsymbol{x}, \boldsymbol{y}) d\boldsymbol{y}$.

Proof. From Proposition 3.3, if $p_{\boldsymbol{\theta}}$ is an exponential family distribution, $\nabla^2 \ell(\boldsymbol{\theta}, \boldsymbol{y})$ is actually independent of $\boldsymbol{y}$. Using Bartlett's second identity Eq. (11.5), we then obtain

$$
\begin{aligned}
\nabla^2 \ell(\boldsymbol{\theta}; \cdot) &= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla^2 \ell(\boldsymbol{\theta}; Y)] \\
&= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla^2 \ell(\boldsymbol{\theta}; Y)] \\
&= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[-\nabla_{\boldsymbol{\theta}}^2 \log p_{\boldsymbol{\theta}}(Y)] \\
&= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y) \otimes \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)] \\
&= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla \ell(\boldsymbol{\theta}; Y) \otimes \nabla \ell(\boldsymbol{\theta}; Y)],
\end{aligned}
$$

where we used $\cdot$ to indicate that the results holds for all $\boldsymbol{y}$. Plugging the result back in the Fisher information matrix concludes the proof. $\quad\square$

8.4   Inverse-Hessian vector product

8.4.1   Definition as a linear map

We saw in Section 16.1 that Newton's method uses iterations as

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \nabla^2 L(\boldsymbol{w}^t)^{-1} \nabla L(\boldsymbol{w}^t).$$

The inverse is well-defined if for example L is strictly convex. Otherwise, we saw that some additional regularization can be added. Newton's method therefore requires to access **inverse-Hessian vector products** (IHVPs), as defined below.

> **Definition 8.3** (Inverse-Hessian vector product)**.** For a twice differentiable function $L : \mathbb{R}^P \to \mathbb{R}$, we define the **inverse-Hessian Vector Product** (IHVP) of L at $\boldsymbol{w} \in \mathbb{R}^P$ as the linear map
>
> $$\boldsymbol{u} \mapsto \nabla^2 L(\boldsymbol{w})^{-1} \boldsymbol{u},$$
>
> provided that it exists. In other words, it is the linear map which to $\boldsymbol{u}$ associates $\boldsymbol{v}$ such that $\nabla^2 L(\boldsymbol{w}) \boldsymbol{v} = \boldsymbol{u}$.

8.4.2   Implementation with matrix-free linear solvers

Numerous direct methods exist to compute the inverse of a matrix, such as the Cholesky decomposition, QR decomposition and Gaussian elimination. However, these algorithms require accessing elementary entries of the matrix, while an autodiff framework gives access to the Hessian through HVPs. Fortunately, there exists so-called **matrix-free** algorithms, that can solve a linear system of equations

$$H[\boldsymbol{v}] = \boldsymbol{u}$$

by only accessing the linear map $\boldsymbol{v} \mapsto H[\boldsymbol{v}]$ for any $\boldsymbol{v}$. Among such algorithms, we have the **conjugate gradient** (CG) method, that applies for H positive-definite, i.e., such that $\langle \boldsymbol{v}, H[\boldsymbol{v}] \rangle > 0$ for all $\boldsymbol{v} \neq 0$, or the **generalized minimal residual** (GMRES) method, that applies for any invertible H. A longer list of solvers can be found in public software such as SciPy (Virtanen *et al.*, 2020). The IHVP of a striclty convex

function (ensuring that the Hessian is positive definite) can therefore be computed by instantiating CG on the HVP,

$$\nabla^2 L(\boldsymbol{w})^{-1}\boldsymbol{u} \approx \text{CG}(\nabla^2 L(\boldsymbol{w})[\cdot], \boldsymbol{u}).$$

Positive-definiteness of the Hessian is indeed guaranteed for strictly convex functions for example, while for generic non-convex functions, such property may be verified around a minimizer but not in general. The conjugate gradient method is recalled in Algorithm 8.1 in its simplest form. In theory, the exact solution of the linear system is found after at most $T = P$ iterations of CG, though in practice numerical errors may prevent from getting an exact solution.

Algorithm 8.1 Conjugate gradient method

    Inputs: linear map $H[\cdot] : \mathbb{R}^P \to \mathbb{R}^P$, target $\boldsymbol{u} \in \mathbb{R}^P$, initialization $\boldsymbol{v}_0$ (default $\boldsymbol{0}$), number of iterations T (default P), target accuracy ε (default machine precision)

1: $\boldsymbol{r}_0 = \boldsymbol{u} - H[\boldsymbol{v}_0]$
2: $\boldsymbol{p}_0 = \boldsymbol{r}_0$
3: **for** $t = 0, \ldots T$ **do**
4:     $\alpha_t = \frac{\langle \boldsymbol{r}_t, \boldsymbol{r}_t \rangle}{\langle \boldsymbol{p}_t, H[\boldsymbol{p}_t] \rangle}$
5:     $\boldsymbol{v}_{t+1} = \boldsymbol{v}_t + \alpha_t \boldsymbol{p}_t$
6:     $\boldsymbol{r}_{t+1} = \boldsymbol{r}_t - \alpha_t H[\boldsymbol{p}_t]$
7:     **if** $\langle \boldsymbol{r}_{t+1}, \boldsymbol{r}_{t+1} \rangle \leq \varepsilon$ **then break**
8:     $\beta_t = \frac{\langle \boldsymbol{r}_{t+1}, \boldsymbol{r}_{t+1} \rangle}{\langle \boldsymbol{r}_t, \boldsymbol{r}_t \rangle}$
9:     $\boldsymbol{p}_{t+1} = \boldsymbol{r}_{t+1} + \beta_t \boldsymbol{p}_t$

    Output: $\boldsymbol{v}_T$, such that $H[\boldsymbol{v}_T] \approx \boldsymbol{u}$

8.4.3 Complexity

For a given matrix $H \in \mathbb{R}^{P \times P}$, solving $H\boldsymbol{v} = \boldsymbol{u}$ can be done with decomposition methods (LU, QR, Cholesky) in $O(P^3)$ time. For matrix-free methods such as CG or GMRES, the cost per iteration is $O(P^2)$. Since they theoretically solve the linear system in $O(P)$ iterations, the cost to obtain an exact solution is theoretically the same, $O(P^3)$.

However, CG or GMRES differ from decomposition methods in that they are iterative methods, meaning that, at each iteration, they get closer to a solution. Unlike decomposition methods, this means that we can stop them before an exact solution is found. In practice, the number of iterations required to find a good approximate solution depends on the matrix. Well conditioned matrices require only few iterations. Badly conditioned matrices lead to some numerical instabilities for CG, so that more than P iterations may be needed to get a good solution. In contrast, decomposition methods proceed in two steps: first they build a decomposition of H at a cost of $O(P^3)$, and second they solve a linear system at a cost of $O(P^2)$, by leveraging the structure. LU and QR decompositions are known to be generally more stable and are therefore often preferred in practice, when we can access entries of H at no cost.

If we do not have access to the Hessian H, but only to its HVP, accessing entries of H comes at a prohibitive cost. Indeed, entries of H can still be recovered from HVPs, since $e_i^\top H e_j = H_{i,j}$, but accessing each row or column of H costs one HVP (matrix-vector product). To access the information necessary to use a decomposition method, we therefore need P calls to HVPs before being able to actually compute the solution. For the same number of calls, CG or GMRES will already have found an approximate solution. In addition, a CG method does not require to store any memory.

8.5 Second-order backpropagation

8.5.1 Second-order Jacobian chain rule

The essential ingredient to develop forward-mode and reverse-mode autodiff hinged upon the chain rule for composed functions, $h = g \circ f$. For second derivatives, a similar rule can be obtained. To do so, we slightly abuse notations and denote

$$\partial^2 h(\boldsymbol{w})^*[\boldsymbol{u}] := \nabla^2 \langle h, \boldsymbol{u} \rangle (\boldsymbol{w}) \in \mathbb{R}^{P \times P},$$

where $h : \mathbb{R}^P \to \mathbb{R}^Q$, $\boldsymbol{w} \in \mathbb{R}^P$, $\boldsymbol{u} \in \mathbb{R}^Q$, and where we recall the shorthand notation $\langle \boldsymbol{u}, h \rangle (\boldsymbol{w}) := \langle \boldsymbol{u}, h(\boldsymbol{w}) \rangle$. Moreover, we view the above quantity as a linear map. Strictly speaking, the superscript $*$ is

not a linear adjoint anymore, since $\boldsymbol{v}_1, \boldsymbol{v}_2 \mapsto \partial^2 h(\boldsymbol{w})[\boldsymbol{v}_1, \boldsymbol{v}_2]$ is no longer linear but bilinear. However, this superscript plays the same role as the VJP, since it takes an output vector and returns the input derivatives that correspond to infinitesimal variations along that output vector.

Proposition 8.7 (Hessian chain-rule). For two twice differentiable functions $f : \mathbb{R}^P \to \mathbb{R}^M$ and $g : \mathbb{R}^M \to \mathbb{R}^Q$, the second directional derivative of the composition $g \circ f$ is a bilinear map from $\mathbb{R}^P \times \mathbb{R}^P$ to $\mathbb{R}^Q$ along input directions $\boldsymbol{v}_1, \boldsymbol{v}_2 \in \mathbb{R}^P$ of the form

$$\partial^2 (g \circ f)(\boldsymbol{w})[\boldsymbol{v}_1, \boldsymbol{v}_2] = \partial g(f(\boldsymbol{w}))[\partial^2 f(\boldsymbol{w})[\boldsymbol{v}_1, \boldsymbol{v}_2]]$$
$$+ \partial^2 g(f(\boldsymbol{w}))[\partial f(\boldsymbol{w})[\boldsymbol{v}_1], \partial f(\boldsymbol{w})[\boldsymbol{v}_2]].$$

The Hessian of the composition $g \circ f$ along an output direction $\boldsymbol{u} \in \mathbb{R}^Q$ is, seen as a linear map,

$$\partial^2 (g \circ f)(\boldsymbol{w})^*[\boldsymbol{u}] = \partial^2 f(\boldsymbol{w})^*[\partial g(f(\boldsymbol{w}))^*\boldsymbol{u}] \qquad (8.2)$$
$$+ \partial f(\boldsymbol{w})^* \partial^2 g(f(\boldsymbol{w}))^*[\boldsymbol{u}]\partial f(\boldsymbol{w}).$$

For the composition of $f \colon \mathbb{R}^P \to \mathbb{R}^M$ with a scalar-valued function function $\ell \colon \mathbb{R}^M \to \mathbb{R}$, we have in matrix form

$$\nabla^2 (\ell \circ f)(\boldsymbol{w}) = \sum_{j=1}^{M} (\nabla \ell(f(\boldsymbol{w})))_j \nabla^2 f_j(\boldsymbol{w})$$
$$+ \boldsymbol{\partial} f(\boldsymbol{w})^\top \nabla^2 \ell(f(\boldsymbol{w})) \boldsymbol{\partial} f(\boldsymbol{w}).$$

Note that, while the Hessian is usually defined for scalar-valued functions $h \colon \mathbb{R}^P \to \mathbb{R}$, the above definition is for a generalized notion of Hessian that works for any function $h \colon \mathbb{R}^P \to \mathbb{R}^Q$.

The Hessian back-propagation rule in Eq. (8.2) reveals two terms. The first one $\partial^2 f(\boldsymbol{w})^*[\partial g(f(\boldsymbol{w}))^*\boldsymbol{u}]$ simply computes the Hessian of the intermediate function along the output direction normally back-propagated by a VJP. The second term $\partial f(\boldsymbol{w})^* \partial^2 g(f(\boldsymbol{w}))^*[\boldsymbol{u}]\partial f(\boldsymbol{w})$ shows how intermediate first-order variations influence second order derivatives of the output.

Example 8.1 (Composition with an elementwise nonlinear function). Consider the element-wise application of a twice differentiable scalar-valued function $f(\boldsymbol{x}) = (f(x_i))_{i=1}^M$ followed by some twice differentiable function ℓ. Note that $\nabla^2 f_i(\boldsymbol{x}) = f''(x_i)\boldsymbol{e}_i\boldsymbol{e}_i^\top$. Hence, the Hessian of the composition reads

$$\nabla^2(\ell \circ f)(\boldsymbol{x}) = \sum_{i=1}^M (\nabla\ell(f(\boldsymbol{x})))_i f''(x_i)\boldsymbol{e}_i\boldsymbol{e}_i^\top$$
$$+ \mathbf{diag}(f'(\boldsymbol{x}))\nabla^2\ell(f(\boldsymbol{x}))\,\mathbf{diag}(f'(\boldsymbol{x}))$$
$$= \mathbf{diag}(\nabla\ell(f(\boldsymbol{w})) \odot f''(\boldsymbol{x}))$$
$$+ \nabla^2\ell(f(\boldsymbol{x})) \odot (f'(\boldsymbol{x})f'(\boldsymbol{x})^\top),$$

where $f'(\boldsymbol{x}) := (f'(x_i))_{i=1}^M$ and $f''(\boldsymbol{x}) := (f''(x_i))_{i=1}^M$.

Example 8.2 (Hessian of the composition with a linear function). Consider a linear function $f(\boldsymbol{W}) = \boldsymbol{W}\boldsymbol{x}$, for $\boldsymbol{W} \in \mathbb{R}^{M \times D}$, composed with some twice differentiable function $\ell : \mathbb{R}^M \to \mathbb{R}$. From Proposition 8.7, we get, in terms of linear maps,

$$\nabla^2(\ell \circ f)(\boldsymbol{W}) = \partial f(\boldsymbol{W})^*\nabla^2\ell(f(\boldsymbol{W}))\partial f(\boldsymbol{W}).$$

As already noted in Section 2.3, we have that $\partial f(\boldsymbol{W})[\boldsymbol{V}] = \boldsymbol{V}\boldsymbol{x}$ and $\partial f(\boldsymbol{W})^*[\boldsymbol{u}] = \boldsymbol{u}\boldsymbol{x}^\top$. Hence, the Hessian seen as a linear map reads

$$\nabla^2(\ell \circ f)(\boldsymbol{W})[\boldsymbol{V}] = \partial f(\boldsymbol{W})^*[\nabla^2\ell(f(\boldsymbol{W}))[\partial f(\boldsymbol{W})[\boldsymbol{V}]]] \quad = \boldsymbol{H}\boldsymbol{V}\boldsymbol{x}\boldsymbol{x}^\top,$$

where $\boldsymbol{H} := \nabla^2\ell(f(\boldsymbol{W}))$.

8.5.2   Computation chains

For a simple computation chain $f = f_K \circ \ldots \circ f_1$ as in Section 7.1, the formula derived in Proposition 8.7 suffices to develop an algorithm that backpropagates the Hessian, as shown in Algorithm 8.2. Compared to Algorithm 7.2, we simply backpropagate both the vectors $\boldsymbol{r}_k$ and the matrices $\boldsymbol{R}_k$ using intermediate first and second derivatives.

Algorithm 8.2 Hessian backprop for computation chains

    Functions: $f := f_K \circ \ldots \circ f_1$,

    Inputs: input $\boldsymbol{x}$, output direction $\boldsymbol{u}$

1: Initialize and store $\boldsymbol{s}_0 := \boldsymbol{x}$ ▷ Forward pass

2: **for** $k := 1, \ldots, K$ **do**

3:       Compute and store $\boldsymbol{s}_k := f_k(\boldsymbol{s}_{k-1})$

4: Initialize $\boldsymbol{r}_K := \nabla\ell(\boldsymbol{s}_K)$, $\boldsymbol{R}_K := \nabla^2\ell(\boldsymbol{s}_K)$ ▷ Backward pass

5: **for** $k := K, \ldots, 1$ **do**

6:       Compute $\boldsymbol{r}_{k-1} := \partial f_k(\boldsymbol{s}_{k-1})^*[\boldsymbol{r}_k]$

7:       Compute $\boldsymbol{R}_{k-1} := \partial^2 f_k(\boldsymbol{s}_{k-1})^*[\boldsymbol{r}_k] + \partial f_k(\boldsymbol{s}_{k-1})^* \boldsymbol{R}_k \partial f_k(\boldsymbol{s}_{k-1})$

8:       Release $\boldsymbol{s}_{k-1}$ from memory

    Outputs: $\ell(f(\boldsymbol{x})) = \ell(\boldsymbol{s}_K)$, $\nabla(\ell \circ f)(\boldsymbol{x}) = \boldsymbol{r}_0$, $\nabla^2(\ell \circ f)(\boldsymbol{x}) = \boldsymbol{R}_0$

8.5.3   Fan-in and fan-out

For generic computation graphs (see Section 7.3), we saw that multi-input functions (fan-in) were crucial. For Hessian backpropagation in computation graphs, we therefore need to develop a similar formula.

Proposition 8.8 (Hessian chain-rule for fan-in). Consider $n+1$ twice differentiable functions $f_1, \ldots, f_n$ and g with $f_i : \mathbb{R}^P \to \mathbb{R}^{M_i}$ and $g : \mathbb{R}^{M_1} \times \ldots \times \mathbb{R}^{M_n} \to \mathbb{R}^Q$. The Hessian of $g \circ f$ for $f(\boldsymbol{w}) = (f_1(\boldsymbol{w}), \ldots, f_n(\boldsymbol{w}))$ along an output direction $\boldsymbol{u} \in \mathbb{R}^Q$ is given by

$$\partial^2(g \circ f)(\boldsymbol{w})^*[\boldsymbol{u}] = \sum_{i=1}^{n} \partial^2 f_i(\boldsymbol{w})^*[\partial_i g(f(\boldsymbol{w}))^*[\boldsymbol{u}]]$$

$$+ \sum_{i,j=1}^{n} \partial f_i(\boldsymbol{w})^* \partial^2_{i,j} g(f(\boldsymbol{w}))^*[\boldsymbol{u}] \partial f_j(\boldsymbol{w}).$$

    The gradient backpropagation expression for fan-in is simple because the functions f_i are not linked by any path. In contrast, the Hessian backpropagation involves cross-product terms $\partial f_i(\boldsymbol{w})^* \partial^2_{i,j} g(f(\boldsymbol{w}))^*[\boldsymbol{u}] \partial f_j(\boldsymbol{w})$ for $i \neq j$. The nodes associated to the f_i computations cannot be treated independently anymore.

    On the other hand, developing a backpropagation rule for fan-out does not pose any issue, since each output function can be treated

independently.

Proposition 8.9 (Hessian chain-rule for fan-out). Consider $n+1$ twice differentiable functions $g_1, \ldots, g_n$ and f with $g_i : \mathbb{R}^M \to \mathbb{R}^{Q_i}$ and $f : \mathbb{R}^P \to \mathbb{R}^M$. The Hessian of $g \circ f$ for $g(\boldsymbol{w}) = (g_1(\boldsymbol{w}), \ldots, g_n(\boldsymbol{w}))$ along a direction $\boldsymbol{u} = (\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n) \in \mathbb{R}^{Q_1} \times \ldots \times \mathbb{R}^{Q_n}$ is given by

$$\partial^2 (g \circ f)(\boldsymbol{w})^*[\boldsymbol{u}] = \sum_{i=1}^n \partial^2 f(\boldsymbol{w})^*[\partial g_i(f(\boldsymbol{w}))^*[\boldsymbol{u}_i]]$$

$$+ \sum_{i=1}^n \partial f(\boldsymbol{w})^* \partial^2 g_i(f(\boldsymbol{w}))^*[\boldsymbol{u}] \partial f(\boldsymbol{w}).$$

8.6 Block diagonal approximations

Rather than computing the whole Hessian or Gauss-Newton matrices, we can consider computing block-diagonal or diagonal approximations, which are easier to invert. The approximation rules we present in this section build upon the Hessian chain rule studied in Section 8.5.

8.6.1 Feedforward networks

Recall the definition of a feedforward network:

$$\boldsymbol{s}_0 := \boldsymbol{x}$$
$$\boldsymbol{s}_k := f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k) \ \forall k \in \{1, \ldots, K\}$$
$$f(\boldsymbol{x}, \boldsymbol{w}) := \boldsymbol{s}_K,$$

where $\boldsymbol{w} := (\boldsymbol{w}_1, \ldots, \boldsymbol{w}_K)$. Rather than computing the entire Hessian of $\ell \circ f$ w.r.t. $\boldsymbol{w}$, we can compute the Hessians w.r.t. each set of parameters $\boldsymbol{w}_k$. For the case of computation chains, the Hessian backpropagation recursion we used in Algorithm 8.2 was

$$\boldsymbol{R}_{k-1} := \partial^2 f_k(\boldsymbol{s}_{k-1})^*[\boldsymbol{r}_k] + \partial f_k(\boldsymbol{s}_{k-1})^* \boldsymbol{R}_k \partial f_k(\boldsymbol{s}_{k-1}).$$

Extending this recursion to the feedforward network case, we obtain, starting from $\boldsymbol{r}_K := \nabla \ell(\boldsymbol{s}_K)$ and $\boldsymbol{R}_K := \nabla^2 \ell(\boldsymbol{s}_K)$,

$$\boldsymbol{r}_{k-1} := \partial f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k)^* [\boldsymbol{r}_k]$$

$$\begin{pmatrix} \boldsymbol{R}_{k-1} & \sim \\ \sim & \boldsymbol{H}_k \end{pmatrix} := \partial^2 f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k)^* [\boldsymbol{r}_k]$$

$$+ \partial f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k)^* \boldsymbol{R}_k \partial f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k),$$

where we used $\sim$ to indicate that these blocks are not used. The Hessians w.r.t each set of parameters are then

$$\boldsymbol{R}_0 = \nabla^2_{\boldsymbol{x}\boldsymbol{x}} (\ell \circ f)(\boldsymbol{x}, \boldsymbol{w})$$

$$\boldsymbol{H}_1 = \nabla^2_{\boldsymbol{w}_1 \boldsymbol{w}_1} (\ell \circ f)(\boldsymbol{x}, \boldsymbol{w})$$

$$\vdots$$

$$\boldsymbol{H}_K = \nabla^2_{\boldsymbol{w}_K \boldsymbol{w}_K} (\ell \circ f)(\boldsymbol{x}, \boldsymbol{w})).$$

The validity of this result stems from the fact that we can view the Hessian w.r.t. $\boldsymbol{w}_k$ as computing the Hessian w.r.t. $\boldsymbol{w}_k$ of

$$\tilde{f}_K \circ \ldots \circ \tilde{f}_{k+1} \circ f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k)$$

where $\tilde{f}_i := f_i(\cdot, \boldsymbol{w}_k)$, for $i \in \{k+1, \ldots, K\}$. As the computations of the block-wise Hessians share most of the computations, they can be evaluated in a single backward pass just as the gradients.

Example 8.3 (Block-wise computation of the Gauss-Newton matrix). Our blockwise backpropagation scheme can readily be adapted for the Gauss-Newton matrix as

$$\begin{pmatrix} \boldsymbol{R}_{k-1} & \sim \\ \sim & \boldsymbol{G}_k \end{pmatrix} := \partial f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k)^* \boldsymbol{R}_k \partial f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k),$$

starting from $\boldsymbol{R}_K := \nabla^2 \ell(\boldsymbol{s}_K)$. The outputs $\boldsymbol{R}_0, \boldsymbol{G}_0, \ldots, \boldsymbol{G}_K$ give a block-wise approximation of the Gauss-Newton matrix.

Now, consider a simple multilayer perceptron such that

$$f_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k) := \boldsymbol{a}(\boldsymbol{W}_k \boldsymbol{s}_{k-1}) \quad \text{with} \quad \boldsymbol{w}_k := \text{vec}(\boldsymbol{W}_k)$$

Using Example 8.2 and Example 8.1 adapted to the Gauss-Newton

matrix, we can compute the block-wise decomposition of the Gauss-Newton matrix as, for $k = K, \ldots, 1$,

$$\boldsymbol{R}_{k-1} := \boldsymbol{W}_k^\top \boldsymbol{J}_k \boldsymbol{W}_k$$
$$\boldsymbol{J}_k := \boldsymbol{R}_k \odot (\boldsymbol{a}'(\boldsymbol{W}_k \boldsymbol{s}_{k-1}) \boldsymbol{a}'(\boldsymbol{W}_k \boldsymbol{s}_{k-1})^\top)$$
$$\boldsymbol{G}_k := \boldsymbol{J}_k \otimes \boldsymbol{s}_{k-1} \boldsymbol{s}_{k-1}^\top$$

starting from $\boldsymbol{R}_K := \nabla^2 \ell(\boldsymbol{s}_K)$. The outputs $\boldsymbol{G}_1, \ldots, \boldsymbol{G}_K$ correspond to the block-wise elements of the Gauss-Newton matrix of f for the vectorized weights $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_K$. Similar computations were done in KFRA (Botev *et al.*, 2017) and BackPack (Dangel *et al.*, 2019).

8.6.2 Computation graphs

For generic computation graphs, consider a function $f(\boldsymbol{x}, \boldsymbol{w})$ defined by, denoting $i_1, \ldots, i_{p_k} := \text{parents}(k)$,

$$\boldsymbol{s}_k := f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}}) \quad \forall k \in \{1, \ldots, K\}$$

such that $f(\boldsymbol{x}, \boldsymbol{w}) = \boldsymbol{s}_K$, and k is following a topological ordering of the graph (see Section 7.3). We can consider the following backpropagation scheme, for $k = K, \ldots, 1$ and $j \in \text{parents}(k)$

$$\boldsymbol{r}_{i_j} \leftarrow \boldsymbol{r}_{i_j} + \partial_j f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})^*[\boldsymbol{r}_k] \tag{8.3}$$
$$R_{i_j} \leftarrow R_{i_j} + \partial_{jj}^2 f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})^*[\boldsymbol{r}_k]$$
$$+ \partial_j f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})^* R_k \partial_j f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}}), \tag{8.4}$$

starting from $R_K := \nabla^2 \ell(\boldsymbol{s}_K)$ and $\boldsymbol{r}_K := \nabla \ell(\boldsymbol{s}_K)$. Recall that for multiple inputs, the chain-rule presented in Proposition 8.8 involves the cross-derivatives. For this reason the back-propagation scheme in Eq. (8.3) only computes an approximation. For example, one can verify that using Eq. (8.3) to compute the Hessian of $\ell(f_1(\boldsymbol{w}), f_2(\boldsymbol{w}))$ does not provide an exact expression for the Hessian of f. This scheme is easy to implement and may provide a relevant proxy for the Hessian.

8.7 Diagonal approximations

Similarly to the idea of designing a backpropagation scheme that approximates blocks of the Hessian, we can design a backpropagation

scheme that approximates the diagonal of the Hessian. The approach was originally proposed by Becker and Le Cun (1988) for feedforward networks, but our exposition, new to our knowledge, has the benefit that it naturally extends to computational graphs, as we shall see.

8.7.1   Computation chains

The idea stems from modifying the Hessian backpropagation rule in Proposition 8.7 to only keep the diagonal of the Hessian. Formally, given a matrix $\boldsymbol{M} \in \mathbb{R}^{D \times D}$, we denote by $\mathbf{diag}(\boldsymbol{M}) = (\boldsymbol{M}_{ii})_{i=1}^{D} \in \mathbb{R}^{D}$ the vector of diagonal entries of $\boldsymbol{M}$, and for a vector $\boldsymbol{m} \in \mathbb{R}^{D}$, we denote $\mathbf{Diag}(\boldsymbol{m}) = \sum_{i=1}^{D} m_i \boldsymbol{e}_i \boldsymbol{e}_i^{\top}$ the diagonal matrix with entries m_i. For the backpropagation of the Hessian of $\ell \circ f_K \circ \ldots \circ f_1$, we see from Algorithm 8.2 that $\mathbf{diag}(\boldsymbol{H}_{k-1})$ can be expressed in terms of $\boldsymbol{H}_k$ as

$$\begin{aligned} \mathbf{diag}(\boldsymbol{H}_{k-1}) = {} & \mathbf{diag}(\partial^2 f_k(\boldsymbol{s}_{k-1})^* \boldsymbol{r}_k) \\ & + \mathbf{diag}(\boldsymbol{\partial} f_k(\boldsymbol{s}_{k-1})^* \boldsymbol{H}_k \boldsymbol{\partial} f_k(\boldsymbol{s}_{k-1})). \end{aligned}$$

Unfortunately, that recursion needs access to the whole Hessian $\boldsymbol{H}_k$, and would therefore be too expensive. A natural idea is to modify the recursion to approximate $\mathbf{diag}(\boldsymbol{H}_k)$ by backpropagating **vectors**:

$$\begin{aligned} \boldsymbol{d}_{k-1} \coloneqq {} & \mathbf{diag}(\partial^2 f_k(\boldsymbol{s}_{k-1})^* \boldsymbol{r}_k) \\ & + \mathbf{diag}(\boldsymbol{\partial} f_k(\boldsymbol{s}_{k-1})^* \mathbf{Diag}(\boldsymbol{d}_k) \boldsymbol{\partial} f_k(\boldsymbol{s}_{k-1})). \end{aligned}$$

The diagonal matrix $\mathbf{Diag}(\boldsymbol{d}_k)$ serves as a surrogate for $\boldsymbol{H}_k$. Each iteration of this recursion can be computed in linear time in the output dimension D_k since

$$d_{k-1,i} = \sum_{j=1}^{D_k} r_{k,j} \cdot \partial_{i,i}^2 f_{k,j}(\boldsymbol{s}_{k-1}) + \sum_{j=1}^{D_k} d_{k,j} (\partial_i f_{k,j}(\boldsymbol{s}_{k-1}))^2.$$

To initialize the recursion, we can set $\boldsymbol{d}_K \coloneqq \mathbf{diag}(\nabla^2 \ell(\boldsymbol{s}_K))$. As an alternative, as proposed by Elsayed and Mahmood (2022), if $\boldsymbol{H}_K$ has a simple form, we can use $\nabla^2 \ell(\boldsymbol{s}_K)$ instead of $\mathbf{Diag}(\boldsymbol{d}_K)$ at the first iteration. This is the case for instance if f_K is a cross-entropy loss. The recursion is repeated until we obtain the approximate diagonal Hessian $\boldsymbol{d}_0 \approx \mathbf{diag}(\nabla^2 (\ell \circ f)(\boldsymbol{x}))$. The gradients $\boldsymbol{r}_k$, needed to compute $\boldsymbol{d}_k$, are computed along the way and the algorithm can therefore also return $\boldsymbol{r}_0 = \nabla(\ell \circ f)(\boldsymbol{x})$.

8.7.2 Computation graphs

Although this diagonal approximation was originally derived for feedforward networks Becker and Le Cun (1988), it is straightforward to generalize it to computation graphs. Namely, for a function $f(\boldsymbol{x}, \boldsymbol{w})$ decomposed along a computation graph, we can backpropagate a diagonal approximation in reverse topological order as

$$\boldsymbol{r}_{i_j} \leftarrow \boldsymbol{r}_{i_j} + \partial_j f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})^*[\boldsymbol{r}_k]$$
$$\boldsymbol{d}_{i_j} \leftarrow \boldsymbol{d}_{i_j} + \mathbf{diag}(\partial^2_{jj} f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})^*[\boldsymbol{r}_k])$$
$$+ \mathbf{diag}(\partial_j f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})^* \mathbf{Diag}(\boldsymbol{d}_k) \partial_j f_k(\boldsymbol{s}_{i_1}, \ldots, \boldsymbol{s}_{i_{p_k}})), \quad (8.5)$$

for $j \in \text{parents}(k)$, starting from $\boldsymbol{r}_K = \nabla \ell(\boldsymbol{s}_K)$ and $\boldsymbol{d}_K = \mathbf{diag}(\nabla^2 \ell(\boldsymbol{s}_K))$ or $\mathbf{Diag}(\boldsymbol{d}_K) = \nabla^2 \ell(\boldsymbol{s}_K)$. To implement such an algorithm, each elementary function in the computational graph needs to be augmented with an oracle that computes the Hessian diagonal approximation of the current function, given the previous ones. An example with MLPs is presented in Example 8.4.

> **Example 8.4** (Hessian diagonal approximation for MLPs). Consider a multilayer perceptron
>
> $$\boldsymbol{s}_k := \boldsymbol{a}_k(\boldsymbol{W}_k \boldsymbol{s}_{k-1}) \quad \forall k \in \{1, \ldots, K-1\}$$
> $$f(\boldsymbol{w}, \boldsymbol{x}) := \boldsymbol{s}_K$$
>
> starting from $\boldsymbol{s}_0 = \boldsymbol{x}$. Here $\boldsymbol{a}_k$ is the element-wise activation function (potentially the identity) and $\boldsymbol{w}$ encapsulates the weight matrices $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_K$. We consider the derivatives w.r.t. the flattened matrices, so that gradients and diagonal approximations w.r.t. these flattened quantities are vectors. The backpropagation scheme (8.5)

then reduces to, denoting $\boldsymbol{t}_k = \boldsymbol{W}_k \boldsymbol{s}_{k-1}$,

$$\boldsymbol{r}_{k-1} := \boldsymbol{W}_k^\top (\boldsymbol{a}'(\boldsymbol{t}_k) \odot \boldsymbol{r}_k)$$
$$\boldsymbol{g}_k := \mathrm{vec}((\boldsymbol{a}'(\boldsymbol{t}_k) \odot \boldsymbol{r}_k) \boldsymbol{s}_{k-1}^\top)$$
$$\boldsymbol{\delta}_k := \boldsymbol{r}_k \odot \boldsymbol{a}''(\boldsymbol{t}_k) + \boldsymbol{d}_k \odot \boldsymbol{a}'(\boldsymbol{t}_k)^2$$
$$\boldsymbol{d}_{k-1} := \left(\sum_{j=1}^{D_k} \boldsymbol{W}_{k,ij}^2 \delta_{k,j} \right)_{i=1}^{D_k}$$
$$\boldsymbol{h}_k := \mathrm{vec}(\boldsymbol{\delta}_k (\boldsymbol{s}_{k-1}^2)^\top)$$

starting from $\boldsymbol{r}_K = \nabla \ell(\boldsymbol{s}_K)$ and, e.g., $\boldsymbol{d}_K = \mathbf{diag}(\nabla^2 \ell(\boldsymbol{s}_K))$. The algorithm returns $\boldsymbol{g}_1, \ldots, \boldsymbol{g}_K$ as the gradients of f w.r.t. $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_K$, with $\boldsymbol{w}_i = \mathrm{vec}(\boldsymbol{W}_i)$, and $\boldsymbol{h}_1, \ldots, \boldsymbol{h}_K$ as the diagonal approximations of the Hessian w.r.t. $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_K$.

8.8 Randomized estimators

In this section, we describe randomized estimators of the diagonal of the Hessian or Gauss-Newton matrices.

8.8.1 Girard-Hutchinson estimator

We begin with a generic estimator, originally proposed for trace estimation by Girard (1989) and extended by Hutchinson (1989). Let $\boldsymbol{A} \in \mathbb{R}^{P \times P}$ be an arbitrary square matrix, whose matrix-vector product (matvec) is available. Suppose $\boldsymbol{\omega} \in \mathbb{R}^P$ is an isotropic random vector, i.e., such that $\mathbb{E}_{\boldsymbol{\omega} \sim p}[\boldsymbol{\omega} \boldsymbol{\omega}^\top] = I$. For example, two common choices are the Rademacher distribution $p = \mathrm{Uniform}(\{-1, 1\})$ and the standard normal distribution $p = \mathrm{Normal}(0, I)$. Then, we have

$$\mathbb{E}_{\boldsymbol{\omega} \sim p}[\langle \boldsymbol{\omega}, \boldsymbol{A} \boldsymbol{\omega} \rangle] = \mathrm{tr}(\boldsymbol{A}).$$

Applications include generalized cross-validation, computing the Kullback-Leibler divergence between two Gaussians, and computing the derivatives of the log-determinant.

The approach can be extended (Bekas *et al.*, 2007; Baston and Nakatsukasa, 2022; Hallman *et al.*, 2023) to obtain an estimator of the

diagonal of $\boldsymbol{A}$,

$$\mathbb{E}_{\boldsymbol{\omega} \sim p}[\boldsymbol{\omega} \odot \boldsymbol{A}\boldsymbol{\omega}] = \mathbf{Diag}(\boldsymbol{A}),$$

where $\odot$ denotes the Hadamard product (element-wise multiplication). This suggests that we can use the Monte-Carlo method to estimate the diagonal of $\boldsymbol{A}$,

$$\mathbf{Diag}(\boldsymbol{A}) \approx \frac{1}{S} \sum_{i=1}^{S} \boldsymbol{\omega}_i \odot \boldsymbol{A}\boldsymbol{\omega}_i,$$

with equality as $S \to \infty$, since the estimator is unbiased. Since, as reviewed in Section 8.1 and Section 8.2, we know how to multiply efficiently with the Hessian and the Gauss-Newton matrices, we can apply the technique with these matrices. The variance is determined by the number S of samples drawn and therefore by the number of matvecs performed. More elaborated approaches have been proposed to further reduce the variance (Meyer *et al.*, 2021; Epperly *et al.*, 2023).

8.8.2 Bartlett estimator for the factorization

Suppose the objective function is of the form $L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}) := \ell(f(\boldsymbol{w}; \boldsymbol{x}); \boldsymbol{y})$ where ℓ is the negative log-likelihood $\ell(\boldsymbol{\theta}; \boldsymbol{y}) := -\log p_{\boldsymbol{\theta}}(\boldsymbol{y})$ of an exponential family distribution, and $\boldsymbol{\theta} := f(\boldsymbol{w}; \boldsymbol{x})$, for some network f. We saw from the equivalence between the Fisher and Gauss-Newton matrices in Proposition 8.6 (which follows from the Bartlett identity) that

$$\begin{aligned}
\nabla_{\mathrm{GN}}^2 L(\boldsymbol{w}; \boldsymbol{x}, \cdot) &= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\partial f(\boldsymbol{w}; \boldsymbol{x})^* \nabla \ell(\boldsymbol{\theta}; Y) \otimes \nabla \ell(\boldsymbol{\theta}; Y) \partial f(\boldsymbol{w}; \boldsymbol{x})] \\
&= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla L(\boldsymbol{w}; \boldsymbol{x}, Y) \otimes \nabla L(\boldsymbol{w}; \boldsymbol{x}, Y)],
\end{aligned}$$

where $\cdot$ indicates that the result holds for any value of the second argument. This suggests a Monte-Carlo scheme

$$\nabla_{\mathrm{GN}}^2 L(\boldsymbol{w}; \boldsymbol{x}, \cdot) \approx \frac{1}{S} \sum_{j=1}^{S} [\nabla L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}_{i_j}) \otimes \nabla L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}_{i_j})]$$

where $\boldsymbol{y}_{i_1}, \ldots, \boldsymbol{y}_{i_S} \sim p_{\boldsymbol{\theta}}$ and $\boldsymbol{\theta} = f(\boldsymbol{w}, \boldsymbol{x})$. In words, we can approximate the Gauss-Newton matrix with S gradient computations. This factorization can also be used to approximate the GNVP in Eq. (8.1).

8.8.3   Bartlett estimator for the diagonal

Following a similar approach, we obtain

$$\mathbf{diag}(\nabla_{\mathrm{GN}}^2(\boldsymbol{w};\boldsymbol{x},\cdot)) = \mathbb{E}_{Y\sim p_{\boldsymbol{\theta}}}[\nabla L(\boldsymbol{w};\boldsymbol{x},Y) \odot \nabla L(\boldsymbol{w};\boldsymbol{x},Y)],$$

where $\odot$ indicates the element-wise (Hadamard) product. Using a Monte-Carlo scheme, sampling $\boldsymbol{y}_{i_1},\ldots,\boldsymbol{y}_{i_S}$ from $p_{\boldsymbol{\theta}}$, we therefore obtain

$$\mathbf{diag}(\nabla_{\mathrm{GN}}^2(\boldsymbol{w};\boldsymbol{x},\cdot)) \approx \frac{1}{S}\sum_{j=1}^{S} \nabla L(\boldsymbol{w};\boldsymbol{x},\boldsymbol{y}_{i_j}) \odot \nabla L(\boldsymbol{w};\boldsymbol{x},\boldsymbol{y}_{i_j}),$$

with equality when all labels in the support of $p_{\boldsymbol{\theta}}$ have been sampled. That estimator, used for instance in (Wei *et al.*, 2020, Appendix C.1.), requires access to **individual gradients** evaluated at the sampled labels. Another possible estimator of the diagonal is given by

$$\frac{1}{S}\,\mathbf{diag}(\nabla_{\mathrm{GN}}^2 L(\boldsymbol{w};\boldsymbol{x},\cdot))$$

$$= \mathbb{E}_{Y_1,\ldots,Y_S\sim p_{\boldsymbol{\theta}}}\left[\nabla\frac{1}{S}\sum_{i=1}^{S} L(\boldsymbol{w};\boldsymbol{x},Y_i) \odot \nabla\frac{1}{S}\sum_{i=1}^{S} L(\boldsymbol{w};\boldsymbol{x},Y_i)\right].$$

Letting $\gamma_i := \nabla L(\boldsymbol{w};\boldsymbol{x},Y_i)$, this follows from

$$\mathbb{E}\left[\sum_i \gamma_i \odot \sum_j \gamma_j\right] = \mathbb{E}\left[\sum_i \gamma_i \odot \gamma_i + \sum_{i\neq j} \gamma_i \odot \gamma_j\right]$$

$$= \mathbb{E}\left[\sum_i \gamma_i \odot \gamma_i\right]$$

where we used that $\mathbb{E}[\gamma_i \odot \gamma_j] = \mathbb{E}[\gamma_i] \odot \mathbb{E}[\gamma_j] = \mathbf{0}$ since γ_i and γ_j are independent variables for $i \neq j$ and have zero mean, from Bartlett's first identity Eq. (11.4). We can then use the Monte-Carlo method to obtain

$$\frac{1}{S}\,\mathbf{diag}(\nabla_{\mathrm{GN}}^2 L(\boldsymbol{w};\boldsymbol{x},\cdot)) \approx \left(\nabla\frac{1}{S}\sum_{j=1}^{S} L(\boldsymbol{w};\boldsymbol{x},\boldsymbol{y}_{i_j})\right) \odot \left(\nabla\frac{1}{S}\sum_{j=1}^{S} L(\boldsymbol{w};\boldsymbol{x},\boldsymbol{y}_{i_j})\right),$$

with equality when all labels in the support of $p_{\boldsymbol{\theta}}$ have been sampled. This estimator can be more convenient to implement, since it only needs access to the gradient of the **averaged** losses. However, it may suffer from higher variance. A special case of this estimator is used by Liu *et al.* (2023), where they draw only one $\boldsymbol{y}$ for each $\boldsymbol{x}$.

8.9 Summary

By using a Hessian chain rule, we can develop a "Hessian backpropagation". While it is reasonably simple for computation chains, it becomes computationally prohibitive for computation graphs, due to the cross-product terms occurring with fan-in. A better approach is to use Hessian-vector products (HVPs). We saw that there are four possible methods to compute HVPs, but the forward-over-reverse method is a priori the most efficient. Similarly as for computing gradients, computing HVPs is only a constant times more expensive than evaluating the function itself.

The Gauss-Newton matrix associated with the composition $\ell \circ f$ can be seen as an approximation of the Hessian. It is a positive semidefinite matrix if ℓ is convex, and can be used to build a principled quadratic approximation of a function. It is equivalent to the Fisher information matrix in the case of exponential families. Gauss-Newton-vector products can be computed efficiently, like HVPs.

We also described other approximations, such as (block) diagonal approximations, and randomized estimators.

9

Inference in graphical models as differentiation

A graphical model specifies how random variables depend on each other and therefore determines how their joint probability distribution factorizes. In this chapter, we review key concepts in graphical models and how they relate to differentiation, drawing in the process analogies with computation chains and computation graphs.

9.1 Chain rule of probability

The chain rule of probability is a fundamental law in probability theory for computing the **joint probability** of events. In the case of only two events A_1 and A_2, it reduces to the **product rule**

$$\mathbb{P}(A_1 \cap A_2) = \mathbb{P}(A_2|A_1)\mathbb{P}(A_1).$$

For two discrete random variables S_1 and S_2, using the events $A_1 := \{S_1 = s_1\}$ and $A_2 := \{S_2 = s_2\}$, the product rule becomes

$$\mathbb{P}(S_1 = s_1, S_2 = s_2) = \mathbb{P}(S_2 = s_2|S_1 = s_1)\mathbb{P}(S_1 = s_1).$$

More generally, using the product rule, we have for K events

$$\mathbb{P}(A_1 \cap \ldots \cap A_K) = \mathbb{P}(A_K \mid A_1 \cap \ldots \cap A_{K-1})\,\mathbb{P}(A_1 \cap \ldots \cap A_{K-1}).$$

Applying the product rule one more time, we have

$$\mathbb{P}\left(A_1 \cap \ldots \cap A_{K-1}\right) = \mathbb{P}\left(A_{K-1} \mid A_1 \cap \ldots \cap A_{K-2}\right)\mathbb{P}\left(A_1 \cap \ldots \cap A_{K-2}\right).$$

Repeating the process recursively, we arrive at the **chain rule of probability**

$$\mathbb{P}\left(A_1 \cap \ldots \cap A_K\right) = \prod_{j=1}^{K} \mathbb{P}(A_j \mid A_1 \cap \cdots \cap A_{j-1})$$

$$= \prod_{j=1}^{K} \mathbb{P}\left(A_j \,\middle|\, \bigcap_{i=1}^{j-1} A_i\right).$$

For K discrete random variables S_j, using the events $A_j := \{S_j = s_j\}$, the chain rule of probability becomes

$$\mathbb{P}\left(S_1 = s_1, \ldots, S_K = s_K\right) = \prod_{j=1}^{K} \mathbb{P}(S_j = s_j \mid S_1 = s_1, \ldots, S_{j-1} = s_{j-1}).$$

Importantly, this factorization holds without any independence assumption on the variables $S_1, \ldots, S_K$. We can further simplify this expression if we make conditional independence assumptions.

9.2 Conditional independence

We know that if two events A and B are independent, then

$$\mathbb{P}(A|B) = \mathbb{P}(A).$$

Similarly, if two random variables S_1 and S_2 are independent, then

$$\mathbb{P}(S_2 = s_2 | S_1 = s_1) = \mathbb{P}(S_2 = s_2).$$

More generally, if we work with K variables $S_1, \ldots, S_K$, some variables may depend on each other, while others may not. To simplify the notation, given a set $\mathcal{C}$, we define the shorthands

$$S_{\mathcal{C}} := (S_i \colon i \in \mathcal{C})$$

$$s_{\mathcal{C}} := (s_i \colon i \in \mathcal{C}).$$

We say that a variable S_j is independent of $S_{\mathcal{D}}$ **conditioned** on $S_{\mathcal{C}}$, with $\mathcal{C} \cap \mathcal{D} = \emptyset$, if for any $s_j, s_{\mathcal{C}}, s_{\mathcal{D}}$

$$\mathbb{P}(S_j = s_j \mid S_{\mathcal{C}} = s_{\mathcal{C}}, S_{\mathcal{D}} = s_{\mathcal{D}}) = \mathbb{P}(S_j = s_j \mid S_{\mathcal{C}} = s_{\mathcal{C}}).$$

9.3   Inference problems

9.3.1   Joint probability distributions

We consider a collection of K variables $\boldsymbol{s} := (\boldsymbol{s}_1, \ldots, \boldsymbol{s}_K)$, potentially **ordered** or **unordered**. Each $\boldsymbol{s}$ belongs to the **Cartesian product** $\mathcal{S} := \mathcal{S}_1 \times \cdots \times \mathcal{S}_K$. Throughout this chapter, we assume that the sets $\mathcal{S}_k$ are discrete for concreteness, with $\mathcal{S}_k := \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{M_k}\}$. Note that because $\mathcal{S}_k$ is discrete, we can always identify it with $\{1, \ldots, M_k\}$. A graphical model specifies a **joint probability distribution**

$$\mathbb{P}(S = \boldsymbol{s}) = \mathbb{P}(S_1 = \boldsymbol{s}_1, \ldots, S_K = \boldsymbol{s}_K)$$
$$= p(\boldsymbol{s})$$
$$= p(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_K),$$

where p is the probability mass function of the joint probability distribution. Summing over the Cartesian product of all possible configurations, we obtain

$$\sum_{\boldsymbol{s} \in \mathcal{S}} p(\boldsymbol{s}) = \sum_{\boldsymbol{s}_1, \ldots, \boldsymbol{s}_K \in \mathcal{S}} p(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_K) = 1.$$

As we shall see, the graph of a graphical model encodes the **dependencies** between the variables $(S_1, \ldots, S_K)$ and therefore how their joint distribution **factorizes**. Given access to a joint probability distribution, there are several **inference** problems one typically needs to solve.

9.3.2   Likelihood

A trivial task is to compute the **likelihood** of some observations $\boldsymbol{s} = (\boldsymbol{s}_1, \ldots, \boldsymbol{s}_K)$,

$$\mathbb{P}(S_1 = \boldsymbol{s}_1, \ldots, S_k = \boldsymbol{s}_k) = p(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_k).$$

It is also common to compute the **log-likelihood**,

$$\log \mathbb{P}(S_1 = \boldsymbol{s}_1, \ldots, S_k = \boldsymbol{s}_k) = \log p(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_k).$$

9.3.3   Maximum a-posteriori inference

Another common task is to compute the most likely configuration,

$$\underset{\boldsymbol{s}_1 \in \mathcal{S}_1, \ldots, \boldsymbol{s}_K \in \mathcal{S}_K}{\arg\max} \; p(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_K).$$

This is the **mode** of the joint probability distribution.

9.3.4   Marginal inference

The operation of **marginalization** consists in summing (or integrating) over all possible values of a given variable in a joint probability distribution. This allows us to compute the **marginal probability** of the remaining variables. For instance, we may want to marginalize all variables but $S_k = s_k$. To do so, we define the Cartesian product

$$\mathcal{C}_k(s_k) := \underbrace{\mathcal{S}_1 \times \cdots \times \mathcal{S}_{k-1}}_{\mathcal{A}_{k-1}} \times \{s_k\} \times \underbrace{\mathcal{S}_{k+1} \times \cdots \times \mathcal{S}_K}_{\mathcal{B}_{k+1}}. \qquad (9.1)$$

Summing over all variables but S_k, we obtain the marginal probability of $S_k = s_k$ as

$$\mathbb{P}(S_k = s_k) = \sum_{s_1,\ldots,s_K \in \mathcal{C}_k(s_k)} p(s_1,\ldots,s_K)$$

$$= \sum_{s_1,\ldots,s_{k-1} \in \mathcal{A}_{k-1}} \sum_{s_{k+1},\ldots,s_K \in \mathcal{B}_{k+1}} p(s_1,\ldots,s_K)$$

Defining similarly

$$\mathcal{C}_{k,l}(s_k, s_l) := \mathcal{S}_1 \times \cdots \times \{s_k\} \times \cdots \times \{s_l\} \times \cdots \times \mathcal{S}_K,$$

we obtain

$$\mathbb{P}(S_k = s_k, S_l = s_l) = \sum_{s_1,\ldots,s_K \in \mathcal{C}_{k,l}(s_k,s_l)} p(s_1,\ldots,s_K).$$

In particular, we may want to compute the marginal probability of two consecutive variables, $\mathbb{P}(S_{k-1} = s_{k-1}, S_k = s_k)$.

9.3.5   Expectation, convex hull, marginal polytope

Another common operation is to compute the expectation of $\phi(S)$ under a distribution p. It is defined by

$$\boldsymbol{\mu} := \mathbb{E}_{S \sim p}[\phi(S)] = \sum_{s \in \mathcal{S}} p(s)\phi(s) \in \mathcal{M}$$

For the expectation under $p_{\boldsymbol{\theta}}$, we write

$$\mu(\boldsymbol{\theta}) := \mathbb{E}_{S \sim p_{\boldsymbol{\theta}}}[\phi(S)] = \sum_{\boldsymbol{s} \in \mathcal{S}} p_{\boldsymbol{\theta}}(\boldsymbol{s}) \phi(\boldsymbol{s}) \in \mathcal{M}.$$

In exponential family distributions (Section 3.4), the function ϕ is called a **sufficient statistic**. It decomposes as

$$\phi(\boldsymbol{s}) := (\phi_{\mathcal{C}}(\boldsymbol{s}_{\mathcal{C}}))_{\mathcal{C} \in C},$$

where $\mathcal{C} \subseteq [K]$. Intuitively, $\phi(\boldsymbol{s})$ can be thought as an **encoding** or **embedding** of $\boldsymbol{s}$ (a potentially discrete object such as a sequence of integers) in a vector space. Under this decomposition, we can also compute

$$\boldsymbol{\mu}_{\mathcal{C}} := \mathbb{E}_S[\phi_{\mathcal{C}}(S_{\mathcal{C}})] = \sum_{\boldsymbol{s} \in \mathcal{S}} p(\boldsymbol{s}) \phi_{\mathcal{C}}(\boldsymbol{s}_{\mathcal{C}}).$$

Convex hull

The mean $\boldsymbol{\mu}$ belongs to the **convex hull** of $\phi(\mathcal{S}) := \{\phi(\boldsymbol{s}) \colon \boldsymbol{s} \in \mathcal{S}\}$,

$$\mathcal{M} := \text{conv}(\phi(\mathcal{S})) := \left\{ \sum_{\boldsymbol{s} \in \mathcal{S}} p(\boldsymbol{s}) \phi(\boldsymbol{s}) \colon p \in \mathcal{P}(\mathcal{S}) \right\},$$

where $\mathcal{P}(\mathcal{S})$ is the set of all possible probability distributions over $\mathcal{S}$. In other words, $\mathcal{M}$ is the set of all possible convex combinations of $\phi(\boldsymbol{s})$ for $\boldsymbol{s} \in \mathcal{S}$. The vertices of $\mathcal{M}$ are all the $\boldsymbol{s} \in \mathcal{S}$.

Case of binary encodings: the marginal polytope

In the special case of a discrete set $\mathcal{S}_k = \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_M\}$ and of a **binary encoding** (indicator function) $\phi(\boldsymbol{s})$, the set $\mathcal{M}$ is called the **marginal polytope** (Wainwright and Jordan, 2008), because each point $\boldsymbol{\mu} \in \mathcal{M}$ contains marginal probabilities. To see why, consider the **unary** potential

$$[\phi(\boldsymbol{s})]_{k,i} = [\phi_k(\boldsymbol{s}_k)]_i = \mathbb{I}(\boldsymbol{s}_k = \boldsymbol{v}_i) \tag{9.2}$$

where $\mathbb{I}(p) := 1$ if p is true, 0 otherwise. We then obtain the marginal probability of $S_k = v_i$,

$$
\begin{aligned}
[\boldsymbol{\mu}]_{k,i} &= \mathbb{E}_S[\phi(S)_{k,i}] \\
&= \mathbb{E}_{S_k}[\phi_k(S_k)_i] \\
&= \mathbb{E}_{S_k}[\mathbb{I}(S_k = v_i)] \\
&= \sum_{s_k \in \mathcal{S}_k} \mathbb{P}(S_k = s_k)\mathbb{I}(s_k = v_i) \\
&= \mathbb{P}(S_k = v_i).
\end{aligned}
$$

Likewise, consider the **pairwise** potential

$$
[\phi(s)]_{k,l,i,j} = [\phi_{k,l}(s_k, s_l)]_{i,j} = \mathbb{I}(s_k = v_i, s_l = v_j). \tag{9.3}
$$

We then obtain the marginal probability of $S_k = v_i$ and $S_l = v_j$,

$$
\begin{aligned}
[\boldsymbol{\mu}]_{k,l,i,j} &= \mathbb{E}_S[\phi(S)_{k,l,i,j}] \\
&= \mathbb{E}_{S_k,S_l}[\phi_{k,l}(S_k, S_l)_{i,j}] \\
&= \mathbb{E}_{S_k,S_l}[\mathbb{I}(S_k = v_i, S_l = v_j)] \\
&= \sum_{s_k \in \mathcal{S}_k} \sum_{s_l \in \mathcal{S}_l} \mathbb{P}(S_k = s_k, S_l = s_l)\mathbb{I}(s_k = v_i, s_l = v_j) \\
&= \mathbb{P}(S_k = s_k, S_l = v_j).
\end{aligned}
$$

We can do the same with higher-order potential functions.

9.3.6 Complexity of brute force

Apart from computing the likelihood, which is trivial, computing the marginal, mode and expectation by brute force takes $O(\prod_{k=1}^K |\mathcal{S}_k|)$ time. In particular, if $|\mathcal{S}_k| = M \; \forall k \in [K]$, brute force takes $O(M^K)$ time.

9.4 Markov chains

In this section, we briefly review Markov chains. Our notation is chosen to emphasize the analogies with computation chains.

9.4.1   The Markov property

When random variables are organized **sequentially** as $S_1, \ldots, S_K$, a simple example of conditional independence is when each variable $S_k \in \mathcal{S}_k$ only depends on the previous variable $S_{k-1} \in \mathcal{S}_{k-1}$, that is,

$$\mathbb{P}(S_k = s_k \mid S_{k-1} = s_{k-1}, \ldots, S_1 = s_1) = \mathbb{P}(S_k = s_k \mid S_{k-1} = s_{k-1})$$
$$:= p_k(s_k \mid s_{k-1}),$$

A probability distribution satisfying the above is said to satisfy the **Markov property**, and is called a **Markov chain**. A computation chain is specified by the functions f_k, that take s_{k-1} as input and output s_k. In analogy, a Markov chain is specified by the **conditional** probability distributions p_k of S_k given S_{k-1}. We can then define the **generative process**

$$S_0 := s_0$$
$$S_1 \sim p_1(\cdot \mid S_0)$$
$$S_2 \sim p_2(\cdot \mid S_1)$$
$$\vdots$$
$$S_K \sim p_K(\cdot \mid S_{K-1}).$$

Strictly speaking, we should write $S_k \mid S_{k-1} \sim p_k(\cdot \mid S_{k-1})$. We choose our notation both for conciseness and for analogy with computation chains. Furthermore, to simplify the notation, we assume without loss of generality that S_0 is deterministic (if this is not the case, we can always move S_0 to S_1 and add a dummy variable as S_0). That is, $\mathbb{P}(S_0 = s_0) = p_0(s_0) := 1$ and $\mathcal{S}_0 := \{s_0\}$. This amounts to setting the **initial distribution** of S_1 as

$$\mathbb{P}(S_1 = s_1) := \mathbb{P}(S_0 = s_0)\mathbb{P}(S_1 = s_1|S_0 = s_0) = \mathbb{P}(S_1 = s_1|S_0 = s_0).$$
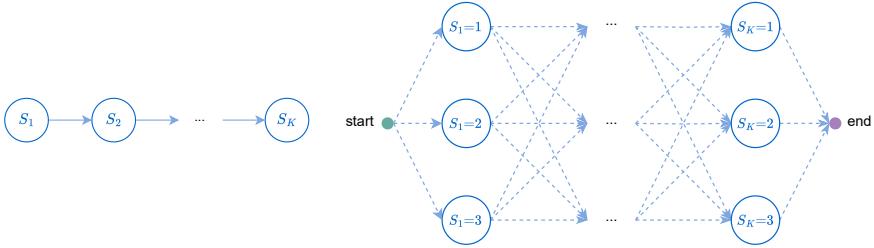
Figure 9.1: Left: Markov chain. **Right:** Computation graph of the forward-backward and the Viterbi algorithms: a lattice.

We can then compute the joint probability of the Markov chain by

$$
\mathbb{P}(S_1 = \boldsymbol{s}_1, \ldots, S_K = \boldsymbol{s}_K) = p(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_K)
$$
$$
= \prod_{k=1}^{K} \mathbb{P}(S_k = \boldsymbol{s}_k \mid S_{k-1} = \boldsymbol{s}_{k-1})
$$
$$
= \prod_{k=1}^{K} p_k(\boldsymbol{s}_k \mid \boldsymbol{s}_{k-1}),
$$

where we left the dependence on $\boldsymbol{s}_0$ implicit, since $p_0(\boldsymbol{s}_0) = 1$. A Markov chain with $\mathcal{S}_k = \{1, 2, 3\}$ is illustrated in Fig. 9.1. A chain defines a **totally ordered set** $\{1, \ldots, K\}$, since two nodes in the graph are necessarily linked to each other by a path.

Example 9.1 (Chain of categorical distributions). Suppose our goal is predict, from $\boldsymbol{x} \in \mathcal{X}$, a sequence of length K, where each S_k belongs to $\mathcal{S}_k = \{1, \ldots, M\}$. In natural language processing, this task is called sequence tagging. We can define

$$
S_k \sim \text{Categorical}(\boldsymbol{\pi}_{k-1, k, S_{k-1}})
$$

where

$$
\boldsymbol{\pi}_{k-1,k,i} := \text{softargmax}(\boldsymbol{\theta}_{k-1,k,i}) \in \triangle^M
$$
$$
= (\pi_{k-1,k,i,j})_{j=1}^{M}
$$
$$
\boldsymbol{\theta}_{k-1,k,i} := (\theta_{k-1,k,i,j})_{j=1}^{M} \in \mathbb{R}^M
$$
$$
\theta_{k-1,k,i,j} := f_{k-1,k}(\boldsymbol{x}, i, j, \boldsymbol{w}_k) \in \mathbb{R}.
$$

We therefore have

$$\mathbb{P}(S_k = j \mid S_{k-1} = i) = p_k(j \mid i)$$
$$= \pi_{k-1,k,i,j}$$
$$= [\mathrm{softargmax}(\boldsymbol{\theta}_{k-1,k,i})]_j$$
$$= \frac{\exp(\theta_{k-1,k,i,j})}{\sum_{j'} \exp(\theta_{k-1,k,i,j'})}$$

and

$$\log \mathbb{P}(S_k = j \mid S_{k-1} = i) = \log p_k(j \mid i)$$
$$= \theta_{k-1,k,i,j} - \mathrm{logsumexp}(\boldsymbol{\theta}_{k-1,k,i})$$
$$= \theta_{k-1,k,i,j} - \log \sum_{j'} \exp(\theta_{k-1,k,i,j'}).$$

We emphasize that because $k - 1$ and k are always consecutive, the representation $\theta_{k-1,k,i,j}$ is inefficient; we could use $\theta_{k,i,j}$ instead. Our notation is designed for consistency with Markov random fields.

9.4.2   Time-homogeneous Markov chains

A **time-homogeneous** discrete-time Markov chain corresponds to the case when the distribution of S_k given S_{k-1} is the same regardless of k:

$$p_1 = \cdots = p_K = p.$$

The **finite-space** case corresponds to when each $S_k \in \mathcal{S}$ can take a finite set of values $\mathcal{S} = \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_M\}$ and

$$\mathbb{P}(S_k = \boldsymbol{v}_j \mid S_{k-1} = \boldsymbol{v}_i) = p(\boldsymbol{v}_j | \boldsymbol{v}_i) = \pi_{i,j},$$

where $\pi_{i,j} \in [0,1]$ is the **transition probability** from $\boldsymbol{v}_i$ to $\boldsymbol{v}_j$. Because the set $\mathcal{S} = \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_M\}$ is discrete, we can always identify it with $\{1, \ldots, M\}$. That is, we can instead write

$$\mathbb{P}(S_k = j \mid S_{k-1} = i) = p(j|i) = \pi_{i,j}.$$

9.4.3 Higher-order Markov chains

More generally, a nth-order Markov chain may depend, not only on the last variable, but on the last n variables,

$$
\begin{aligned}
&\mathbb{P}(S_k = \boldsymbol{s}_k \mid S_{k-1} = \boldsymbol{s}_{k-1}, \ldots, S_1 = \boldsymbol{s}_1) \\
=&\mathbb{P}(S_k = \boldsymbol{s}_k \mid S_{k-1} = \boldsymbol{s}_{k-1}, \ldots, S_{k-n} = \boldsymbol{s}_{k-n}) \\
=&p_k(\boldsymbol{s}_k|\boldsymbol{s}_{k-1}, \ldots, \boldsymbol{s}_{k-n}).
\end{aligned}
$$

Autoregressive models such as Transformers can be seen as specifying a higher-order Markov chain, with a context window of size n. The larger context makes exact inference using dynamic programming computationally intractable. This is why practitioners use **beam search** or **ancestral sampling** (Section 9.5.3) instead.

9.5 Bayesian networks

In this section, we briefly review Bayesian networks. Our notation is chosen to emphasize the analogies with computation graphs.

9.5.1 Expressing variable dependencies using DAGs

Markov chains and more generally higher-order Markov chains are a special case of Bayesian network. Similarly to computation graphs reviewed in Section 7.3, variable dependencies can be expressed using a directed acylic graph (DAG) $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where the vertices $\mathcal{V} = \{1, \ldots, K\}$ represent variables and edges $\mathcal{E}$ represent variable dependencies. The set $\{i_1, \ldots, i_{n_k}\} = \text{parents}(k) \subseteq \mathcal{V}$, where $n_k := |\text{parents}(k)|$, indicates the variables $S_{i_1}, \ldots, S_{i_{n_k}}$ that S_k depends on. This defines a **partially ordered set** (poset). For notational simplicity, we again assume without loss of generality that S_0 is deterministic. A computation graph is specified by functions $f_1, \ldots, f_K$ in topological order. In analogy, a **Bayesian network** is specified by **conditional** probability distributions p_k of S_k given $S_{\text{parents}(k)}$. We can then define the **generative**

process

$$S_0 := \boldsymbol{s}_0$$
$$S_1 \sim p_1(\cdot \mid S_0)$$
$$S_2 \sim p_2(\cdot \mid S_{\text{parents}(2)})$$
$$\vdots$$
$$S_K \sim p_K(\cdot \mid S_{\text{parents}(K)}).$$

Using the chain rule of probability and variable independences expressed by the DAG, the **joint probability distribution** is then (assuming a topological order for $S_0, S_1, \ldots, S_K$)

$$\mathbb{P}(S = \boldsymbol{s}) := \mathbb{P}(S_1 = \boldsymbol{s}_1, \ldots, S_K = \boldsymbol{s}_K)$$
$$= \prod_{k=1}^{K} \mathbb{P}(S_k = s_k | S_{\text{parents}(k)} = \boldsymbol{s}_{\text{parents}(k)})$$
$$:= \prod_{k=1}^{K} p_k(s_k | \boldsymbol{s}_{\text{parents}(k)})$$

This representation is well suited to express **causal** relationships between random variables.

9.5.2   Parameterizing Bayesian networks

In a Bayesian framework, observed data, latent variables, parameters and noise variables are all treated as random variables. If the conditional distribution p_k associated to node k depends on some parameters, they can be provided to p_k as conditioning, using parent nodes.

A Bayesian network is specified by the conditional distributions p_k. Therefore, unlike computation graphs, there is no notion of function f_k in a Bayesian network. However, the root nodes of the Bayesian network can be the output of a neural network. For instance, autoregressive models, such as RNNs or Transformers, specify the conditional probability distribution of a token given past tokens, and the chain rule of probability is used to obtain a probability distribution over entire sequences.

9.5.3 Ancestral sampling

A major advantage of Bayesian networks is that, provided that each conditional distribution p_k is normalized, the joint distribution of $S = (S_1, \ldots, S_K)$ is automatically normalized. This means that we can very easily draw i.i.d. samples from the joint distribution, by following the generative process: we follow the topological order $k = 1, \ldots, K$ and on iteration k we draw a value $s_k \sim p_k(\cdot | \boldsymbol{s}_{\mathrm{parents}(k)})$ conditioned on the previous values $\boldsymbol{s}_{\mathrm{parents}(k)}$. This is known as **ancestral sampling**.

9.6 Markov random fields

9.6.1 Expressing factors using undirected graphs

A Markov random field (MRF), a.k.a. undirected graphical model, specifies a distribution that factorizes as

$$\mathbb{P}(S = \boldsymbol{s}) = p(\boldsymbol{s}) := \frac{1}{Z} \prod_{\mathcal{C} \in C} \psi_{\mathcal{C}}(\boldsymbol{s}_{\mathcal{C}}),$$

where C is the set of maximal **cliques** of $\mathcal{G}$, that is, subsets of $\mathcal{V}$ that are fully connected, Z is a normalization constant defined by

$$Z := \sum_{\boldsymbol{s} \in \mathcal{S}} \prod_{\mathcal{C} \in C} \psi_{\mathcal{C}}(\boldsymbol{s}_{\mathcal{C}}),$$

and $\psi_{\mathcal{C}} : \mathcal{S}_{\mathcal{C}} \to \mathbb{R}_+$ is a **potential function** (a.k.a. compatibility function), with $\mathcal{S}_{\mathcal{C}} := (\mathcal{S}_j)_{j \in \mathcal{C}}$. According to the Hammersley-Clifford theorem, an MRF can be equivalently defined in terms of Markov properties; we refer the interested reader to Wainwright and Jordan (2008). For the sake of this chapter, the definition above is sufficient for our purposes.

Example 9.2 (Markov chains as Markov random fields). For a chain, letting $S = (S_1, \ldots, S_K)$ and $\boldsymbol{s} = (\boldsymbol{s}_1, \ldots, \boldsymbol{s}_K)$, recall that

$$\mathbb{P}(S = \boldsymbol{s}) = \prod_{k=1}^{K} p_k(\boldsymbol{s}_k \mid \boldsymbol{s}_{k-1}).$$

This is equivalent to an MRF with $Z = 1$ (since a chain is auto-

matically normalized),

$$C := \{\{0, 1\}, \{1, 2\}, \dots, \{K - 1, K\}\}$$

and with potential function

$$\psi_{\{k-1,k\}}(\boldsymbol{s}_{k-1}, \boldsymbol{s}_k) := p_k(\boldsymbol{s}_k | \boldsymbol{s}_{k-1}).$$

More generally, a Bayesian network can be similarly written as an MRF by creating appropriate potential functions corresponding to the parents of each node.

9.6.2 MRFs as exponential family distributions

Let us define the potential functions

$$\psi_C(\boldsymbol{s}_C; \boldsymbol{\theta}_C) := \exp(\langle \boldsymbol{\theta}_C, \phi_C(\boldsymbol{s}_C) \rangle)$$

for some sufficient statistic function $\phi_C \colon \mathcal{S}_C \to \Theta_C$ and parameters $\boldsymbol{\theta}_C \in \Theta_C$. Then,

$$
\begin{aligned}
p_{\boldsymbol{\theta}}(\boldsymbol{s}) &:= \frac{1}{Z(\boldsymbol{\theta})} \prod_{C \in C} \psi_C(\boldsymbol{s}_C; \boldsymbol{\theta}_C) \\
&= \frac{1}{Z(\boldsymbol{\theta})} \prod_{C \in C} \exp(\langle \boldsymbol{\theta}_C, \phi_C(\boldsymbol{s}_C) \rangle) \\
&= \frac{1}{Z(\boldsymbol{\theta})} \exp\left(\sum_{C \in C} \langle \boldsymbol{\theta}_C, \phi_C(\boldsymbol{s}_C) \rangle \right) \\
&= \frac{1}{Z(\boldsymbol{\theta})} \exp\left(\langle \boldsymbol{\theta}, \phi(\boldsymbol{s}) \rangle \right) \\
&= \exp\left(\langle \boldsymbol{\theta}, \phi(\boldsymbol{s}) \rangle - A(\boldsymbol{\theta}) \right)
\end{aligned}
$$

where

$$\phi(\boldsymbol{s}) := (\phi_{\mathcal{C}}(\boldsymbol{s}_{\mathcal{C}}))_{\mathcal{C} \in C}$$

$$\boldsymbol{\theta} := (\boldsymbol{\theta}_{\mathcal{C}})_{\mathcal{C} \in C}$$

$$Z(\boldsymbol{\theta}) := \sum_{\boldsymbol{s} \in \mathcal{S}} \prod_{\mathcal{C} \in C} \psi_{\mathcal{C}}(\boldsymbol{s}_{\mathcal{C}}; \boldsymbol{\theta}_{\mathcal{C}})$$

$$= \sum_{\boldsymbol{s} \in \mathcal{S}} \exp\left(\langle \boldsymbol{\theta}, \phi(\boldsymbol{s}) \rangle\right)$$

$$A(\boldsymbol{\theta}) := \log Z(\boldsymbol{\theta})$$

Therefore, for this choice of potential functions, we can view an MRF as an exponential family distribution (Section 3.4) with **natural parameters** $\boldsymbol{\theta}$, **sufficient statistic** ϕ and **log-partition** function $A(\boldsymbol{\theta})$.

Example 9.3 (Ising model). The Ising model is a classical example of MRF. Let $Y = (Y_1, \ldots, Y_M) \in \{0, 1\}^M$ be an unordered collection of binary variables $Y_i \in \{0, 1\}$. This forms a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V} = [M]$ and $\mathcal{E} \subseteq V^2$, such that $(i, j) \in \mathcal{E}$ means that Y_i interacts with Y_j. In statistical physics, Y_i may indicate the presence or absence of particles, or the orientation of magnets. In image processing, Y_i may represent a black and white pixel. In multi-label classification, Y_i may indicate the presence or absence of a label. The probability of $\boldsymbol{y} = (y_1, \ldots, y_M) \in \{0, 1\}^M$ is then

$$\mathbb{P}(Y = \boldsymbol{y}) = p_{\boldsymbol{\theta}}(\boldsymbol{y})$$

$$= \exp\left(\sum_{i \in \mathcal{V}} \theta_i y_i + \sum_{(i,j) \in \mathcal{E}} \theta_{i,j} y_i y_j - A(\boldsymbol{\theta})\right)$$

$$= \exp\left(\sum_{\mathcal{C} \in C} \langle \boldsymbol{\theta}_{\mathcal{C}}, \phi_{\mathcal{C}}(\boldsymbol{y}) \rangle - A(\boldsymbol{\theta})\right),$$

where $C := \mathcal{V} \cup \mathcal{E}$ and $\boldsymbol{\theta} \in \mathbb{R}^{|\mathcal{V}| + |\mathcal{E}|}$ is the concatenation of $(\theta_i)_{i \in \mathcal{V}}$ and $(\theta_{i,j})_{(i,j) \in \mathcal{E}}$. These models are also known as **Boltzmann machines** in a neural network context. MAP inference in general Ising models is know to be NP-hard, but when the interaction weights $\theta_{i,j}$ are non-negative, MAP inference can be reduced to graph cut algorithms

(Greig *et al.*, 1989). There are two ways the above equation can be extended. First, we can use higher-order interactions, such as $y_i y_j y_k$ for $(i, j, k) \in \mathcal{V}^3$. Second, we may want to use categorical variables, which leads to the **Potts model**.

9.6.3   Conditional random fields

Conditional random fields (Lafferty *et al.*, 2001; Sutton, McCallum, *et al.*, 2012) are a special case of Markov random field, in which a conditioning variable is **explicitly** incorporated. For example, when the goal is to predict a variable $\boldsymbol{y}$ conditioned on a variable $\boldsymbol{x}$, CRFs are defined as

$$\mathbb{P}(Y = \boldsymbol{y} \mid X = \boldsymbol{x}) = p(\boldsymbol{y} \mid \boldsymbol{x}) = \frac{1}{Z(\boldsymbol{x})} \prod_{\mathcal{C} \in C} \psi_{\mathcal{C}}(\boldsymbol{y}_{\mathcal{C}}, \boldsymbol{x}).$$

Note that the potential functions $\Psi_{\mathcal{C}}$ are allowed to depend on the whole $\boldsymbol{x}$, as $\boldsymbol{x}$ is just a conditioning variable.

9.6.4   Sampling

Contrary to Bayesian networks, MRFs require an explicit normalization constant Z. As a result, sampling from a distribution represented by a general MRF is usually more involved than for Bayesian networks. A commonly-used technique is **Gibbs sampling**.

9.7   Inference on chains

In this section, we review how to perform marginal inference and maximum a-posteriori inference on joint distributions of the form

$$p(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_K) = \frac{1}{Z} \prod_{k=1}^{K} \psi_k(\boldsymbol{s}_{k-1}, \boldsymbol{s}_k),$$

where

$$Z := \sum_{s \in \mathcal{S}} \prod_{k=1}^{K} \psi_k(\boldsymbol{s}_{k-1}, \boldsymbol{s}_{k-1})$$

and where we used ψ_k as a shorthand for $\psi_{k-1,k}$, since $k-1$ and k are consecutive. As explained in Example 9.2, this also includes Markov

chains by setting

$$\psi_k(s_{k-1}, s_k) := p_k(s_k \mid s_{k-1}),$$

in which case $Z = 1$.

9.7.1 The forward-backward algorithm

The key idea of the forward-backward algorithm is to use the **distributivity** of multiplication over addition to write

$$Z = \sum_{s_1 \in \mathcal{S}_1} \psi_1(s_0, s_1) \sum_{s_2 \in \mathcal{S}_2} \psi_2(s_1, s_2) \cdots \sum_{s_K \in \mathcal{S}_K} \psi_K(s_{K-1}, s_K).$$

We can compute these sums recursively, either **forward** or **backward**. Recalling the definitions of $\mathcal{A}_{k-1}$ and $\mathcal{B}_{k+1}$ in Eq. (9.1), we define the summations **up to** and **down to** k,

$$\alpha_k(s_k) := \sum_{s_1, \dots, s_{k-1} \in \mathcal{A}_{k-1}} \prod_{j=1}^{k} \psi_j(s_{j-1}, s_j)$$

$$= \sum_{s_{k-1} \in \mathcal{S}_{k-1}} \psi_k(s_{k-1}, s_k) \cdots \sum_{s_1 \in \mathcal{S}_1} \psi_2(s_1, s_2)\psi_1(s_0, s_1)$$

$$\beta_k(s_k) := \sum_{s_{k+1}, \dots, s_K \in \mathcal{B}_{k+1}} \prod_{j=k+1}^{K} \psi_j(s_{j-1}, s_j)$$

$$= \sum_{s_{k+1} \in \mathcal{S}_{k+1}} \psi_{k+1}(s_k, s_{k+1}) \cdots \sum_{s_K \in \mathcal{S}_K} \psi_K(s_{K-1}, s_K).$$

We can compute the two quantities by recursing forward and backward

$$\alpha_k(s_k) = \sum_{s_{k-1} \in \mathcal{S}_{k-1}} \psi_k(s_{k-1}, s_k)\alpha_{k-1}(s_{k-1})$$

$$\beta_k(s_k) = \sum_{s_{k+1} \in \mathcal{S}_{k+1}} \psi_{k+1}(s_k, s_{k+1})\beta_{k+1}(s_{k+1})$$

where we defined the initializations

$$\alpha_1(s_1) := \psi_1(s_0, s_1) \quad \forall s_1 \in \mathcal{S}_1$$

$$\beta_K(s_K) := 1 \quad \forall s_K \in \mathcal{S}_K.$$

The **normalization** term can then be computed by

$$Z = \sum_{s_K \in \mathcal{S}_K} \alpha_K(s_K)\beta_K(s_K) = \sum_{s_1 \in \mathcal{S}_1} \alpha_1(s_1)\beta_1(s_1)$$

and the **marginal probabilities** by

$$\mathbb{P}(S_k = s_k) = \frac{1}{Z}\alpha_k(s_k)\beta_k(s_k)$$

$$\mathbb{P}(S_{k-1} = s_{k-1}, S_k = s_k) = \frac{1}{Z}\alpha_{k-1}(s_{k-1})\psi_k(s_{k-1}, s_k)\beta_k(s_k).$$

We can also compute the conditional probabilities by

$$\begin{aligned}
\mathbb{P}(S_k = s_k \mid S_{k-1} = s_{k-1}) &= \frac{\mathbb{P}(S_{k-1} = s_{k-1}, S_k = s_k)}{\mathbb{P}(S_{k-1} = s_{k-1})} \\
&= \frac{\alpha_{k-1}(s_{k-1})\psi_k(s_{k-1}, s_k)\beta_k(s_k)}{\alpha_{k-1}(s_{k-1})\beta_{k-1}(s_{k-1})} \\
&= \frac{\psi_k(s_{k-1}, s_k)\beta_k(s_k)}{\beta_{k-1}(s_{k-1})}.
\end{aligned}$$

In practice, the two recursions are often implemented in the **log-domain** for numerical stability,

$$\log \alpha_k(s_k) = \log \sum_{s_{k-1} \in \mathcal{S}_{k-1}} \exp(\log \psi_k(s_{k-1}, s_k) + \log \alpha_{k-1}(s_{k-1}))$$

$$\log \beta_k(s_k) = \log \sum_{s_{k+1} \in \mathcal{S}_{k+1}} \exp(\log \psi_{k+1}(s_k, s_{k+1}) + \log \beta_{k+1}(s_{k+1})).$$

We recognize the **log-sum-exp** operator, which can be implemented in a numerically stable way (Section 4.4.2). The overal **dynamic programming** procedure, a.k.a. **forward-backward** algorithm (Baum and Petrie, 1966; Rabiner, 1989), is summarized in Algorithm 9.1. We notice that the forward and backward passes are actually independent of each other, and can therefore be performed in parallel.

9.7.2 The Viterbi algorithm

Similarly, using the distributivity of multiplication over maximization,

$$\max_{s_1 \in \mathcal{S}_1, \dots, s_K \in \mathcal{S}_K} \prod_{k=1}^{K} \psi_k(s_{k-1}, s_k)$$

$$= \max_{s_K \in \mathcal{S}_K} \max_{s_{K-1} \in \mathcal{S}_{K-1}} \psi_K(s_{K-1}, s_K) \dots \max_{s_1 \in \mathcal{S}_1} \psi_2(s_1, s_2)\psi_1(s_0, s_1).$$

Algorithm 9.1 Marginal inference on a chain

   Potential functions: $\psi_1, \ldots, \psi_K$
   Input: s_0
1: Initialize $\alpha_1(s_1) := \psi_1(s_0, s_1) \; \forall s_1 \in \mathcal{S}_1$
2: **for** $k := 2, \ldots, K$ **do** $\triangleright$ Forward pass
3:     **for** $s_k \in \mathcal{S}_k$ **do**
4:         $\alpha_k(s_k) := \displaystyle\sum_{s_{k-1} \in \mathcal{S}_{k-1}} \psi_k(s_{k-1}, s_k) \alpha_{k-1}(s_{k-1})$

5: Initialize $\beta_K(s_K) := 1 \; \forall s_K \in \mathcal{S}_K$
6: **for** $k := K - 1, \ldots, 1$ **do** $\triangleright$ Backward pass
7:     **for** $s_k \in \mathcal{S}_k$ **do**
8:         $\beta_k(s_k) := \displaystyle\sum_{s_{k+1} \in \mathcal{S}_{k+1}} \psi_{k+1}(s_k, s_{k+1}) \beta_{k+1}(s_{k+1})$

9: Compute $Z = \displaystyle\sum_{s_K \in \mathcal{S}_K} \alpha_K(s_K) \beta_K(s_K) = \sum_{s_K \in \mathcal{S}_K} \alpha_K(s_K)$
   Outputs: $\forall k \in [K]$:
   $\mathbb{P}(S_k = s_k) = \frac{1}{Z} \alpha_k(s_k) \beta_k(s_k)$
   $\mathbb{P}(S_{k-1} = s_{k-1}, S_k = s_k) = \frac{1}{Z} \alpha_{k-1}(s_{k-1}) \psi_k(s_{k-1}, s_k) \beta_k(s_k)$

Let us define for $k \in [K]$

$$\delta_k(s_k) := \max_{s_{k-1} \in \mathcal{S}_{k-1}} \psi_k(s_{k-1}, s_k) \ldots \max_{s_1 \in \mathcal{S}_1} \psi_2(s_1, s_2) \psi_1(s_0, s_1).$$

We can compute these quantities recursively, since for $k \in [K]$

$$\delta_k(s_k) = \max_{s_{k-1} \in \mathcal{S}_{k-1}} \psi_k(s_{k-1}, s_k) \delta_{k-1}(s_{k-1}),$$

with $\delta_1(s_k) := \psi(s_0, s_k)$. We finally have

$$\max_{s_1 \in \mathcal{S}_1, \ldots, s_K \in \mathcal{S}_K} p(s_1, \ldots, s_K) = \frac{1}{Z} \max_{s_K \in \mathcal{S}_K} \delta_K(s_K).$$

In practice, for numerical stability, we often implement the forward recursion in the **log-domain**. Using the fact that the logarithm is monotonic, we indeed have for all $k \in [K]$

$$\log \delta_k(s_k) = \max_{s_{k-1} \in \mathcal{S}_{k-1}} \log \psi_k(s_{k-1}, s_k) + \log \delta_{k-1}(s_{k-1}).$$

To enable efficient **backtracking**, during the forward pass, we compute

$$q_k(s_k) := \underset{s_{k-1} \in \mathcal{S}_{k-1}}{\arg\max} \psi_k(s_{k-1}, s_k)\delta_{k-1}(s_{k-1})$$

which can be thought as **backpointers** from $s_k^\star$ to $s_{k-1}^\star$.

The resulting dynamic programming procedure, a.k.a. **Viterbi algorithm** (Viterbi, 1967; Forney, 1973), is summarized in Algorithm 9.2.

Algorithm 9.2 MAP inference on a chain

Potential functions: $\psi_1, \ldots, \psi_K$
Input: s_0
1: Initialize $\delta_1(s_1) := \psi_1(s_0, s_1) \; \forall s_1 \in \mathcal{S}_1$
2: **for** $k := 2, \ldots, K$ **do**   ▷ Forward pass
3:     **for** $s_k \in \mathcal{S}_k$ **do**
4:         $\delta_k(s_k) := \underset{s_{k-1} \in \mathcal{S}_{k-1}}{\max} \psi_k(s_{k-1}, s_k)\delta_{k-1}(s_{k-1})$
5:         $q_k(s_k) := \underset{s_{k-1} \in \mathcal{S}_{k-1}}{\arg\max} \psi_k(s_{k-1}, s_k)\delta_{k-1}(s_{k-1})$
6: $\delta^\star := \underset{s_K \in \mathcal{S}_K}{\max} \delta_K(s_K)$
7: $s_K^\star := \underset{s_K \in \mathcal{S}_K}{\arg\max} \delta_K(s_K)$
8: **for** $k := K - 1, \ldots, 1$ **do**   ▷ Backtracking
9:     $s_k^\star := q_{k+1}(s_{k+1}^\star)$
Outputs: $\underset{s_1 \in \mathcal{S}_1, \ldots, s_K \in \mathcal{S}_K}{\max} p(s_1, \ldots, s_K) \propto \delta^\star$
         $\underset{s_1 \in \mathcal{S}_1, \ldots, s_K \in \mathcal{S}_K}{\arg\max} p(s_1, \ldots, s_K) = (s_1^\star, \ldots, s_K^\star)$

9.8   Inference on trees

More generally, efficient inference based on dynamic programming can be performed when dependencies between variables are expressed using a **tree** or **polytree**. The resulting marginal inference and MAP inference algorithms are often referred to as the **sum-product** and **max-sum** algorithms. The sum-product algorithm is also known as **belief propagation** or **message passing**, since it can be interpreted as propagating "local messages" through the graph. See for instance (Wainwright and Jordan, 2008, Section 2.5.1) for more details.

9.9 Inference as differentiation

In this section, we review the profound connections between differentiating the log-partition function of an exponential family distribution on one hand, and performing marginal inference (as well as maximum a-posteriori inference in the zero-temperature limit) on the other hand.

9.9.1 Inference as gradient of the log-partition

We first discuss a well-known fact in the graphical model literature: when using a binary encoding as the sufficient statistic ϕ in an exponential family distribution, the gradient $\nabla A(\boldsymbol{\theta})$ of the log-partition $A(\boldsymbol{\theta})$ gathers all the marginals (Wainwright and Jordan, 2008).

To see why, recall from Section 3.4 the definition of an exponential family distribution

$$p_{\boldsymbol{\theta}}(\boldsymbol{s}) = h(\boldsymbol{s}) \exp\left[\langle \boldsymbol{\theta}, \phi(\boldsymbol{s}) \rangle - A(\boldsymbol{\theta})\right]$$

and of its log-partition

$$A(\boldsymbol{\theta}) := \log \sum_{s \in \mathcal{S}} h(\boldsymbol{s}) \exp\left[\langle \boldsymbol{\theta}, \phi(\boldsymbol{s}) \rangle\right].$$

From Proposition 3.2,

$$\mu(\boldsymbol{\theta}) := \nabla A(\boldsymbol{\theta}) = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\phi(Y)] \in \mathcal{M}.$$

Therefore, with the **binary encodings** in Eq. (9.2) and Eq. (9.3),

$$\mathbb{P}(S_k = \boldsymbol{v}_i) = [\nabla A(\boldsymbol{\theta})]_{k,i}$$
$$\mathbb{P}(S_k = \boldsymbol{v}_i, S_l = \boldsymbol{v}_j) = [\nabla A(\boldsymbol{\theta})]_{k,l,i,j}.$$

Put differently, if we have an efficient algorithm for computing $A(\boldsymbol{\theta})$, we can perform **reverse-mode autodiff** on $A(\boldsymbol{\theta})$ to obtain $\nabla A(\boldsymbol{\theta})$, and therefore obtain the marginal probabilities. Following Section 7.3.3, the complexity of computing all marginal probabilities is therefore roughly the same as that of computing $A(\boldsymbol{\theta})$.

In the special case of chains, we obtain

$$\mathbb{P}(S_k = \boldsymbol{v}_i) = [\nabla A(\boldsymbol{\theta})]_{k,i} = \frac{1}{Z} \alpha_k(\boldsymbol{v}_i) \beta_k(\boldsymbol{v}_i)$$

$$\mathbb{P}(S_{k-1} = \boldsymbol{v}_i, S_k = \boldsymbol{v}_j) = [\nabla A(\boldsymbol{\theta})]_{k-1,k,i,j} = \frac{1}{Z} \alpha_{k-1}(\boldsymbol{v}_i) \psi_k(\boldsymbol{v}_i, \boldsymbol{v}_j) \beta_k(\boldsymbol{v}_j),$$

where we left the dependence of Z, α and β on $\boldsymbol{\theta}$ implicit.

If we define $A_\varepsilon(\boldsymbol{\theta}) \coloneqq \varepsilon A(\boldsymbol{\theta}/\varepsilon)$, in the zero-temperature limit $\varepsilon \to 0$, we obtain that $\boldsymbol{\mu}(\boldsymbol{\theta})$ is a binary encoding of the mode, i.e., of the maximum a-posteriori inference solution.

We now show i) how to unify the forward pass of the forward-backward and Viterbi algorithms using semirings and softmax operators ii) how to compute the gradient of the log-partition using backpropagation.

9.9.2 Semirings and softmax operators

The forward passes in the forward-backward and Viterbi algorithms are clearly similar. In fact, they can be formally linked to each other using **semirings**.

> **Definition 9.1** (Semiring). A semiring is a set $\mathbb{K}$ equipped with two binary operations $(\oplus, \otimes)$ such that
>
> - $\otimes$ is commutative and associative,
>
> - $\oplus$ is associative and distributive over $\oplus$,
>
> - $\otimes$ and $\oplus$ have identity element $\bar{0}$ and $\bar{1}$, respectively.

We use the notations $\oplus$, $\otimes$, $\bar{0}$ and $\bar{1}$ to clearly distinguish them from the classical addition, multiplication, 0 and 1.

We recall the following laws for binary operations:

- **Commutativity** of $\oplus$: $a \oplus b = b \oplus a$,

- **Associativity** of $\oplus$: $a \oplus (b \oplus c) = (a \oplus b) \oplus c$,

- **Distributivity** of $\otimes$ over $\oplus$: $a \otimes (b \oplus c) = (a \otimes b) \oplus (a \otimes c)$.

A set equipped with a binary operation supporting associativity and an identity element is called a **monoid**. A monoid such that every element has an inverse element is called a **group**. The difference between a ring and a semiring is that the latter only requires $(\mathbb{K}, \oplus)$ and $(\mathbb{K}, \otimes)$ to be monoids, not groups.

Equipped with these definitions, we can interpret the forward passes in the Viterbi and forward-backward algorithms as follows:

- the forward-backward algorithm in the exponential domain uses the semiring $\mathbb{R}_+$ equipped with $(+, \times)$ and identity elements $(0, 1)$;

- the Viterbi algorithm in the log domain uses the semiring $\mathbb{R}$ equipped with $(\max, +)$ and identity elements $(-\infty, 0)$;

- the forward-backward algorithm in the log domain uses the semiring $\mathbb{R}$ equipped with $(\max_\varepsilon, +)$ and identity elements $(-\infty, 0)$, where we defined the soft max operator (log-add-exp)

$$\max{}_\varepsilon(a, b) := \varepsilon \log((\exp(a) + \exp(b))/\varepsilon),$$

with $\varepsilon := 1$ by default.

It can be checked that indeed $\max_\varepsilon$ is commutative, associative, and addition is distributive over $\max_\varepsilon$. Its identity element is $-\infty$. By associativity,

$$\max{}_\varepsilon(a_1, \max{}_\varepsilon(a_2, a_3)) = \operatorname{logsumexp}_\varepsilon(a_1, a_2, a_3)$$
$$= \varepsilon \log \sum_i \exp(a_i/\varepsilon).$$

In constrast, note that the sparsemax in Section 12.4.2 is not associative.

Thanks to associativity, we can introduce the shorthand notations

$$\max{}_\varepsilon_{\boldsymbol{v} \in \mathcal{V}} f(\boldsymbol{v}) := \varepsilon \log \sum_{\boldsymbol{v} \in \mathcal{V}} \exp(f(\boldsymbol{v})/\varepsilon) \in \mathbb{R}.$$

and

$$\operatorname{argmax}_\varepsilon_{\boldsymbol{v} \in \mathcal{V}} f(\boldsymbol{v}) := \left(\exp(f(\boldsymbol{v}')/\varepsilon) / \sum_{\boldsymbol{v} \in \mathcal{V}} \exp(f(\boldsymbol{v})/\varepsilon) \right)_{\boldsymbol{v}' \in \mathcal{V}} \in \mathcal{P}(\mathcal{V}).$$

Many algorithms can be generalized thanks to the use of semirings; see among others Aji and McEliece (2000) and Mohri *et al.* (2008). The distributive and associative properties play a key role in breaking down large problems into smaller ones (Verdu and Poor, 1987).

9.9.3   Inference as backpropagation

In this section, we show that, algorithmically, backtracking is recovered as a special case of backpropagation. See also (Eisner, 2016; Mensch and Blondel, 2018).

For notation simplicity, we assume $\mathcal{S}_0 = \{1\}$ and $\mathcal{S}_k = \{1, \ldots, M\}$ for all $k \in [K]$. We focus on the case

$$\log \psi_k(i, j) = \langle \boldsymbol{\theta}_k, \phi_k(i, j) \rangle = \theta_{k,i,j}.$$

We also introduce the shorthands

$$a_{1,j} := \log \alpha_1(j) = \theta_{1,1,j}$$
$$a_{k,j} := \log \alpha_k(j) = \max_{\substack{\varepsilon \\ i \in [M]}} \theta_{k,i,j} + a_{k-1,i}$$

and

$$q_{k,j} := \operatorname*{argmax}_{\substack{\varepsilon \\ i \in [M]}} \theta_{k,i,j} + a_{k-1,i}.$$

Our goal is to compute the gradient w.r.t. $\boldsymbol{\theta} \in \mathbb{R}^{K \times M \times M}$ of

$$\log Z = A = \max_{\substack{\varepsilon \\ j \in [M]}} a_{K,j}.$$

The soft argmax counterpart of this quantity is

$$Q := \operatorname*{argmax}_{\substack{\varepsilon \\ j \in [M]}} a_{K,j} \in \triangle^M,$$

where we used $\mathcal{P}([M]) = \triangle^M$.

Computing the gradient of A is similar to computing the gradient of a feedforward network, in the sense that $\boldsymbol{\theta}_k$ influences not only a_k but also $a_{k+1}, \ldots, a_K$. Let us introduce the adjoint variable

$$r_{k,i} := \frac{\partial A}{\partial a_{k,i}},$$

which we initialize as

$$r_{K,i} = \frac{\partial A}{\partial a_{K,i}} = Q_i.$$

Since $\theta_{k,i,j}$ directly influences $a_{k,j}$, we have for $k \in [K]$, $i \in [M]$ and $j \in [M]$

$$
\begin{aligned}
\mu_{k,i,j} &:= \frac{\partial A}{\partial \theta_{k,i,j}} \\
&= \frac{\partial A}{\partial a_{k,j}} \cdot \frac{\partial a_{k,j}}{\partial \theta_{k,i,j}} \\
&= r_{k,j} \cdot q_{k,j,i}.
\end{aligned}
$$

Since $a_{k,i}$ directly influences $a_{k+1,j}$ for $j \in [M]$, we have for $k \in \{1, \ldots, K-1\}$ and $i \in [M]$

$$
\begin{aligned}
r_{k,i} = \frac{\partial A}{\partial a_{k,i}} &= \sum_{j \in [M]} \frac{\partial A}{\partial a_{k+1,j}} \frac{\partial a_{k+1,j}}{\partial a_{k,i}} \\
&= \sum_{j \in [M]} r_{k+1,j} q_{k+1,j,i} \\
&= \sum_{j \in [M]} \mu_{k+1,i,j}.
\end{aligned}
$$

We summarize the procedure in Algorithm 9.3. The forward pass uses the softmax operator $\max_\varepsilon$ and the softargmax operator $\text{argmax}_\varepsilon$. In the hard max case, in Algorithm 9.2, we used q to store backpointers from integer to integer. In the soft max case, in Algorithm 9.3, we used $\boldsymbol{q}$ to store **soft backpointers**, that is, discrete probability distributions. In the zero-temperature limit, backpropagation outputs a binary encoding of the solution of backtracking.

Algorithm 9.3 Inference on a chain as backprop with max operators

---

    Input: $\boldsymbol{\theta} \in \mathbb{R}^{K \times M \times M}$

    Max operator: $\max_{\varepsilon}$

 1: Initialize $a_{1,j} := \theta_{1,1,j} \;\forall j \in [M]$

 2: **for** $k := 2, \ldots, K$ **do**   ▷ Forward pass

 3:     **for** $j \in [M]$ **do**

 4:         $a_{k,j} := \max_{\varepsilon} \limits_{i \in [M]} \theta_{k,i,j} + a_{k-1,j} \in \mathbb{R}$

 5:         $\boldsymbol{q}_{k,j} := \operatorname{argmax}_{\varepsilon} \limits_{i \in [M]} \theta_{k,i,j} + a_{k-1,j} \in \triangle^M$

 6: $A := \max_{\varepsilon} \limits_{i \in [M]} a_{K,i} \in \mathbb{R}$

 7: $\boldsymbol{Q} := \operatorname{argmax}_{\varepsilon} \limits_{i \in [M]} a_{K,i} \in \triangle^M$

 8: Initialize $r_{K,j} = Q_j \quad \forall j \in [K]$

 9: **for** $k := K - 1, \ldots, 1$ **do**   ▷ Backward pass

10:     **for** $i \in [M]$ **do**

11:         **for** $j \in [M]$ **do**

12:             $\mu_{k+1,i,j} = r_{k+1,j} \cdot q_{k+1,j,i}$

13:             $r_{k,i} \leftarrow \mu_{k+1,i,j}$

    Outputs: $\max_{\varepsilon} \limits_{i_1, \ldots, i_K \in [M]^K} \theta_{1,1,i_1} + \sum_{k=2}^{K} \theta_{k,i_{k-1},i_k} = A, \; \nabla A(\boldsymbol{\theta}) = \mu$

9.10   Summary

Graphical models represent the conditional dependencies between variables and therefore specify how their joint distribution factorizes. We saw clear analogies between the worlds of functions and of distributions: the counterparts of computation chains and computation graphs are Markov chains and Bayesian networks. Inference on chains and more generally on trees, for exponential family distributions, is equivalent, both statistically and algorithmically, to differentiating the log-partition function. The forward-backward algorithm can be seen as using a sum-product algebra, while the Viterbi algorithm can be seen as using a max-plus algebra. Equivalently, in the log domain, we can see the former as using a soft max, and the latter as using a hard max.

10

Differentiating through optimization

In this chapter, we study how to differentiate through optimization problems, and more generally through nonlinear systems of equations.

10.1 Implicit functions

Implicit functions are functions that do not enjoy an explicit decomposition into elementary functions, for which automatic differentiation, as studied in Chapter 7, can therefore not be directly applied. We describe in this chapter techniques to differentiate through such functions and how to integrate them into an autodiff framework.

Formally, we will denote an implicit function by $w^\star(\lambda)$, where $w^\star \colon \Lambda \to \mathcal{W}$. One question is then how to compute the Jacobian $\partial w^\star(\lambda)$. As a first application one can consider **sensitivity analysis** of a system. For example, $w^\star(\lambda)$ could correspond to the equilibrium state of a physical system and in this case, $\partial w^\star(\lambda)$ would tell us about the sensitivity of the system to some parameters $\lambda \in \Lambda$.

10.1.1   Optimization problems

Another example is a function implicitly defined as the solution (assumed unique) of an optimization problem

$$\boldsymbol{w}^\star(\boldsymbol{\lambda}) = \arg\max_{\boldsymbol{w} \in \mathcal{W}} f(\boldsymbol{w}, \boldsymbol{\lambda}),$$

where $f\colon \mathcal{W} \times \Lambda \to \mathbb{R}$ and $\mathcal{W}$ denotes a constraint set. Note that we use an arg max for convenience, but the same applies when using an arg min.

10.1.2   Nonlinear equations

More generally, $\boldsymbol{w}^\star(\boldsymbol{\lambda})$ can be defined as the root of some function $F\colon \mathcal{W} \times \Lambda \to \mathcal{W}$, i.e., $\boldsymbol{w}^\star(\boldsymbol{\lambda})$ is implicitly defined as the function satisfying the (potentially nonlinear) system of equations

$$F(\boldsymbol{w}, \boldsymbol{\lambda}) = \boldsymbol{0}$$

for all $\boldsymbol{\lambda} \in \Lambda$.

10.1.3   Application to bilevel optimization

Besides sensitivity analysis, another example of application is **bilevel optimization**. Many times, we want to minimize a function defined as the composition of a fixed function and the solution of an optimization problem. Formally, let $f, g\colon \mathcal{W} \times \Lambda \to \mathbb{R}$. We consider the composition $h(\boldsymbol{\lambda})$ defined as

$$h(\boldsymbol{\lambda}) \coloneqq g(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}), \quad \text{where} \quad \boldsymbol{w}^\star(\boldsymbol{\lambda}) = \arg\max_{\boldsymbol{w} \in \mathcal{W}} f(\boldsymbol{w}, \boldsymbol{\lambda}). \quad (10.1)$$

This includes for instance hyperparameter optimization, where f is an inner log-likelihood objective, g is an outer validation loss, $\boldsymbol{w} \in \mathcal{W}$ are model parameters and $\boldsymbol{\lambda} \in \Lambda$ are model hyperparameters, such as regularization strength. To minimize $h(\boldsymbol{\lambda})$ one generally resorts to a gradient descent scheme w.r.t. $\boldsymbol{\lambda}$, which requires computing $\nabla h(\boldsymbol{\lambda})$. Assuming that $\boldsymbol{w}^\star(\boldsymbol{\lambda})$ is differentiable at $\boldsymbol{\lambda}$, by the chain rule, we obtain the Jacobian

$$\partial h(\boldsymbol{\lambda}) = \partial_1 g(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}) \partial \boldsymbol{w}^\star(\boldsymbol{\lambda}) + \partial_2 g(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}).$$
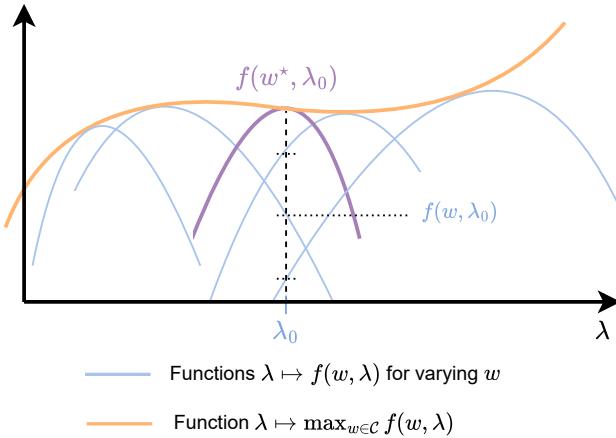
Figure 10.1: The graph of $h(\boldsymbol{\lambda}) = \max_{\boldsymbol{w} \in \mathcal{W}} f(\boldsymbol{w}, \boldsymbol{\lambda})$ is the upper-envelope of the graphs of the functions $\boldsymbol{\lambda} \mapsto f(\boldsymbol{w}, \boldsymbol{\lambda})$ for all $\boldsymbol{w} \in \mathcal{W}$.

Using $\partial h(\boldsymbol{\lambda})^{\top} = \nabla h(\boldsymbol{\lambda})$ (see Remark 2.3), we obtain the gradient

$$\nabla h(\boldsymbol{\lambda}) = \partial \boldsymbol{w}^{\star}(\boldsymbol{\lambda})^{\top} \nabla_1 g(\boldsymbol{w}^{\star}(\boldsymbol{\lambda}), \boldsymbol{\lambda}) + \nabla_2 g(\boldsymbol{w}^{\star}(\boldsymbol{\lambda}), \boldsymbol{\lambda}).$$

The only problematic term is $\partial \boldsymbol{w}^{\star}(\boldsymbol{\lambda})$, as it requires **argmax** differentiation. Indeed, most of the time, there is no explicit formula for $\boldsymbol{w}^{\star}(\boldsymbol{\lambda})$ and it does not decompose into elementary functions.

10.2 Envelope theorems

In the special case $g = f$, the composition h defined in Eq. (10.1) is simply given by

$$h(\boldsymbol{\lambda}) = f(\boldsymbol{w}^{\star}(\boldsymbol{\lambda}), \boldsymbol{\lambda}) = \max_{\boldsymbol{w} \in \mathcal{W}} f(\boldsymbol{w}, \boldsymbol{\lambda}).$$

That is, we no longer need **argmax** differentiation, but only **max** differentiation, which, as we shall now see is much easier. The function h is often called a **value function** (Fleming and Rishel, 2012). The reason for the name "envelope" is illustrated in Fig. 10.1. We emphasize that there is not one, but several envelope theorems, depending on the assumptions on f.

10.2.1 Danskin's theorem

When f is concave-convex, we can use Danskin's theorem.

Theorem 10.1 (Danskin's theorem). Let $f \colon \mathcal{W} \times \Lambda \to \mathbb{R}$ and $\mathcal{W}$ be a compact convex set. Let

$$h(\boldsymbol{\lambda}) := \max_{\boldsymbol{w} \in \mathcal{W}} f(\boldsymbol{w}, \boldsymbol{\lambda})$$

and

$$\boldsymbol{w}^{\star}(\boldsymbol{\lambda}) := \arg\max_{\boldsymbol{w} \in \mathcal{W}} f(\boldsymbol{w}, \boldsymbol{\lambda}).$$

If f is **concave** in $\boldsymbol{w}$, **convex** in $\boldsymbol{\lambda}$, and the maximum $\boldsymbol{w}^{\star}(\boldsymbol{\lambda})$ is unique, then the function h is differentiable with gradient

$$\nabla h(\boldsymbol{\lambda}) = \nabla_2 f(\boldsymbol{w}^{\star}(\boldsymbol{\lambda}), \boldsymbol{\lambda}).$$

If the maximum is not unique, we get a subgradient.

Informally, Danskin's theorem means that we can treat $\boldsymbol{w}^{\star}(\boldsymbol{\lambda})$ as if it were a constant of $\boldsymbol{\lambda}$, i.e., we do not need to differentiate through it, even though it depends on $\boldsymbol{\lambda}$. Danskin's theorem can also be used to differentiate through a minimum, $h(\boldsymbol{\lambda}) = \min_{\boldsymbol{w} \in \mathcal{W}} f(\boldsymbol{w}, \boldsymbol{\lambda})$, if $f(\boldsymbol{w}, \boldsymbol{\lambda})$ is convex in $\boldsymbol{w}$ and concave in $\boldsymbol{\lambda}$, as we now illustrate.

Example 10.1 (Ilustration of Danskin's theorem). Let us define $h(\lambda) = \min_{w \in \mathbb{R}} f(w, \lambda)$, where $f(w, \lambda) = \frac{\lambda}{2}w^2 + bw + c$ and $\lambda > 0$. Let $w^{\star}(\lambda)$ be the minimum. The derivative of f w.r.t. λ is $\frac{1}{2}w^2$. From Danskin's theorem, we have $h'(\lambda) = \frac{1}{2}w^{\star}(\lambda)$. Let us check that this result is correct. The derivative of f w.r.t. w is $\lambda w + b$. Setting it to zero, we get $w^{\star}(\lambda) = -\frac{b}{\lambda}$. We thus obtain $h'(\lambda) = \frac{1}{2}\frac{b^2}{\lambda^2}$. Let's check that the result is indeed correct. Plugging $w^{\star}(\lambda)$ back into $f(w, \lambda)$, we get $h(\lambda) = -\frac{1}{2}\frac{b^2}{\lambda} + c$. Using $(\frac{1}{\lambda})' = -\frac{1}{\lambda^2}$, we indeed obtain the same result for $h'(\lambda)$.

Danskin's theorem has a simple interpretation for functions that are linear in $\boldsymbol{\lambda}$ as shown below.

Example 10.2 (Convex conjugate). Let $f(\boldsymbol{w}, \boldsymbol{\lambda}) := \langle \boldsymbol{w}, \boldsymbol{\lambda} \rangle - \Omega(\boldsymbol{w})$ with Ω convex. We then have $h(\boldsymbol{\lambda}) = \max_{\boldsymbol{w} \in \mathcal{W}} \langle \boldsymbol{w}, \boldsymbol{\lambda} \rangle - \Omega(\boldsymbol{w}) =: \Omega^*(\boldsymbol{\lambda})$, where Ω^* denotes the convex conjugate of Ω. Since f satisfies the conditions of Danskin's theorem and since we have $\nabla_2 f(\boldsymbol{w}, \boldsymbol{\lambda}) = \boldsymbol{w}$, we obtain $\nabla h(\boldsymbol{\lambda}) = \nabla \Omega^*(\boldsymbol{\lambda}) = \boldsymbol{w}^\star(\boldsymbol{\lambda})$. In other words, in this special case, the gradient of the max is equal to the argmax. This is due to the fact that $f(\boldsymbol{w}, \boldsymbol{\lambda})$ is linear in $\boldsymbol{\lambda}$.

Another application is saddle point optimization.

Example 10.3 (Saddle point problem). Consider the saddle point problem $\min_{\boldsymbol{\lambda} \in \Lambda} \max_{\boldsymbol{w} \in \mathcal{W}} f(\boldsymbol{w}, \boldsymbol{\lambda})$. If it is difficult to minimize w.r.t. $\boldsymbol{\lambda}$ but easy to maximize w.r.t. $\boldsymbol{w}$, we can rewrite the problem as $\min_{\boldsymbol{\lambda} \in \Lambda} h(\boldsymbol{\lambda})$, where $h(\boldsymbol{\lambda}) := \max_{\boldsymbol{w} \in \mathcal{W}} f(\boldsymbol{w}, \boldsymbol{\lambda})$, and use $\nabla h(\boldsymbol{\lambda})$ to perform (projected) gradient descent w.r.t. $\boldsymbol{\lambda}$.

10.2.2 Rockafellar's theorem

A related theorem can be proved under different assumptions about f, in particular without concavity w.r.t. $\boldsymbol{w}$.

Theorem 10.2 (Rockafellar's envelope theorem). Let $f \colon \mathcal{W} \times \Lambda \to \mathbb{R}$ and $\mathcal{W}$ be a compact convex set. Let

$$h(\boldsymbol{\lambda}) := \max_{\boldsymbol{w} \in \mathcal{W}} f(\boldsymbol{w}, \boldsymbol{\lambda})$$

and

$$\boldsymbol{w}^\star(\boldsymbol{\lambda}) := \arg\max_{\boldsymbol{w} \in \mathcal{W}} f(\boldsymbol{w}, \boldsymbol{\lambda}).$$

If f is continuously differentiable in $\boldsymbol{\lambda}$ for all $\boldsymbol{w} \in \mathcal{W}$, $\nabla_1 f$ is continuous and the maximum $\boldsymbol{w}^\star(\boldsymbol{\lambda})$ is unique, then the function h is differentiable with gradient

$$\nabla h(\boldsymbol{\lambda}) = \nabla_2 f(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}).$$

See Rockafellar and Wets (2009, Theorem 10.31). Compared to Danskin's theorem, Rockafellar's theorem does not require f to be concave-convex, but requires stronger assumptions on the differentiability of f.

10.3   Implicit function theorem

10.3.1   Univariate functions

The implicit function theorem (IFT) provides conditions under which an implicit relationship of the form $F(x, \lambda) = 0$ can be rewritten as a function $x = x^\star(\lambda)$ locally, and provides a way to compute its derivative w.r.t. λ.

Theorem 10.3 (Implicit function theorem, univariate case). Let $F \colon \mathbb{R} \times \mathbb{R} \to \mathbb{R}$. Assume $F(x, \lambda)$ is a continuously differentiable function in a neighborhood $\mathcal{U}$ of (x_0, λ_0) such that $F(x_0, \lambda_0) = 0$ and $\partial_1 F(x_0, \lambda_0) \neq 0$. Then there exists a neighborhood $\mathcal{V} \subseteq \mathcal{U}$ of (x_0, λ_0) in which there is a function $x^\star(\lambda)$ such that

- $x^\star(\lambda_0) = x_0$,

- $F(x^\star(\lambda), \lambda) = 0$ for all λ in the neighborhood $\mathcal{V}$,

- $\partial x^\star(\lambda) = -\frac{\partial_2 F(x^\star(\lambda), \lambda)}{\partial_1 F(x^\star(\lambda), \lambda)}$.

We postpone the proof to the multivariate case and begin with a classical example of application of the theorem.

Example 10.4 (Equation of the unit circle). We use $w \equiv x$ and $\lambda \equiv y$ for clarity. Let $F(x, y) := x^2 + y^2 - 1$. In general, we cannot rewrite the unit circle equation $F(x, y) = 0$ as a function from y to x, because for every $y \in [-1, 1]$, there are always two possible x values, namely, $x = \sqrt{1 - y^2}$ or $x = -\sqrt{1 - y^2}$. However, locally around some point (x_0, y_0), e.g., such that $x_0 > 0$ and $y_0 > 0$ (upper-right quadrant), the function $x = x^\star(y) = \sqrt{1 - y^2}$ is well-defined. Using $\partial_1 F(x, y) = 2x$ and $\partial_2 F(x, y) = 2y$, we get $\partial x^\star(y) = -\frac{2y}{2x^\star(y)} = -\frac{y}{\sqrt{1-y^2}}$ in that neighborhood (the upper right quadrant in this case). This is indeed the same derivative expression as if we used the chain rule on $\sqrt{1 - y^2}$ and is well-defined on $y \in [0, 1)$.

In the above simple example, we can easily derive an explicit function relating y to x in a given neighborhood, but this is not always the case. The IFT gives us conditions guaranteeing that such function **exists** and

a way to **differentiate** it, but not a way to **construct** such a function. In fact, finding $x^\star(\lambda)$ such that $F(x^\star(\lambda), \lambda) = 0$ typically involves a root finding algorithm, an optimization algorithm, a nonlinear system solver, etc.

> **Example 10.5** (Polynomial). Let $F(w, \lambda) = w^5 + w^3 + w - \lambda$. According to the Abel-Ruffini theorem (Tignol, 2015), quintics (polynomials of degree 5) do no enjoy roots in terms of radicals and one must resort to numerical root finding. In addition, odd-degree polynomials have real roots. Moreover, $\partial_1 F(w, \lambda) = 5w^4 + 3w^2 + 1$ is strictly positive. Therefore, by the intermediate value theorem, there must be only one root $w^\star(\lambda)$ such that $F(w^\star(\lambda), \lambda) = 0$. This unique root can for example be found by bisection. Using the IFT, its derivative is found to be $\partial w^\star(\lambda) = (5w^\star(\lambda)^4 + 3w^\star(\lambda)^2 + 1)^{-1}$.

While an implicit function is differentiable at a point if the assumptions of the IFT hold in a neighborhood of that point, the reciprocal is not true: failure of the IFT assumptions does not necessarily mean that the implicit function is not differentiable, as we now illustrate.

> **Example 10.6** (IFT conditions are not necessary for differentiability). Consider $F(w, \lambda) = (w - \lambda)^2$. We clearly have that $F(w^\star(\lambda), \lambda) = 0$ if we define $w^\star(\lambda) = \lambda$, the identity function. It is clearly differentiable for all λ, yet the assumptions of the IFT fail, since we have $\partial_1 F(w, \lambda) = 2(w - \lambda)$ and therefore $\partial_1 F(0, 0) = 0$.

10.3.2   Multivariate functions

We now present the IFT in the general multivariate setting. Informally, if $F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}) = \boldsymbol{0}$, then by the chain rule, we have

$$\partial_1 F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}) \partial \boldsymbol{w}^\star(\boldsymbol{\lambda}) + \partial_2 F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}) = \boldsymbol{0},$$

meaning that the Jacobian $\partial \boldsymbol{w}^\star(\boldsymbol{\lambda})$, assuming that it exists, satisfies

$$-\partial_1 F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}) \partial \boldsymbol{w}^\star(\boldsymbol{\lambda}) = \partial_2 F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}).$$

The IFT gives us conditions for the existence of $\partial \boldsymbol{w}^\star(\boldsymbol{\lambda})$.

Theorem 10.4 (Implicit function theorem, multivariate case). Let us define $F \colon \mathcal{W} \times \Lambda \to \mathcal{W}$. Assume $F(\boldsymbol{w}, \boldsymbol{\lambda})$ is a continuously differentiable function in a neighborhood of $(\boldsymbol{w}_0, \boldsymbol{\lambda}_0)$ such that $F(\boldsymbol{w}_0, \boldsymbol{\lambda}_0) = \boldsymbol{0}$ and $\partial_1 F(\boldsymbol{w}_0, \boldsymbol{\lambda}_0)$ is invertible, i.e., its determinant is nonzero. Then there exists a neighborhood of $\boldsymbol{\lambda}_0$ in which there is a function $\boldsymbol{w}^\star(\boldsymbol{\lambda})$ such that

- $\boldsymbol{w}^\star(\boldsymbol{\lambda}_0) = \boldsymbol{w}_0$,

- $F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}) = \boldsymbol{0}$ for all $\boldsymbol{\lambda}$ in the neighborhood,

- $-\partial_1 F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}) \partial \boldsymbol{w}^\star(\boldsymbol{\lambda}) = \partial_2 F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda})$
  $\iff \partial \boldsymbol{w}^\star(\boldsymbol{\lambda}) = -\partial_1 F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda})^{-1} \partial_2 F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda})$.

We begin with a simple unconstrained optimization algorithm.

Example 10.7 (Unconstrained optimization). Assume we want to differentiate through $\boldsymbol{w}^\star(\boldsymbol{\lambda}) = \arg\min_{\boldsymbol{w} \in \mathbb{R}^P} f(\boldsymbol{w}, \boldsymbol{\lambda})$, where f is strictly convex in $\boldsymbol{w}$, which ensures that the solution is unique. From the stationary conditions, if we define $F(\boldsymbol{w}, \boldsymbol{\lambda}) \coloneqq \nabla_1 f(\boldsymbol{w}, \boldsymbol{\lambda})$, then $\boldsymbol{w}^\star(\boldsymbol{\lambda})$ is uniquely characterized as the root of F in the first argument, i.e., $F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}) = \boldsymbol{0}$. We have $\partial_1 F(\boldsymbol{w}, \boldsymbol{\lambda}) = \nabla_1^2 f(\boldsymbol{w}, \boldsymbol{\lambda})$, the Hessian of f in $\boldsymbol{w}$, and $\partial_2 F(\boldsymbol{w}, \boldsymbol{\lambda}) = \partial_2 \nabla_1 f(\boldsymbol{w}, \boldsymbol{\lambda})$, the cross derivatives of f. Therefore, assuming that the Hessian is well-defined and invertible at $(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda})$, we can use the IFT to differentiate through $\boldsymbol{w}^\star(\boldsymbol{\lambda})$ and obtain $\partial \boldsymbol{w}^\star(\boldsymbol{\lambda}) = -\nabla_1^2 f(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}) \partial_2 \nabla_1 f(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda})$.

Next, we generalize the previous example, by allowing constraints in the optimization problem.

Example 10.8 (Constrained optimization). Now, assume we want to differentiate through $\boldsymbol{w}^\star(\boldsymbol{\lambda}) = \arg\min_{\boldsymbol{w} \in \mathcal{C}} f(\boldsymbol{w}, \boldsymbol{\lambda})$, where f is strictly convex in $\boldsymbol{w}$ and $\mathcal{C} \subseteq \mathcal{W}$ is a convex set. A solution is characterized by the fixed point equation $\boldsymbol{w}^\star(\boldsymbol{\lambda}) = P_{\mathcal{C}}(\boldsymbol{w}^\star(\boldsymbol{\lambda}) - \eta \nabla_1 f(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}))$, for any $\eta > 0$, where $P(\boldsymbol{y}) \coloneqq \arg\min_{\boldsymbol{x} \in \mathcal{C}} \|\boldsymbol{x} - \boldsymbol{y}\|_2^2$ is the Euclidean projection of $\boldsymbol{y}$ onto $\mathcal{C}$. Therefore, $\boldsymbol{w}^\star(\boldsymbol{\lambda})$ is the root of $F(\boldsymbol{w}, \boldsymbol{\lambda}) = \boldsymbol{w} - P_{\mathcal{C}}(\boldsymbol{w} - \eta \nabla_1 f(\boldsymbol{w}, \boldsymbol{\lambda}))$ (see Chapter 15). We

can differentiate through $\boldsymbol{w}^\star(\boldsymbol{\lambda})$ using the IFT, assuming that the conditions of the theorem apply. Note that $\partial_1 F(\boldsymbol{w}, \boldsymbol{\lambda})$ requires the expression of the Jacobian $\partial P_{\mathcal{C}}(\boldsymbol{y})$. Fortunately, $P_{\mathcal{C}}(\boldsymbol{y})$ and its Jacobian are easy to compute for many sets $\mathcal{C}$ (Blondel *et al.*, 2021).

10.3.3   JVP and VJP of implicit functions

To integrate an implicit function $\boldsymbol{w}^\star(\boldsymbol{\lambda})$ in an autodiff framework, we need to be able to compute its JVP or VJP. This is the purpose of the next proposition.

Proposition 10.1 (JVP and VJP of implicit functions). Let $\boldsymbol{w}^\star \colon \Lambda \to \mathcal{W}$ be a function implicitly defined as the solution of $F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}) = \boldsymbol{0}$, for some function $F \colon \mathcal{W} \times \Lambda \to \mathcal{W}$. Define

$$A \coloneqq -\partial_1 F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda})$$
$$B \coloneqq \partial_2 F(\boldsymbol{w}^\star(\boldsymbol{\lambda}), \boldsymbol{\lambda}).$$

Assume the assumptions of the IFT hold. The JVP $\boldsymbol{t} \coloneqq \partial \boldsymbol{w}^\star(\boldsymbol{\lambda})\boldsymbol{v}$ in the input direction $\boldsymbol{v} \in \Lambda$ is obtained by solving the linear system

$$A\boldsymbol{t} = B\boldsymbol{v}.$$

The VJP $\partial \boldsymbol{w}^\star(\boldsymbol{\lambda})^* \boldsymbol{u}$ in the output direction $\boldsymbol{u} \in \mathcal{W}$ is obtained by solving the linear system

$$A^* \boldsymbol{r} = \boldsymbol{u}.$$

Using the solution $\boldsymbol{r}$, we get

$$\partial \boldsymbol{w}^\star(\boldsymbol{\lambda})^* \boldsymbol{u} = \partial \boldsymbol{w}^\star(\boldsymbol{\lambda})^* A^* \boldsymbol{r} = B^* \boldsymbol{r}.$$

Note that in the above linear systems, we can access to A and B as linear maps, the JVPs of F. Their adjoints, A^* and B^*, correspond to the VJPs of F. To solve these systems, we can therefore use **matrix-free** solvers as detailed in Section 8.4. For example, when A is symmetric positive semi-definite, we can use the conjugate gradient method (Hestenes, Stiefel, *et al.*, 1952). When A is not symmetric positive definite, we can

use GMRES (Saad and Schultz, 1986) or BiCGSTAB (Vorst and Vorst, 1992).

10.3.4   Proof of the implicit function theorem

We prove the theorem using the inverse function theorem presented in Theorem 10.5. Define

$$f(\boldsymbol{\lambda}, \boldsymbol{w}) = (\boldsymbol{\lambda}, F(\boldsymbol{w}, \boldsymbol{\lambda}))$$

which goes from $\mathbb{R}^Q \times \mathbb{R}^P$ onto $\mathbb{R}^Q \times \mathbb{R}^P$. The Jacobian of f is

$$\boldsymbol{\partial} f(\boldsymbol{\lambda}, \boldsymbol{w}) = \begin{pmatrix} \mathrm{I} & 0 \\ \boldsymbol{\partial}_2 F(\boldsymbol{w}, \boldsymbol{\lambda}) & \boldsymbol{\partial}_1 F(\boldsymbol{w}, \boldsymbol{\lambda}) \end{pmatrix}.$$

So at $\boldsymbol{w}_0, \boldsymbol{\lambda}_0$, we have $\det(\boldsymbol{\partial} f(\boldsymbol{\lambda}_0, \boldsymbol{w}_0)) = \det(\mathrm{I}) \det(\boldsymbol{\partial}_1 F(\boldsymbol{w}_0, \boldsymbol{\lambda}_0)) > 0$ since we assumed $\partial_1 F(\boldsymbol{w}_0, \boldsymbol{\lambda}_0)$ invertible. By the inverse function theorem, the function f is then invertible in a neighborhood N of $f(\boldsymbol{\lambda}_0, \boldsymbol{w}_0) = (\boldsymbol{\lambda}_0, \boldsymbol{0})$. In particular, it is invertible in $N \cap \{(\boldsymbol{\lambda}, \boldsymbol{0}), \boldsymbol{\lambda} \in \mathbb{R}^Q\}$. The solution of the implicit equation in a neighborhood of $\boldsymbol{\lambda}_0$ is then $(\boldsymbol{\lambda}, \boldsymbol{w}^*(\boldsymbol{\lambda})) = f^{-1}(\boldsymbol{\lambda}, \boldsymbol{0})$. By the inverse function theorem, f^{-1} is continuously differentiable inverse and so is $\boldsymbol{w}^*(\boldsymbol{\lambda})$. The derivative $\partial \boldsymbol{w}^*(\boldsymbol{\lambda})$ from the differential of the inverse as

$$\begin{pmatrix} \overset{\sim}{\partial \boldsymbol{w}^*(\boldsymbol{\lambda})} & \overset{\sim}{} \end{pmatrix} = \partial f^{-1}(\boldsymbol{\lambda}, \boldsymbol{0}),$$

and by the inverse function theorem, we have $\partial f^{-1}(\boldsymbol{\lambda}, \boldsymbol{0}) = (\partial f(\boldsymbol{\lambda}, \boldsymbol{w}^*(\boldsymbol{\lambda})))^{-1}$. So using block matrix inversions formula

$$\begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{C} & \boldsymbol{D} \end{pmatrix}^{-1} = \begin{pmatrix} \overset{\sim}{} & \overset{\sim}{} \\ -(\boldsymbol{D} - \boldsymbol{C} \boldsymbol{A}^{-1} \boldsymbol{B})^{-1} \boldsymbol{C} \boldsymbol{A}^{-1} & \overset{\sim}{} \end{pmatrix},$$

we get the claimed expression. Though we expressed the proof in terms of Jacobians and matrices, the result naturally holds for the corresponding linear operators, JVPs, VJPs, and their inverses.

10.4   Adjoint state method

10.4.1   Differentiating nonlinear equations

We describe in this section the adjoint state method (a.k.a. adjoint method, method of adjoints, adjoint sensitivity method). The method

can be used to compute the gradient of the composition of an explicit function and an **implicit function**, defined through an **equality constraint** (e.g., a **nonlinear equation**). The method dates back to Céa (1986).

Suppose a variable $s \in \mathcal{S}$ (which corresponds to a **state** in optimal control) is implicitly defined given some parameters $w \in \mathcal{W}$ through the (potentially nonlinear) equation $c(s, w) = 0$, where $c \colon \mathcal{S} \times \mathcal{W} \to \mathcal{S}$. Assuming s is **uniquely** determined for all $w \in \mathcal{W}$, this defines an **implicit function** $s^\star(w)$ from $\mathcal{W}$ to $\mathcal{S}$ such that $c(s^\star(w), w) = 0$. Given an objective function $L \colon \mathcal{S} \times \mathcal{W} \to \mathbb{R}$, the goal of the adjoint state method is then to compute the gradient of

$$L(w) := L(s^\star(w), w).$$

However, this is not trivial as $s^\star(w)$ is an implicit function. For instance, this can be used to convert the **equality-constrained** problem

$$\min_{w \in \mathcal{W}} L(s, w) \quad \text{s.t.} \quad c(s, w) = 0.$$

into the **unconstrained** problem

$$\min_{w \in \mathcal{W}} L(s^\star(w), w).$$

Access to $\nabla L(w)$ allows us to solve this problem by gradient descent.

> **Proposition 10.2** (Adjoint state method). Let $c : \mathcal{S} \times \mathcal{W} \to \mathcal{S}$ be a mapping defining constraints of the form $c(s, w)$. Assume that for each $w \in \mathcal{W}$, there exists a unique $s^\star(w)$ satisfying $c(s^\star(w), w) = 0$ and that $s^\star(w)$ is differentiable. The gradient of
>
> $$L(w) := L(s^\star(w), w),$$
>
> for some differentiable function $L : \mathcal{S} \times \mathcal{W} \to \mathbb{R}$, is given by
>
> $$\nabla L(w) = \nabla_2 L(s^\star(w), w) + \partial_2 c(s^\star(w), w)^* r^\star(w),$$
>
> where $r^\star(w)$ is the solution of the linear system
>
> $$\partial_1 c(s^\star(w), w)^* r = -\nabla_1 L(s^\star(w), w).$$

As shown in the proof below, $r^\star(w)$ corresponds to a **Lagrange multiplier**. The linear system can be solved using matrix-free solvers.

10.4.2   Relation with envelope theorems

Because s is uniquely determined for any $w \in \mathcal{W}$ by $c(s, w) = 0$, we can alternatively rewrite $L(w)$ as the trivial minimization or maximization,

$$L(w) = \min_{s \in \mathcal{S}} L(s, w) \quad \text{s.t.} \quad c(s, w) = 0$$
$$= \max_{s \in \mathcal{S}} L(s, w) \quad \text{s.t.} \quad c(s, w) = 0.$$

Therefore, the adjoint state method can be seen as an envelope theorem for computing $\nabla L(w)$, for the case when w is involved in **both** the objective function and in the **equality constraint**.

10.4.3   Proof using the method of Lagrange multipliers

Classically, the adjoint state method is derived using the method of Lagrange multipliers. Let us introduce the **Lagrangian** associated with L and c,

$$\mathcal{L}(s, w, r) := L(s, w) + \langle r, c(s, w) \rangle,$$

where $r \in \mathcal{S}$ is the **Lagrange multiplier** associated with the equality constraint $c(s, w) = 0$. In the optimal control literature, r is often called the **adjoint variable** or **adjoint state**. The gradients of the Lagrangian are

$$\nabla_s \mathcal{L}(s, w, r) = \nabla_1 L(s, w) + \partial_1 c(s, w)^* r$$
$$\nabla_w \mathcal{L}(s, w, r) = \nabla_2 L(s, w) + \partial_2 c(s, w)^* r$$
$$\nabla_r \mathcal{L}(s, w, r) = c(s, w),$$

where $\partial_i c(s, w)^*$ are the **adjoint operators**. Setting $\nabla_r \mathcal{L}(s, w, r)$ to zero gives the constraint $c(s, w) = 0$. Setting $\nabla_s \mathcal{L}(s, w, r)$ to zero gives the so-called **adjoint state equation**

$$\partial_1 c(s, w)^* r = -\nabla_1 L(s, w).$$

Solving this linear system w.r.t. r at $s = s^\star(w)$ gives the adjoint variable $r^\star(w)$. We then get

$$\nabla L(w) = \nabla_2 \mathcal{L}(s^\star(w), w, r^\star(w))$$
$$= \nabla_2 L(s^\star(w), w) + \partial_2 c(s^\star(w), w)^* r^\star(w),$$

which concludes the proof.

10.4.4 Proof using the implicit function theorem

A more direct proof is possible thanks to the implicit function theorem (Section 10.3). Using the chain rule, we get

$$\nabla L(\boldsymbol{w}) = \nabla_2 L(\boldsymbol{s}^\star(\boldsymbol{w}), \boldsymbol{w}) + \partial \boldsymbol{s}^\star(\boldsymbol{w})^* \nabla_1 L(\boldsymbol{s}^\star(\boldsymbol{w}), \boldsymbol{w}),$$

where $\partial \boldsymbol{s}^\star(\boldsymbol{w})^*$ is the VJP of $\boldsymbol{s}^\star$, a linear map from $\mathcal{S}$ to $\mathcal{W}$.

Computationally, the main difficulty is to apply $\partial \boldsymbol{s}^\star(\boldsymbol{w})^*$ to the vector $\boldsymbol{u} = \nabla_1 L(\boldsymbol{s}^\star(\boldsymbol{w}), \boldsymbol{w}) \in \mathcal{S}$. Using the implicit function theorem (Section 10.3) on the implicit function $c(\boldsymbol{s}^\star(\boldsymbol{w}), \boldsymbol{w}) = \boldsymbol{0}$, and Proposition 10.1, we get the linear system $A^* \boldsymbol{r} = \boldsymbol{u}$, where $A^* \coloneqq \partial_1 c(\boldsymbol{s}^\star(\boldsymbol{w}), \boldsymbol{w})^*$ is a linear map from $\mathcal{S}$ to $\mathcal{S}$. After solving for $\boldsymbol{r}$, we get $\partial \boldsymbol{s}^\star(\boldsymbol{w})^* \boldsymbol{u} = B^* \boldsymbol{r}$, where $B^* \coloneqq \partial_2 c(\boldsymbol{s}^\star(\boldsymbol{w}), \boldsymbol{w})^*$ is a linear map from $\mathcal{S}$ to $\mathcal{W}$. Putting everything together, we get

$$\nabla L(\boldsymbol{w}) = \nabla_2 L(\boldsymbol{s}^\star(\boldsymbol{w}), \boldsymbol{w}) + \partial_2 c(\boldsymbol{s}^\star(\boldsymbol{w}), \boldsymbol{w})^* \boldsymbol{r}.$$

10.4.5 Reverse mode as adjoint method with backsubstitution

In this section, we revisit reverse-mode autodiff from the perspective of the adjoint state method. For clarity, we focus our exposition on feedforward networks with input $\boldsymbol{x} \in \mathcal{X}$ and network weights $\boldsymbol{w} = (\boldsymbol{w}_1, \ldots, \boldsymbol{w}_k) \in \mathcal{W}_1 \times \ldots \times \mathcal{W}_K$,

$$\begin{aligned}
\boldsymbol{s}_0 &\coloneqq \boldsymbol{x} \in \mathcal{X} \\
\boldsymbol{s}_1 &\coloneqq f_1(\boldsymbol{s}_0, \boldsymbol{w}_1) \in \mathcal{S}_1 \\
&\ \ \vdots \\
\boldsymbol{s}_K &\coloneqq f_K(\boldsymbol{s}_{K-1}, \boldsymbol{w}_K) \in \mathcal{S}_K \\
f(\boldsymbol{w}) &\coloneqq \boldsymbol{s}_K.
\end{aligned} \tag{10.2}$$

Here we focus on gradients with respect to the parameters $\boldsymbol{w}$, hence the notation $f(\boldsymbol{w})$. We can use the adjoint state method to recover reverse-mode autodiff, and prove its **correctness** in the process. While we focus for simplicity on feedforward networks, our exposition can be generalized to computation graphs.

Feedforward networks as the solution of a nonlinear equation

While we defined the set of intermediate computations $\boldsymbol{s} = (\boldsymbol{s}_1, \ldots, \boldsymbol{s}_K) \in \mathcal{S}_1 \times \ldots \times \mathcal{S}_K$ as a sequence of operations, they can also be defined as the unique solution of the **nonlinear equation** $c(\boldsymbol{s}, \boldsymbol{w}) = \boldsymbol{0}$, where

$$c(\boldsymbol{s}, \boldsymbol{w}) := \begin{pmatrix} \boldsymbol{s}_1 - f_1(\boldsymbol{x}, \boldsymbol{w}_1) \\ \boldsymbol{s}_2 - f_2(\boldsymbol{s}_1, \boldsymbol{w}_2) \\ \vdots \\ \boldsymbol{s}_K - f_K(\boldsymbol{s}_{K-1}, \boldsymbol{w}_K) \end{pmatrix}.$$

This defines an **implicit function** $\boldsymbol{s}^\star(\boldsymbol{w}) = (\boldsymbol{s}_1^\star(\boldsymbol{w}), \ldots, \boldsymbol{s}_K^\star(\boldsymbol{w}))$, the solution of this nonlinear system, which is given by the variables $\boldsymbol{s}_1, \ldots, \boldsymbol{s}_K$ defined in (10.2). The output of the feedforward network is then $f(\boldsymbol{w}) = \boldsymbol{s}_K^\star(\boldsymbol{w})$.

In machine learning, the final layer $\boldsymbol{s}_K^\star(\boldsymbol{w})$ is typically fed into a loss ℓ, to define

$$L(\boldsymbol{w}) := \ell(\boldsymbol{s}_K^\star(\boldsymbol{w}); \boldsymbol{y}).$$

Note that an alternative is to write $L(\boldsymbol{w})$ as

$$L(\boldsymbol{w}) = \min_{\boldsymbol{s} \in \mathcal{S}} \ell(\boldsymbol{s}; \boldsymbol{y}) \quad \text{s.t.} \quad c(\boldsymbol{s}, \boldsymbol{w}) = \boldsymbol{0}.$$

More generally, if we just want to compute the VJP of $\boldsymbol{s}_K^\star(\boldsymbol{w})$ in some direction $\boldsymbol{u}_K \in \mathcal{S}_K$, we can define the scalar-valued function

$$L(\boldsymbol{w}) := \ell(\boldsymbol{s}_K^\star(\boldsymbol{w}); \boldsymbol{u}_K) := \langle \boldsymbol{s}_K^\star(\boldsymbol{w}), \boldsymbol{u}_K \rangle$$

so that

$$\partial f(\boldsymbol{w})^* \boldsymbol{u}_K = \nabla L(\boldsymbol{w}).$$

Let us define $\boldsymbol{u} \in \mathcal{S}_1 \times \cdots \times \mathcal{S}_{K-1} \times \mathcal{S}_K$ as $\boldsymbol{u} := (\boldsymbol{0}, \ldots, \boldsymbol{0}, \nabla_1 \ell(f(\boldsymbol{w}); \boldsymbol{y}))$ (gradient of the loss ℓ case) or $\boldsymbol{u} := (\boldsymbol{0}, \ldots, \boldsymbol{0}, \boldsymbol{u}_K)$ (VJP of f in the direction $\boldsymbol{u}_K$ case). Using the adjoint state method, we know that the gradient of this objective is obtained as

$$\nabla L(\boldsymbol{w}) = \partial_2 c(\boldsymbol{s}(\boldsymbol{w}), \boldsymbol{w})^* \boldsymbol{r}^\star(\boldsymbol{w}),$$

for $\boldsymbol{r}^\star(\boldsymbol{w})$ the solution of the linear system

$$\partial_1 c(\boldsymbol{s}(\boldsymbol{w}), \boldsymbol{w})^* \boldsymbol{r} = -\boldsymbol{u}.$$

Solving the linear system using backsubtitution

The JVP of the constraint function c at $s^\star(w)$, materialized as a matrix, takes the form of a **block lower-triangular matrix**

$$\partial_1 c(s^\star(w), w) = \begin{pmatrix} I & 0 & \cdots & \cdots & 0 \\ -A_1 & I & \ddots & & \vdots \\ 0 & -A_2 & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -A_K & I \end{pmatrix},$$

where $A_k := \partial_1 f_k(s_{k-1}, w_k)$. Crucially the triangular structure of the JVP stems from the fact that each intermediate activation only depends from the past intermediate activations. Therefore, the constraints, corresponding to the lines of the Jacobian, cannot introduce non-zero values beyond its diagonal. The VJP takes the form of a **block upper-triangular matrix**

$$\partial_1 c(s^\star(w), w)^* = \begin{pmatrix} I & -A_1^* & 0 & \cdots & 0 \\ 0 & I & -A_2^* & \ddots & \vdots \\ \vdots & \ddots & I & \ddots & 0 \\ \vdots & & \ddots & \ddots & -A_K^* \\ 0 & \cdots & \cdots & 0 & I \end{pmatrix}.$$

Solving an upper triangular system like $\partial_1 c(s(w), w)^* r = u$ can then be done efficiently by **backsubstitution**. Starting from the last adjoint state $r_K = u$, we can compute each adjoint state r_k from that computed at $k+1$. Namely, for $k \in (K-1, \ldots, 1)$, we have

$$r_k - A_{k+1}^* r_{k+1} = 0 \iff r_k = \partial f_{k+1}(s_k, w_{k+1})^* r_{k+1}.$$

The VJPs with respect to the parameters are then obtained by

$$\partial_2 c(s(w), w)^* r = \begin{pmatrix} \partial_2 f_1(x, w_1)^* r_1 \\ \partial_2 f_2(s_1(w), w_2)^* r_2 \\ \vdots \\ \partial_2 f_K(s_1(w), w_K)^* r_K \end{pmatrix},$$

recovering reverse-mode autodiff.

The Lagrangian perspective of backpropagation for networks with separate parameters $\boldsymbol{w} = (\boldsymbol{w}_1, \ldots, \boldsymbol{w}_K)$ is well-known; see for instance LeCun (1988) or Recht (2016). The Lagrangian perspective of back-propagation through time (Werbos, 1990) for networks with shared parameter $\boldsymbol{w}$ is discussed for instance by Franceschi *et al.* (2017). Our exposition uses the adjoint state method, which can itself be proved either using the method of Lagrange multipliers (Section 10.4.3) or by the implicit function theorem (Section 10.4.4), combined with backsub-titution for solving the upper-triangular linear system. Past works often minimize over $\boldsymbol{w}$ but we do not require this, as gradients are not neces-sarily used for optimization. Our exposition also supports computing the VJP of any vector-valued function f, while existing works derive the gradient of a scalar-valued loss function.

10.5   Inverse function theorem

10.5.1   Differentiating inverse functions

In some cases (see for instance Section 11.4.3), it is useful to compute the Jacobian of an inverse function f^{-1}. The inverse function theorem below allows us to relate the Jacobian of f^{-1} with the Jacobian of f.

Theorem 10.5 (Inverse function theorem)**.** Assume $f \colon \mathcal{W} \to \mathcal{W}$ is continuously differentiable with invertible Jacobian $\partial f(\boldsymbol{w}_0)$ at $\boldsymbol{w}_0$. Then f is bijective from a neighborhood of $\boldsymbol{w}_0$ to a neighborhood of $f(\boldsymbol{w}_0)$. Moreover, the inverse f^{-1} is continuously differentiable near $\boldsymbol{\omega}_0 = f(\boldsymbol{w}_0)$ and the Jacobian of the inverse $\partial f^{-1}(\boldsymbol{\omega})$ is

$$\partial f(\boldsymbol{w}) \partial f^{-1}(\boldsymbol{\omega}) = I \Leftrightarrow \partial f^{-1}(\boldsymbol{\omega}) = (\partial f(\boldsymbol{w}))^{-1},$$

with $\boldsymbol{w} = f^{-1}(\boldsymbol{\omega})$.

10.5.2   Link with the implicit function theorem

The inverse function theorem can be used to prove the implicit function theorem; see proof of Theorem 10.4. Conversely, recall that, in order to use the implicit function theorem, we need to choose a root objective

$F\colon \mathcal{W} \times \Lambda \to \mathcal{W}$. If we set $\mathcal{W} = \Lambda = \mathbb{R}^Q$ and $F(\boldsymbol{w}, \boldsymbol{\omega}) = f(\boldsymbol{w}) - \boldsymbol{\omega}$, with $f\colon \mathbb{R}^Q \to \mathbb{R}^Q$, then we have that the root $\boldsymbol{w}^\star(\boldsymbol{\omega})$ satisfying $F(\boldsymbol{w}^\star(\boldsymbol{\omega}), \boldsymbol{\omega}) = \boldsymbol{0}$ is exactly $\boldsymbol{w}^\star(\boldsymbol{\omega}) = f^{-1}(\boldsymbol{\omega})$. Moreover, $\partial_1 F(\boldsymbol{w}, \boldsymbol{\omega}) = \partial f(\boldsymbol{w})$ and $\partial_2 F(\boldsymbol{w}, \boldsymbol{\omega}) = -I$. By applying the implicit function theorem with this F, we indeed recover the inverse function theorem.

10.5.3 Proof of inverse function theorem

We first give a proof of the formula assuming that f^{-1} is well-defined and continuously differentiable in a neighborhood of $f(\boldsymbol{w}_0)$. In that case, we have for any $\boldsymbol{\omega}$ in a neighborhood of $f(\boldsymbol{w}_0)$,

$$f \circ f^{-1}(\boldsymbol{\omega}) = \boldsymbol{\omega}.$$

Differentiating both sides w.r.t. $\boldsymbol{\omega}$, we get

$$\partial f(f^{-1}(\boldsymbol{\omega}))\partial f^{-1}(\boldsymbol{\omega}) = I,$$

where I is the identity function in $\mathbb{R}^Q$. In particular, for $\boldsymbol{w} = f^{-1}(\boldsymbol{\omega})$ we recover the formula presented in the statement.

Now, it remains to show that invertibility of the JVP ensures that the function is invertible in a neighborhood of $f(\boldsymbol{w}_0)$ and that the inverse is continuously differentiable. For that, denote $\boldsymbol{l} = \partial f(\boldsymbol{w}_0)$ such that $\boldsymbol{l}^{-1}$ is well-defined by definition. f is invertible with continuously differentiable inverse, if and only if $\boldsymbol{l}^{-1}(f(\boldsymbol{w})) - f(\boldsymbol{w}_0)$ is invertible with continuously differentiable inverse. So without loss of generality, we consider $\partial f(\boldsymbol{w}_0) = I$, $f(\boldsymbol{w}_0) = 0$, $\boldsymbol{w}_0 = 0$.

As f is continuously differentiable, there exists a neighborhood $N = \{\boldsymbol{w} : \|\boldsymbol{w} - \boldsymbol{w}_0\|_2 \le \delta\}$ on which we have $\|\partial f(\boldsymbol{w}) - I\|_2 \le 1/2$. In this neighborhood, the function $g(\boldsymbol{w}) = f(\boldsymbol{w}) - \boldsymbol{w}$ is contractive by the mean value theorem with contraction factor $1/2$. For any $\boldsymbol{\omega}$ such that $\|\boldsymbol{\omega} - f(\boldsymbol{w}_0)\|_2 \le \delta/2$, the sequence $\boldsymbol{w}_{k+1} = \boldsymbol{w}_k - f(\boldsymbol{w}_k) - \boldsymbol{\omega}'$ remains in N and converges (since it is a Cauchy sequence by the contraction of g) to a unique fixed point $\boldsymbol{w}_\infty$ satisfying $\boldsymbol{w}_\infty = \boldsymbol{w}_\infty - f(\boldsymbol{w}_\infty) - \boldsymbol{\omega} \iff f(\boldsymbol{w}_\infty) = \boldsymbol{\omega}$. This shows the existence of the inverse in the neighborhood $M = \{\boldsymbol{\omega} : \|\boldsymbol{\omega} - \boldsymbol{\omega}_0\|_2 \le \delta/2\}$ of $\boldsymbol{\omega}_0 = f(\boldsymbol{w}_0)$ onto N.

We tackle now the differentiability (hence the continuity) of f^{-1}. For any $\boldsymbol{\omega}$ in the neighborhood of $\boldsymbol{\omega}_0$ with inverse $\boldsymbol{w} := f^{-1}(\boldsymbol{\omega}) \in N$,

the JVP of f at $\boldsymbol{w}$ satisfies by assumption $\|\partial f(\boldsymbol{w}) - \mathrm{I}\,\|_2 \le 1/2$. Hence, $\boldsymbol{a} = \partial f(\boldsymbol{w}) - \mathrm{I}$ defines a convergent series $\boldsymbol{b} = \sum_{k=0}^{+\infty} \boldsymbol{a}^k$ and one verifies easily that $\boldsymbol{b} = \partial f(\boldsymbol{w})^{-1}$, that is $\partial f(\boldsymbol{w})$ is invertible and $\|\partial f(\boldsymbol{w})^{-1}\| \le 2$. To compute the JVP of the inverse, we consider then $\partial f(\boldsymbol{w})^{-1}$ as the candidate JVP and examine

$$\frac{\|f^{-1}(\boldsymbol{\omega} + \boldsymbol{\eta}) - f(\boldsymbol{\omega}) - (\partial f(\boldsymbol{w}))^{-1}\boldsymbol{\eta}\|_2}{\|\boldsymbol{\eta}\|_2}.$$

Denote then $\boldsymbol{v}$ such that $f^{-1}(\boldsymbol{\omega} + \boldsymbol{\eta}) = \boldsymbol{w} + \boldsymbol{v}$. As $g(\boldsymbol{w}) = f(\boldsymbol{w}) - \boldsymbol{w}$ is $1/2$-contractive in N, we have $\|\boldsymbol{v} - \boldsymbol{\eta}\|_2 = \|g(\boldsymbol{w}+\boldsymbol{v}) - g(\boldsymbol{w})\|_2 \le 1/2\|\boldsymbol{v}\|_2$. So $\|\boldsymbol{v}\|_2 \ge \|\boldsymbol{\eta}\|/2$. We then get

$$\frac{\|f^{-1}(\boldsymbol{\omega} + \boldsymbol{\eta}) - f(\boldsymbol{\omega}) - (\partial f(\boldsymbol{w}))^{-1}\boldsymbol{\eta}\|_2}{\|\boldsymbol{\eta}\|_2}$$
$$= \frac{\|\boldsymbol{v} - (\partial f(\boldsymbol{w}))^{-1}(f(\boldsymbol{w} + \boldsymbol{v}) - f(\boldsymbol{w}))\|_2}{\|\boldsymbol{\eta}\|_2}$$
$$\le 4\frac{\|f(\boldsymbol{w} + \boldsymbol{v}) - f(\boldsymbol{w}) - \partial f(\boldsymbol{w})\boldsymbol{v}\|_2}{\|u\|_2}$$

As $\|\boldsymbol{\eta}\|_2 \to 0$, we have $\|\boldsymbol{v}\|_2 \to 0$ and so $\|f(\boldsymbol{w}+\boldsymbol{v}) - f(\boldsymbol{w}) - \partial f(\boldsymbol{w})\boldsymbol{v}\|_2/\|\boldsymbol{v}\|_2 \to 0$. Hence, f^{-1} is differentiable with JVP $\partial f^{-1}(\boldsymbol{\omega}) = (\partial f(\boldsymbol{w}))^{-1} = (\partial f(f^{-1}(\boldsymbol{\omega})))^{-1}$. This shows that f^{-1} is continuous and so $\partial f^{-1}(\boldsymbol{\omega})$ is continuous as a composition of continuous functions.

10.6   Summary

Implicit functions are functions that cannot be decomposed into elementary operations and for which autodiff can therefore not be directly applied. Examples are optimization problems and nonlinear equations. Envelope theorems can be used for differentiating through the min or max value (not solution) of a function. More generally, the implicit function theorem allows us to differentiate through such implicit functions. It gives conditions for the existence of derivatives and how to obtain them. The adjoint state method can be used to obtain the gradient of the composition of an explicit function and of an implicit function, specified by equality constraints. It can be used to prove the correctness of reverse-mode autodiff. The inverse function theorem can be used to

differentiate function inverses. In a sense, the implicit function theorem can be thought as the mother theorem, as it can be used to prove envelope theorems, the adjoint state method and the inverse function theorem.

11

Differentiating through integration

In this chapter, we study how to differentiate through integrals, with a focus on expectations and solutions of ordinary differential equations.

11.1   Differentiation under the integral sign

Given two Euclidean spaces Θ and $\mathcal{Y}$, and a function $f : \Theta \times \mathcal{Y} \to \mathbb{R}$, we often want to differentiate an integral of the form

$$F(\boldsymbol{\theta}) := \int_{\mathcal{Y}} f(\boldsymbol{\theta}, \boldsymbol{y}) d\boldsymbol{y}.$$

Provided that we can swap integration and differentiation, we have

$$\nabla F(\boldsymbol{\theta}) = \int_{\mathcal{Y}} \nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}, \boldsymbol{y}) d\boldsymbol{y}.$$

The conditions enabling us to do so are best examined in the context of measure theory. We refer the reader to e.g. (Cohn, 2013) for a course on measure theory and Flanders (1973) for an in-depth study of the differentiation under the integral sign. Briefly, if $\Theta = \mathcal{Y} = \mathbb{R}$, the following conditions are sufficient.

1. f is measurable in both its arguments, and $f(\theta, \cdot)$ is integrable for almost all $\theta \in \Theta$ fixed,

2. $f(\cdot, y)$ is absolutely continuous for almost all $y \in \mathcal{Y}$, that is, there exists an integrable function $g(\cdot, y)$ such that $f(\theta, y) = f(\theta_0, y) + \int_{\theta_0}^{\theta} g(\tau, y) d\tau$,

3. $\partial_1 f(\theta, y)$ (which exists almost everywhere if $f(\cdot, y)$ is absolutely continuous), is locally integrable, that is, for any closed interval $[\theta_0, \theta_1]$, the integral $\int_{\theta_0}^{\theta_1} \int |\partial_1 f(\theta, y)| dy d\theta$ is finite.

Any differentiable function $f : \Theta \times \mathcal{Y} \to \mathbb{R}$ is absolutely continuous. However, the conditions also hold if f is just absolutely continuous, that is, if $f(\cdot, y)$ is differentiable for almost all y. This weaker assumption can be used to smooth out differentiable almost-everywhere functions, such as the ReLu, as we study in Section 13.4.

11.2 Differentiating through expectations

A special case of differentiating through integrals is differentiating through expectations. Consider an expectation of the form

$$E(\boldsymbol{\theta}) := \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y)], \tag{11.1}$$

where $Y \in \mathcal{Y} \subseteq \mathbb{R}^M$ is a random variable, distributed according to a distribution $p_{\boldsymbol{\theta}}$ parameterized by $\boldsymbol{\theta} \in \Theta$ and where $g \colon \mathbb{R}^M \to \mathbb{R}$ is, depending on the setting, potentially a blackbox function (i.e., we do not have access to its gradients). Typically, $\boldsymbol{\theta} \in \Theta$ could be parameters we wish to estimate, or it could indirectly be generated by $\boldsymbol{\theta} = f(\boldsymbol{x}, \boldsymbol{w}) \in \Theta$, where f is a neural network with parameters $\boldsymbol{w} \in \mathcal{W}$ we wish to estimate. The operation of computing the expectation over Y removes Y from the computational graph and, depending on the choice of $p_{\boldsymbol{\theta}}$, it can smooth out g. In this chapter, we review estimation techniques to (approximately) compute $\nabla E(\boldsymbol{\theta})$, allowing us to optimize $\boldsymbol{\theta}$ (or $\boldsymbol{w}$ using the chain rule) by gradient-based algorithms.

The main difficulty in computing $\nabla E(\boldsymbol{\theta})$ stems from the fact that $\boldsymbol{\theta}$ are the parameters of the distribution $p_{\boldsymbol{\theta}}$. Estimating an expectation $E(\boldsymbol{\theta}) = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y)]$ using Monte-Carlo estimation requires us to sample from $p_{\boldsymbol{\theta}}$. However, it is not clear how to differentiate E w.r.t. $\boldsymbol{\theta}$ if $\boldsymbol{\theta}$ is involved in the sampling process.

11.2.1   The easy case

If instead, we consider an expected function where $\boldsymbol{\theta}$ are the parameters of E, not of p, the situation is very much different. Formally, consider the function

$$\boldsymbol{\theta} \mapsto \mathbb{E}_{Y \sim p}[g(Y, \boldsymbol{\theta})],$$

where p does not depend on $\boldsymbol{\theta}$. Then, under mild conditions recalled in Section 11.1, we can swap differentiation and integration to obtain

$$\nabla_{\boldsymbol{\theta}} \mathbb{E}_{Y \sim p}[g(Y, \boldsymbol{\theta})] = \mathbb{E}_{Y \sim p}[\nabla_{\boldsymbol{\theta}} g(Y, \boldsymbol{\theta})].$$

Because the gradient is itself an expectation, we can easily obtain an unbiased estimate of it by Monte-Carlo estimation. That is, we draw m i.i.d. samples $Y_1, \ldots, Y_m$ from p, compute $\nabla_{\boldsymbol{\theta}} g(Y_i, \boldsymbol{\theta})$ for each Y_i and average the results.

11.2.2   Exact gradients

Continuous case

When $\mathcal{Y}$ is a continuous set (that is, $p_{\boldsymbol{\theta}}(\boldsymbol{y})$ is a probability density function), we can rewrite Eq. (11.1) as

$$E(\boldsymbol{\theta}) = \int_{\mathcal{Y}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) g(\boldsymbol{y}) d\boldsymbol{y}.$$

Provided that we can swap integration and differentiation (see Section 11.1), we then have

$$\nabla E(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \int_{\mathcal{Y}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) g(\boldsymbol{y}) d\boldsymbol{y}$$
$$= \int_{\mathcal{Y}} \nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) g(\boldsymbol{y}) d\boldsymbol{y}.$$

Discrete case

When $\mathcal{Y}$ is a discrete set (that is, $p_{\boldsymbol{\theta}}(\boldsymbol{y})$ is a probability mass function), we can rewrite Eq. (11.1) as

$$E(\boldsymbol{\theta}) = \sum_{\boldsymbol{y} \in \mathcal{Y}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) g(\boldsymbol{y}).$$

We then obtain

$$\nabla E(\boldsymbol{\theta}) = \sum_{\boldsymbol{y} \in \mathcal{Y}} g(\boldsymbol{y}) \nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\boldsymbol{y}). \tag{11.2}$$

We notice that, as written in Eq. (11.2), $\nabla E(\boldsymbol{\theta})$ is not an expectation. We therefore cannot use Monte-Carlo estimation to estimate (11.2). Instead, we can compute it by brute force, i.e., by summing over all possible $\boldsymbol{y} \in \mathcal{Y}$. However, this is clearly only computationally tractable if $|\mathcal{Y}|$ is small or if $p_{\boldsymbol{\theta}}$ is designed to have sparse support, i.e., so that the set $\{\boldsymbol{y} \in \mathcal{Y} \colon p_{\boldsymbol{\theta}}(\boldsymbol{y}) \neq 0\}$ is small. Moreover, even if these conditions hold, summing over $\boldsymbol{y}$ could be problematic if $g(\boldsymbol{y})$ is expensive to compute. Therefore, exact gradients are seldom used in practice.

11.2.3 Application to expected loss functions

This framework is particularly useful to work with expected loss functions of the form

$$L(\boldsymbol{\theta}; \boldsymbol{y}) := \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\ell(Y, \boldsymbol{y})],$$

where $\boldsymbol{y}$ is some ground truth. Equivalently, we can set $\ell = -r$, where r is a **reward function**. As we shall see, some gradient estimators will support a discrete loss function $\ell \colon \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$, while others will require a differentiable loss function $\ell \colon \mathbb{R}^M \times \mathcal{Y} \to \mathbb{R}$. Intuitively, $L(\boldsymbol{\theta}; \boldsymbol{y})$ will be low if $p_{\boldsymbol{\theta}}$ assigns high probability to predictions $\widehat{\boldsymbol{y}}$ with low loss value $\ell(\widehat{\boldsymbol{y}}, \boldsymbol{y})$.

In the classification setting, where $\mathcal{Y} = [M]$, $p_{\boldsymbol{\theta}}$ is often chosen to be the **Gibbs distribution**, which is a categorical distribution induced by a softargmax

$$p_{\boldsymbol{\theta}}(Y = y) := \frac{\exp(\theta_y)}{\sum_{i \in [M]} \exp(\theta_i)} = [\text{softmax}(\boldsymbol{\theta})]_y \in (0, 1),$$

where $\theta_y := f(\boldsymbol{x}, y, \boldsymbol{w}) \in \mathbb{R}$ are logits produced by a neural network f. More generally, in the structured prediction setting, where $\mathcal{Y} \subseteq \mathbb{R}^M$ but $|\mathcal{Y}| \gg M$, we often use the distribution

$$p_{\boldsymbol{\theta}}(Y = \boldsymbol{y}) := \frac{\exp(\langle \phi(\boldsymbol{y}), \boldsymbol{\theta} \rangle)}{\sum_{\boldsymbol{y} \in \mathcal{Y}} \exp(\langle \phi(\boldsymbol{y}), \boldsymbol{\theta} \rangle)}.$$

where $\boldsymbol{\theta} = f(\boldsymbol{x}, \boldsymbol{w}) \in \mathbb{R}^M$. Given a distribution ρ over $\mathcal{X} \times \mathcal{Y}$, we then want to minimize the expected loss function, also known as **risk**,

$$R(\boldsymbol{w}) := \mathbb{E}_{(X,Y)\sim\rho}[L(f(X, \boldsymbol{w}); Y)].$$

Typically, minimizing $R(\boldsymbol{w})$ is done through some form of gradient descent, which requires us to be able to compute

$$\begin{aligned} \nabla R(\boldsymbol{w}) &= \mathbb{E}_{(X,Y)\sim\rho}[\nabla_{\boldsymbol{w}} L(f(X, \boldsymbol{w}); Y)] \\ &= \mathbb{E}_{(X,Y)\sim\rho}[\partial_2 f(\boldsymbol{x}, \boldsymbol{w})^* \nabla L(f(X, \boldsymbol{w}); Y)]. \end{aligned}$$

Computing $\nabla R(\boldsymbol{w})$ therefore boils down to computing the gradient of $L(\boldsymbol{\theta}; \boldsymbol{y})$, which is of the same form as Eq. (11.1).

11.2.4   Application to experimental design

In experimental design, we wish to minimize a function $g(\boldsymbol{\lambda})$, which we assume costly to evaluate. As an example, evaluating $g(\boldsymbol{\lambda})$ could require us to run a scientific experiment with parameters $\boldsymbol{\lambda} \in \mathbb{R}^Q$. As another example, in hyperparameter optimization, evaluating $g(\boldsymbol{\lambda})$ would require us to run a learning algorithm with hyperparameters $\boldsymbol{\lambda} \in \mathbb{R}^Q$. Instead of solving the problem $\arg\min_{\boldsymbol{\lambda}\in\mathbb{R}^Q} g(\boldsymbol{\lambda})$, we can lift the problem to probability distributions and solve $\arg\min_{\boldsymbol{\theta}\in\mathbb{R}^M} E(\boldsymbol{\theta})$, where $E(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\lambda}\sim p_{\boldsymbol{\theta}}}[g(\boldsymbol{\lambda})]$. This requires the probability distribution $p_{\boldsymbol{\theta}}$ to assign high probability to $\boldsymbol{\lambda}$ values that achieve small $g(\boldsymbol{\lambda})$ value. Solving this problem by stochastic gradient descent requires us to be able to compute estimates of $\nabla E(\boldsymbol{\theta})$. This can be done for instance with SFE explained in Section 11.3, which does not require gradients of g, unlike implicit differentiation explained in Chapter 10. This approach also requires us to choose a distribution $p_{\boldsymbol{\theta}}$ over $\boldsymbol{\lambda}$. For continuous hyperparameters, a natural choice would be the normal distribution $\boldsymbol{\lambda} \sim \text{Normal}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, setting $\boldsymbol{\theta} = (\boldsymbol{\mu}, \boldsymbol{\Sigma})$. Once we obtained $\boldsymbol{\theta}$ by minimizing $E(\boldsymbol{\theta})$, we need a way to recover $\boldsymbol{\lambda}$. This can be done for example by choosing the mode of the distribution, i.e., $\arg\max_{\boldsymbol{\lambda}\in\mathbb{R}^Q} p_{\boldsymbol{\theta}}(\boldsymbol{\lambda})$, or the mean of the distribution $\mathbb{E}_{\boldsymbol{\lambda}\sim p_{\boldsymbol{\theta}}(\boldsymbol{\lambda})}[\boldsymbol{\lambda}]$. Of course, in the case of the normal distribution, they coincide.

11.3 Score function estimators, REINFORCE

11.3.1 Scalar-valued functions

The key idea of the **score function estimator** (SFE), also known as REINFORCE, is to rewrite $\nabla E(\boldsymbol{\theta})$ as an expectation. The estimator is based on the **logarithmic derivative identity**

$$\nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\boldsymbol{y}) = \frac{\nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\boldsymbol{y})}{p_{\boldsymbol{\theta}}(\boldsymbol{y})} \iff \nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) = p_{\boldsymbol{\theta}}(\boldsymbol{y}) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\boldsymbol{y}).$$

This is known as the **score function**, hence the estimator name. Using this identity, we obtain the following gradient estimator.

> **Proposition 11.1** (SFE for scalar-valued functions). Let
> $$E(\boldsymbol{\theta}) := \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y)] = \int_{\mathcal{Y}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) g(\boldsymbol{y}) d\boldsymbol{y},$$
> where $Y \in \mathcal{Y} \subseteq \mathbb{R}^M$ and $g \colon \mathcal{Y} \to \mathbb{R}$. Then,
> $$\nabla E(\boldsymbol{\theta}) = \mathbb{E}_{Y \sim \boldsymbol{p_{\theta}}}[g(Y) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)].$$

Proof.
$$\begin{aligned}
\nabla E(\boldsymbol{\theta}) &= \int_{\mathcal{Y}} \nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) g(\boldsymbol{y}) d\boldsymbol{y} \\
&= \int_{\mathcal{Y}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) g(\boldsymbol{y}) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\boldsymbol{y}) d\boldsymbol{y} \\
&= \mathbb{E}_{Y \sim \boldsymbol{p_{\theta}}}[g(Y) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)].
\end{aligned}$$
□

SFE is suitable when two requirements are met: it is easy to sample from $p_{\boldsymbol{\theta}}$ and the gradient of the log-PDF, $\nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\boldsymbol{y})$, is available in closed form. Since the SFE gradient is an expectation, we can use Monte-Carlo estimation to compute an unbiased estimator of $\nabla E(\boldsymbol{\theta})$:

$$\nabla E(\boldsymbol{\theta}) \approx \boldsymbol{\gamma}_n(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^{n} g(\boldsymbol{y}_i) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\boldsymbol{y}_i), \qquad (11.3)$$

where $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n$ are sampled from $p_{\boldsymbol{\theta}}$. Interestingly, the gradient of g is not needed in this estimator. Therefore, there is no differentiability assumption about g. This is why SFE is useful when g is a discrete loss function or more generally a blackbox function.

Example 11.1 (SFE with a language model). In a language model, the probability of a sentence $\boldsymbol{y} = (y_1, \ldots, y_L)$ is typically factored using the chain rule of probability

$$p_{\boldsymbol{\theta}}(\boldsymbol{y}) \coloneqq p_{\boldsymbol{\theta}}(y_1) p_{\boldsymbol{\theta}}(y_2|y_1) \ldots p_{\boldsymbol{\theta}}(y_L|y_1, \ldots, y_{L-1}),$$

where $p_{\boldsymbol{\theta}}$ is modeled using a transformer or RNN. Note that the probabilities are normalized by construction, so there is no need for an explicit normalization constant. Thanks to this factorization, it is easy to sample from $p_{\boldsymbol{\theta}}$ and the log-probability enjoys the simple expression

$$\nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) = \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(y_1) + \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(y_2|y_1) + \cdots + \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(y_L|y_1, \ldots, y_{L-1}).$$

This gradient is easy to compute, since the token-wise distributions $p_{\boldsymbol{\theta}}(y_j|y_1, \ldots, y_{j-1})$ are typically using a softargmax. We can therefore easily compute $\nabla E(\boldsymbol{\theta})$ under $p_{\boldsymbol{\theta}}$ using SFE. This is for instance useful to optimize an expected reward, in order to finetune or align a language model (Ziegler *et al.*, 2019).

Another example when $\nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\boldsymbol{y})$ is available in closed form is in the context of reinforcement learning, where $p_{\boldsymbol{\theta}}(\boldsymbol{y})$ is a Markov Decision Process (MDP) and is called the policy. Applying the SFE leads to the (vanilla) policy gradient method (Sutton *et al.*, 1999) and can then be used to compute the gradient of an expected cumulative reward. However, SFE is more problematic when used with the Gibbs distribution, due to the explicit normalization constant.

Example 11.2 (SFE with a Gibbs distribution). The Gibbs distribution is parameterized as

$$p_{\boldsymbol{\theta}}(y) \coloneqq \exp(\theta_y/\gamma - A(\boldsymbol{\theta})) = \exp(\theta_y/\gamma)/\exp(A(\boldsymbol{\theta}))$$

where we defined the log-partition function

$$A(\boldsymbol{\theta}) \coloneqq \log \sum_{y \in \mathcal{Y}} \exp(\theta_y/\gamma).$$

A typical parametrization is $\theta_{\boldsymbol{y}} = f(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{w})$. We then have

$$\log p_{\boldsymbol{\theta}}(y) = \theta_y/\gamma - A(\boldsymbol{\theta}),$$

so that

$$\nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(y) = \boldsymbol{e}_y/\gamma - \nabla A(\boldsymbol{\theta}).$$

We therefore see that $\nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(y)$ crucially depends on $\nabla A(\boldsymbol{\theta})$, the gradient of the log-partion. This gradient is available for some structured sets $\mathcal{Y}$ but not in general.

As another example, we apply SFE in Section 13.4 to derive the gradient of perturbed functions.

Differentiating through both the distribution and the function

Suppose both the distribution and the function now depend on $\boldsymbol{\theta}$. When g is scalar-valued and differentiable w.r.t. $\boldsymbol{\theta}$, we want to differentiate

$$E(\boldsymbol{\theta}) := \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y, \boldsymbol{\theta})].$$

Using the product rule, we obtain

$$\nabla E(\boldsymbol{\theta}) = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y, \boldsymbol{\theta}) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)] + \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla_{\boldsymbol{\theta}} g(Y, \boldsymbol{\theta})].$$

Differentiating through joint distributions

Suppose we now want to differentiate through

$$E(\boldsymbol{\theta}) := \mathbb{E}_{Y_1 \sim p_{\boldsymbol{\theta}}, Y_2 \sim q_{\boldsymbol{\theta}}}[g(Y_1, Y_2)].$$

The gradient is then given by

$$\nabla E(\boldsymbol{\theta}) = \mathbb{E}_{Y_1 \sim p_{\boldsymbol{\theta}}, Y_2 \sim q_{\boldsymbol{\theta}}}[(\nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y_1) + \nabla \log p_{\boldsymbol{\theta}}(Y_2)) g(Y_1, Y_2)],$$

which is easily seen by applying Proposition 11.1 on the joint distribution $\rho_{\boldsymbol{\theta}} := p_{\boldsymbol{\theta}} \cdot q_{\boldsymbol{\theta}}$. The extension to more than two variables is straightforward.

11.3.2 Variance reduction

Bias and variance

Recall the definition of $\boldsymbol{\gamma}_n$ in Eq. (11.3). SFE is an **unbiased** estimator, meaning that

$$\nabla E(\boldsymbol{\theta}) = \mathbb{E}[\boldsymbol{\gamma}_n(\boldsymbol{\theta})],$$

where the expectation is taken with respect to the n samples drawn. Since the gradient is vector-valued, we need to define a scalar-valued notion of variance. We do so by using the squared Euclidean distance in the usual variance definition to define

$$\mathbb{V}[\boldsymbol{\gamma}_n(\boldsymbol{\theta})] := \mathbb{E}[\|\boldsymbol{\gamma}_n(\boldsymbol{\theta}) - \nabla E(\boldsymbol{\theta})\|_2^2]$$
$$= \mathbb{E}[\|\boldsymbol{\gamma}_n(\boldsymbol{\theta})\|_2^2] - \|\nabla E(\boldsymbol{\theta})\|_2^2.$$

This is equivalent to the trace of the covariance matrix. The variance goes to zero as $n \to \infty$.

Baseline

SFE is known to suffer from **high variance** (Mohamed *et al.*, 2020). This means that this estimator may require us to draw many samples from the distribution $p_{\boldsymbol{\theta}}$ to work well in practice. One of the simplest variance reduction technique consists in shifting the function g with a constant β, called a **baseline**, to obtain

$$\nabla E(\boldsymbol{\theta}) = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[(g(Y) - \beta)\nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)].$$

The reason this is still a valid estimator of $\nabla E(\boldsymbol{\theta})$ stems from

$$\mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)] = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}\left[\frac{\nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(Y)}{p_{\boldsymbol{\theta}}(Y)}\right]$$
$$= \nabla_{\boldsymbol{\theta}} \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\mathbf{1}]$$
$$= \nabla_{\boldsymbol{\theta}} \mathbf{1}$$
$$= \mathbf{0},$$

for any valid distribution $p_{\boldsymbol{\theta}}$. The baseline β is often set to the running average of past values of the function g, though it is neither optimal nor does it guarantee to lower the variance (Mohamed *et al.*, 2020).

Control variates

Another general technique are **control variates**. Let us denote the expectation of a function $h \colon \mathbb{R}^M \to \mathbb{R}$ under the distribution $p_{\boldsymbol{\theta}}$ as

$$H(\boldsymbol{\theta}) := \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[h(Y)].$$

Suppose that $H(\boldsymbol{\theta})$ and its gradient $\nabla H(\boldsymbol{\theta})$ are known in closed form. Then, for any $\gamma \geq 0$, we clearly have

$$
\begin{aligned}
E(\boldsymbol{\theta}) &= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y)] \\
&= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y) - \gamma(h(Y) - H(\boldsymbol{\theta}))] \\
&= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y) - \gamma h(Y)] + \gamma H(\boldsymbol{\theta})
\end{aligned}
$$

and therefore

$$
\nabla E(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y) - \gamma h(Y)] + \gamma \nabla H(\boldsymbol{\theta}).
$$

Applying SFE, we then obtain

$$
\nabla E(\boldsymbol{\theta}) = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[(g(Y) - \gamma h(Y)) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)] + \gamma \nabla H(\boldsymbol{\theta}).
$$

Examples of h include a bound on f or a second-order Taylor expansion of f, assuming that these approximations are easier to integrate than f (Mohamed *et al.*, 2020).

11.3.3 Vector-valued functions

It is straightforward to extend the SFE to vector-valued functions.

Proposition 11.2 (SFE for vector-valued functions). Let

$$
\boldsymbol{E}(\boldsymbol{\theta}) := \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y)] = \int_{\mathcal{Y}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) g(\boldsymbol{y}) d\boldsymbol{y},
$$

where $Y \in \mathcal{Y}$, $g \colon \mathcal{Y} \to \mathcal{G}$ and $\boldsymbol{\theta} \in \Theta \mapsto p_{\boldsymbol{\theta}}(\boldsymbol{y}) \in [0, 1]$. Then,

$$
\partial \boldsymbol{E}(\boldsymbol{\theta}) = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y) \otimes \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)].
$$

The Jacobian $\partial \boldsymbol{E}(\boldsymbol{\theta})$ is a linear map from Θ to $\mathcal{G}$ such that

$$
\partial \boldsymbol{E}(\boldsymbol{\theta}) \boldsymbol{u} = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\langle \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y), \boldsymbol{u} \rangle g(Y)] \in \mathcal{G} \quad \forall \boldsymbol{u} \in \Theta.
$$

Proof.

$$\partial E(\boldsymbol{\theta}) = \partial_{\boldsymbol{\theta}} \int_{\mathcal{Y}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) g(\boldsymbol{y}) d\boldsymbol{y}$$

$$= \int_{\mathcal{Y}} \partial_{\boldsymbol{\theta}} [p_{\boldsymbol{\theta}}(\boldsymbol{y}) g(\boldsymbol{y})] d\boldsymbol{y}$$

$$= \int_{\mathcal{Y}} g(\boldsymbol{y}) \otimes \nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) d\boldsymbol{y}$$

$$= \int_{\mathcal{Y}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) g(\boldsymbol{y}) \otimes \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\boldsymbol{y}) d\boldsymbol{y}$$

$$= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}} [g(Y) \otimes \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)].$$

$\square$

Differentiating through both the distribution and the function

If $\boldsymbol{\theta}$ now influences both the distribution and the function,

$$E(\boldsymbol{\theta}) := \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}} [g(Y, \boldsymbol{\theta})],$$

then, we obtain

$$\partial E(\boldsymbol{\theta}) = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}} [g(Y, \boldsymbol{\theta}) \otimes \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)] + \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}} [\partial_{\boldsymbol{\theta}} g(Y, \boldsymbol{\theta})].$$

11.3.4 Second derivatives

Using the previous subsection with $g(\boldsymbol{y}, \boldsymbol{\theta}) = g(\boldsymbol{y}) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\boldsymbol{\theta})$, we easily obtain an estimator of the Hessian.

> **Proposition 11.3** (SFE for the Hessian). Let us define the scalar-valued function $E(\boldsymbol{\theta}) := \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}} [g(Y)]$. Then,
>
> $$\nabla^2 E(\boldsymbol{\theta}) = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}} [g(Y) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y) \otimes \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)] +$$
> $$\mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}} [g(Y) \nabla_{\boldsymbol{\theta}}^2 \log p_{\boldsymbol{\theta}}(Y)].$$

This can also be derived using the second-order log-derivative

$$\nabla_{\boldsymbol{\theta}}^2 \log p_{\boldsymbol{\theta}}(\boldsymbol{y}) = \frac{1}{p_{\boldsymbol{\theta}}(\boldsymbol{y})} \nabla_{\boldsymbol{\theta}}^2 p_{\boldsymbol{\theta}}(\boldsymbol{y}) - \frac{1}{p_{\boldsymbol{\theta}}(\boldsymbol{y})^2} \nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) \otimes \nabla_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\boldsymbol{y})$$

so that

$$\nabla_{\boldsymbol{\theta}}^2 p_{\boldsymbol{\theta}}(\boldsymbol{y}) = p_{\boldsymbol{\theta}}(\boldsymbol{y}) \left[\nabla_{\boldsymbol{\theta}}^2 \log p_{\boldsymbol{\theta}}(\boldsymbol{y}) + \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\boldsymbol{y}) \otimes \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\boldsymbol{y}) \right].$$

Link with the Bartlett identities

The Bartlett identities are expressions relating the moments of the score function (gradient of the log-likelihood function). Using Proposition 11.1 with $g(\boldsymbol{y}) = 1$ and $\int_{\mathcal{Y}} p_{\boldsymbol{\theta}}(\boldsymbol{y}) d\boldsymbol{y} = 1$, we obtain

$$\mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)] = \boldsymbol{0}, \tag{11.4}$$

which is known as Bartlett's first identity. Similarly, using Proposition 11.3, we obtain

$$
\begin{aligned}
&\mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla_{\boldsymbol{\theta}}^2 \log p_{\boldsymbol{\theta}}(Y)] + \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y) \otimes \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(Y)] \\
&= \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla_{\boldsymbol{\theta}}^2 \log p_{\boldsymbol{\theta}}(Y)] + \text{cov}[\log p_{\boldsymbol{\theta}}(Y)] \\
&= \boldsymbol{0},
\end{aligned}
\tag{11.5}
$$

which is known as Bartlett's second identity.

11.4 Path gradient estimators, reparametrization trick

As we saw previously, the main difficulty in computing gradients of expectations arises when the parameters $\boldsymbol{\theta}$ play a role in the distribution $p_{\boldsymbol{\theta}}$ being sampled. The key idea of the path gradient estimator (PGE), also known as reparametrization trick, is to rewrite the expectation in such a way that the parameters are moved from the distribution to the function, using a **change of variable**.

11.4.1 Location-scale transforms

For example, let us set $p_{\boldsymbol{\theta}} \coloneqq \text{Normal}(\mu, \sigma^2)$, where $\boldsymbol{\theta} \coloneqq (\mu, \sigma)$ and Normal is a univariate normal distribution. If $U \sim p_{\boldsymbol{\theta}}$, then it is easy to check that $U = \mu + \sigma Z$, where $Z \sim \text{Normal}(0, 1)$. We can therefore write

$$
\begin{aligned}
E(\boldsymbol{\theta}) &\coloneqq \mathbb{E}_{U \sim \text{Normal}(\mu, \sigma^2)}[g(U)] \\
&= \mathbb{E}_{Z \sim \text{Normal}(0,1)}[g(\mu + \sigma Z)] \\
&= \mathbb{E}_{Z \sim \text{Normal}(0,1)}[g(t(Z, \boldsymbol{\theta}))],
\end{aligned}
$$

where we defined the **location-scale transformation**

$$U = T(Z, \boldsymbol{\theta}) \coloneqq \mu + \sigma Z. \tag{11.6}$$

Such a transformation exists, not only for the normal distribution, but for **location-scale family** distributions. The key advantage is that we can now easily compute $\nabla E(\boldsymbol{\theta})$, since $\boldsymbol{\theta}$ is no longer involved in the distribution. We can generalize this idea, as summarized below.

Proposition 11.4 (Path gradient estimator). Let us define

$$E(\boldsymbol{\theta}) \coloneqq \mathbb{E}_{U \sim p_{\boldsymbol{\theta}}}[g(U)],$$

where $U \in \mathcal{U} \subseteq \mathbb{R}^M$ and $g \colon \mathbb{R}^M \to \mathbb{R}$ is differentiable. Suppose there is a differentiable transformation $T \colon \mathbb{R}^M \times \mathbb{R}^Q \to \mathbb{R}^M$ such that if $Z \sim p$ (where p does not depend on $\boldsymbol{\theta}$) and $U = T(Z, \boldsymbol{\theta})$, then $U \sim p_{\boldsymbol{\theta}}$. Then, we have

$$E(\boldsymbol{\theta}) = \mathbb{E}_{Z \sim p}[h(Z, \boldsymbol{\theta})] = \mathbb{E}_{Z \sim p}[g(T(Z, \boldsymbol{\theta}))],$$

where $h(\boldsymbol{z}, \boldsymbol{\theta}) \coloneqq g(T(\boldsymbol{z}, \boldsymbol{\theta}))$. This implies

$$\begin{aligned}
\nabla E(\boldsymbol{\theta}) &= \mathbb{E}_{Z \sim p}[\nabla_2 h(Z, \boldsymbol{\theta})] \\
&= \mathbb{E}_{Z \sim p}[\partial_2 T(Z, \boldsymbol{\theta})^* \nabla g(T(Z, \boldsymbol{\theta}))].
\end{aligned}$$

The reparametrization trick gives an **unbiased estimator** of $\nabla E(\boldsymbol{\theta})$. It has however two key disadvantages. First, it assumes that g is **differentiable** (almost everywhere), which may not always be the case. Second, it assumes that g is well-defined on $\mathbb{R}^M$, not on $\mathcal{U}$, which could be problematic for some discrete loss functions, such as the zero-one loss function or ranking loss functions.

11.4.2 Inverse transforms

The inverse transform method can be used for sampling from a probability distribution, given access to its associated **quantile function**. Recall that the cumulative distribution function (CDF) associated with a random variable Y is the function $F_Y \colon \mathbb{R} \to [0, 1]$ defined by

$$F_Y(y) \coloneqq \mathbb{P}(Y \leq y).$$

The quantile function is then a function $Q \colon [0, 1] \to \mathbb{R}$ such that $Q(\pi) = y$ for $\pi = F_Y(y)$. Assuming F_Y is continuous and strictly increasing, we

have that Q is the **inverse CDF**,

$$Q(\pi) = F_Y^{-1}(\pi).$$

In the general case of CDF functions that are not strictly increasing, the quantile function is usually defined as

$$Q(\pi) := \inf\{y \in \mathbb{R} \colon \pi \leq F_Y(y)\}.$$

Given access to the quantile function $Q(\pi)$ associated with a distribution p, inverse transform sampling allows us to sample from p by first drawing a sample from the **uniform distribution** and then making this sample go through the quantile function.

> **Proposition 11.5** (Inverse transform sampling). Suppose $Y \sim p$, where p is a distribution with quantile function $Q(\pi)$. If $\pi \sim$ Uniform$(0,1)$, then $Q(\pi) \sim p$.

If the quantile function is differentiable, we can therefore use it as a **transformation** within the **reparametrization trick**. Indeed, if $Y \sim p_{\boldsymbol{\theta}}$, where $p_{\boldsymbol{\theta}}$ is a distribution with parameter $\boldsymbol{\theta}$ and quantile function $Q(\pi, \boldsymbol{\theta})$, then we have

$$E(\boldsymbol{\theta}) = \mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[g(Y)] = \mathbb{E}_{\pi \sim \text{Uniform}(0,1)}[g(Q(\pi, \boldsymbol{\theta}))]$$

and therefore, by the reparametrization trick (Proposition 11.4),

$$\nabla E(\boldsymbol{\theta}) = \mathbb{E}_{\pi \sim \text{Uniform}(0,1)}[\partial_2 Q(\pi, \boldsymbol{\theta})^* \nabla g(Q(\pi, \boldsymbol{\theta}))].$$

> **Example 11.3** (Examples of quantile functions). If $Y \sim$ Exponential(λ), the CDF of Y is $\pi = F_Y(y) = 1 - \exp(-\lambda y)$ for $y \geq 0$ and therefore the quantile function is $Q(\pi, \lambda) = -\frac{\log(1-\pi)}{\lambda}$. If $Y \sim$ Normal(μ, σ^2), the CDF is $F_Y(y) = \frac{1}{2}\left[1 + \text{erf}\left(\frac{y-\mu}{\sigma\sqrt{2}}\right)\right]$ and the quantile function is $Q(\pi, \boldsymbol{\theta}) = \mu + \sigma\sqrt{2} \cdot \text{erf}^{-1}(2\pi - 1)$, where $\boldsymbol{\theta} = (\mu, \sigma)$. This therefore defines an alternative transformation to the location-scale transformation in Eq. (11.6).

Note that, in the above example, the error function erf and its inverse do not enjoy analytical expressions but autodiff packages usually

provide numerical routines to compute them and differentiate through them. Nonetheless, one caveat of the inverse transform is that it indeed requires access to (approximations of) the quantile function and its derivatives, which may be difficult for complicated distributions.

11.4.3 Pushforward operators

Pushforward distributions

We saw so far that the reparametrization trick is based on using a change of variables in order to differentiate an expectation w.r.t. the parameters of the distribution. In this section, we further formalize that approach using pushforward distributions.

> **Definition 11.1** (Pushforward distribution). Suppose $Z \sim p$, where p is a distribution over $\mathcal{Z}$. Given a continuous map $T \colon \mathcal{Z} \to \mathcal{U}$, the pushforward distribution of p through T is the distribution q according to which $U \coloneqq T(Z) \in \mathcal{U}$ is distributed, i.e., $U \sim q$.

Although not explicit in the above, the transformation T can depend on some learnable parameters, for example if T is a neural network. Intuitively, the pushforward distribution is obtained by moving the position of all the points in the support of p. Inverse transform sampling studied in Section 11.4.2 can be seen as performing the pushforward of the uniform distribution through $T = Q$, where Q is the quantile function. The Gumbel trick studied in Section 13.5 can be seen as a the pushforward of Gumbel noise through $T = \text{argmax}$ (a discontinuous function) and Gumbel noise can itself be obtained by pushing forward the uniform distribution through $T = -\log(-\log(\cdot))$ (Remark 13.2). In a generative modeling setting, we use the pushforward of Gaussian noise through a parametrized transformation $\boldsymbol{x} = T(\boldsymbol{z}, \boldsymbol{w})$ called a generator, typically a neural network.

A crucial aspect of the pushforward distribution q is that it can be **implicitly** defined, meaning that we do not necessarily need to know the explicit form of the associated PDF. In fact, it is easy to to **sample** from q, provided that it is easy to sample from p:

$$U \sim q \iff Z \sim p, U \coloneqq T(Z).$$

Hence the usefulness of the pushforward distribution in **generative modeling**. Furthermore, if p has associated PDF p_Z, we can compute the expectation of a function f according to q as

$$\mathbb{E}_{U \sim q}[f(U)] = \mathbb{E}_{Z \sim p}[f(T(Z))] = \int_{\mathcal{Z}} f(T(\boldsymbol{z})) p_Z(\boldsymbol{z}) d\boldsymbol{z},$$

even though we do not know the explicit form of the PDF of q.

Pushforward measures

More generally, we can define the notion of pushforward, in the language of measures. A **measure** $\alpha \in \mathcal{M}(\mathcal{Z})$, that has a density $d\alpha(\boldsymbol{z}) \coloneqq p_Z(\boldsymbol{z}) d\boldsymbol{z}$, can be integrated against as

$$\int_{\mathcal{Z}} f(\boldsymbol{z}) d\alpha(\boldsymbol{z}) = \int_{\mathcal{Z}} f(\boldsymbol{z}) p_Z(\boldsymbol{z}) d\boldsymbol{z}.$$

A measure α is called a probability measure if it is positive and satisfies $\alpha(\mathcal{Z}) = \int_{\mathcal{Z}} d\alpha(\boldsymbol{z}) = \int_{\mathcal{Z}} p_Z(\boldsymbol{z}) d\boldsymbol{z} = 1$. See Peyré and Cuturi (2019, Chapter 2) for a concise introduction.

> **Definition 11.2** (Pushforward operator and measure). Given a continuous map $T \colon \mathcal{Z} \to \mathcal{U}$ and some measure $\alpha \in \mathcal{M}(\mathcal{Z})$, the pushforward measure $\beta = T_\sharp \alpha \in \mathcal{M}(\mathcal{U})$ is such that for all functions $f \in \mathcal{C}(\mathcal{U})$
> $$\int_{\mathcal{U}} f(\boldsymbol{u}) d\beta(\boldsymbol{u}) = \int_{\mathcal{Z}} f(T(\boldsymbol{z})) d\alpha(\boldsymbol{z}).$$
> Equivalently, for any measurable set $\mathcal{A} \subset \mathcal{U}$, we have
> $$\beta(\mathcal{A}) = \alpha(\{\boldsymbol{z} \in \mathcal{Z} \colon T(\boldsymbol{z}) \in \mathcal{A}\}) = \alpha(T^{-1}(\mathcal{A})).$$

Importantly, the pushforward operator preserves positivity and mass, therefore if α is a probability measure, then so is $T_\sharp \alpha$. The pushforward of a probability measure therefore defines a pushforward distribution (since a distribution can be parametrized by a probability measure).

11.4.4 Change-of-variables theorem

Assuming a transformation T is invertible, we have $Z = T^{-1}(U)$ and therefore for $\mathcal{A} \subseteq \mathcal{U}$, we have

$$\mathbb{P}(U \in \mathcal{A}) = \mathbb{P}(Z \in T^{-1}(\mathcal{A})) = \int_{T^{-1}(\mathcal{A})} p_Z(\boldsymbol{z})d\boldsymbol{z}.$$

Using the **change-of-variables theorem** from multivariate calculus, assuming T^{-1} is available, we can give an explicit formula for the PDF of the pushforward distribution.

> **Proposition 11.6** (PDF of the pushforward distribution). Suppose $Z \sim p$, where p is a distribution over $\mathcal{Z}$, with PDF p_Z. Given a **diffeomorphism** $T \colon \mathcal{Z} \to \mathcal{U}$ (i.e., an invertible and differentiable map), the pushforward distribution of p through T is the distribution q such that $U := T(Z) \sim q$ and its PDF is
>
> $$q_U(\boldsymbol{u}) = |\det(\partial T^{-1}(\boldsymbol{u}))|p_Z(T^{-1}(\boldsymbol{u})),$$
>
> where $\partial T^{-1}(\boldsymbol{u})$ is the Jacobian of $T^{-1} \colon \mathcal{U} \to \mathcal{Z}$.

Using this formula, we obtain

$$\begin{aligned}
\mathbb{P}(U \in \mathcal{A}) &= \int_{\mathcal{A}} p_U(\boldsymbol{u})d\boldsymbol{u} \\
&= \int_{\mathcal{A}} |\det(\partial T^{-1}(\boldsymbol{u}))|p_Z(T^{-1}(\boldsymbol{u}))d\boldsymbol{u}.
\end{aligned}$$

Using the inverse function theorem (Theorem 10.5), we then have

$$\partial T^{-1}(\boldsymbol{u}) = (\partial T(T^{-1}(\boldsymbol{u})))^{-1},$$

under the assumption that $T(\boldsymbol{z})$ is continuously differentiable and has invertible Jacobian $\partial T(\boldsymbol{z})$. **Normalizing flows** are parametrized transformations T designed such that T^{-1} and its Jacobian ∂T^{-1} are easy to compute; see e.g. Kobyzev *et al.* (2019) and Papamakarios *et al.* (2021) for a review.

11.5 Stochastic programs

A stochastic program is a program that involves some form of randomness. In a stochastic program, the final output, as well as intermediate

variables, may therefore be random variables. In other words, a stochastic program induces a probability distribution over program outputs, as well as over execution trajectories.

11.5.1   Stochastic computation graphs

A stochastic program can be represented by a stochastic computation graph as originally introduced by Schulman *et al.* (2015). Departing from that work, our exposition explicitly supports two types of intermediate operations: sampling from a **conditional distribution** or evaluating a **function**. These operations can produce either **deterministic** variables or **random** variables.

Function and distribution nodes

Formally, we define a stochastic computation graph as a directed acyclic graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V} = \mathcal{V}_f \cup \mathcal{V}_p$, $\mathcal{V}_f$ is the set of function nodes and $\mathcal{V}_p$ is the set of distribution nodes. Similarly to computation graphs reviewed in Section 4.1.3, we number the nodes as $\mathcal{V} = \{0, 1, \ldots, K\}$. Node 0 corresponds to the input $s_0 \in \mathcal{S}_0$, which we assume to be deterministic. It is the variable with respect to which we wish to differentiate. Node K corresponds to the program output $S_K \in \mathcal{S}_K$, which we assume to be a random variable. A node $k \in \{1, \ldots, K\}$ can either be a **function node** $k \in \mathcal{V}_f$ with an associated function f_k or a **distribution node** $k \in \mathcal{V}_p$, with associated conditional distribution p_k. A stochastic program has at least one distribution node, the source of randomness. Otherwise, it is a deterministic program. As for computation graphs, the set of edges $\mathcal{E}$ is used to represent dependences between nodes. We denotes the parents of node k by parents(k).

Deterministic and random variables

We distinguish between two types of intermediate variables: **deterministic** variables s_k and **random** variables S_k. Therefore, a distribution p_k or a function f_k may receive both types of variables as **conditioning** or **input**. It is then convenient to split parents(k) as

$\operatorname{parents}(k) = \operatorname{determ}(k) \cup \operatorname{random}(k)$, where we defined the **determin-istic parents** $\operatorname{determ}(k) \coloneqq \{i_1, \ldots, i_{p_k}\}$ and the **random parents** $\operatorname{random}(k) \coloneqq \{j_1, \ldots, j_{q_k}\}$. Therefore, $s_{i_1}, \ldots, s_{i_{p_k}}$ are the deterministic parent variables and $S_{j_1}, \ldots, S_{j_{q_k}}$ are the random parent variables, of node k.

Executing a stochastic program

We assume that nodes $0, 1, \ldots, K$ are in topological order (if this is not the case, we need to perform a topological sort). Given parent variables $s_{i_1}, \ldots, s_{i_{p_k}}$ and $S_{j_1}, \ldots, S_{j_{q_k}}$, a node $k \in \{1, \ldots, K\}$ produces an output as follows.

- If $k \in \mathcal{V}_p$ (distribution node), the output is

$$S_k \sim p_k(\cdot \mid s_{\operatorname{determ}(k)}, S_{\operatorname{random}(k)})$$
$$\iff S_k \sim p_k(\cdot \mid s_{i_1}, \ldots, s_{i_{p_k}}, S_{j_1}, \ldots, S_{j_{q_k}})$$

  Note that technically p_k is the distribution of S_k conditioned on its parents, not the distribution of S_k. Therefore, we should in principle write $S_k \mid s_{\operatorname{determ}(k)}, S_{\operatorname{random}(k)} \sim p_k(\cdot \mid s_{\operatorname{determ}(k)}, S_{\operatorname{random}(k)})$. We avoid this notation for conciseness and for symmetry with function nodes.

  Contrary to a function node, a distribution node can have no parents. That is, if $k \in \mathcal{V}_p$, it is possible that $\operatorname{parents}(k) = \emptyset$. A good example would be a parameter-free noise distribution.

- If $k \in \mathcal{V}_f$ (function node), the output is in general

$$S_k \coloneqq f_k(s_{\operatorname{determ}(k)}, S_{\operatorname{random}(k)})$$
$$\coloneqq f_k(s_{i_1}, \ldots, s_{i_{p_k}}, S_{j_1}, \ldots, S_{j_{q_k}})$$

  and in the special case $q_k = |\operatorname{random}(k)| = 0$, the output is

$$s_k \coloneqq f_k(s_{\operatorname{determ}(k)})$$
$$\coloneqq f_k(s_{i_1}, \ldots, s_{i_{p_k}}).$$

Unless the associated conditional distribution p_k is a delta distribution, that puts all the probability mass on a single point, the output of a

---

Algorithm 11.1 Executing a stochastic program

Nodes: $1, \ldots, K$ in topological order, where node k is either a function f_k or a conditional distribution p_k

Input: input $\boldsymbol{s}_0 \in \mathcal{S}_0$

1: **for** $k := 1, \ldots, K$ **do**
2:     Retrieve $\text{parents}(k) = \text{determ}(k) \cup \text{random}(k)$
3:     **if** $k \in \mathcal{V}_p$ **then**   ▷ Distribution node
4:         $S_k \sim p_k(\cdot | \boldsymbol{s}_{\text{determ}(k)}, S_{\text{random}(k)})$
5:     **else if** $k \in \mathcal{V}_f$ **then**   ▷ Function node
6:         **if** $|\text{random}(k)| \neq 0$ **then**
7:             $S_k := f_k(\boldsymbol{s}_{\text{determ}(k)}, S_{\text{random}(k)})$ ▷ Output is a R.V.
8:         **else if** $|\text{random}(k)| = 0$ **then**
9:             $\boldsymbol{s}_k := f_k(\boldsymbol{s}_{\text{determ}(k)})$ ▷ Output is deterministic
10: **Output:** $f(\boldsymbol{s}_0) := S_K \in \mathcal{S}_K$

---

distribution node $k \in \mathcal{V}_p$ is necessarily a random variable $S_k \in \mathcal{S}_k$. For function nodes $k \in \mathcal{V}_f$, the output of the function f_k is a random variable $S_k \in \mathcal{S}_k$ if at least one of the parents of k produces a random variable. Otherwise, if all parents of k produce deterministic variables, the output of f_k is a deterministic variable $\boldsymbol{s}_k \in \mathcal{S}_k$.

The entire procedure is summarized in Algorithm 11.1. We emphasize that $S_K = f(\boldsymbol{s}_0) \in \mathcal{S}_K$ is a random variable. Therefore, a stochastic program (implicitly) induces a distribution over S_K, and also over intermediate random variables S_k. Executing the stochastic program allows us to draw samples from that distribution.

Special cases
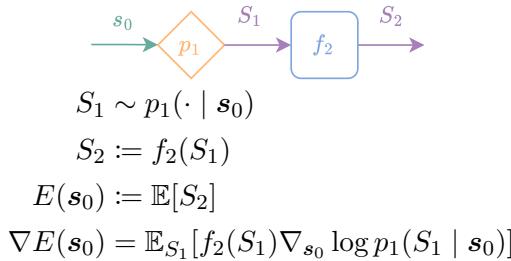
If all nodes are function nodes, we recover computation graphs, reviewed in Section 4.1.3. If all nodes are distribution nodes, we recover Bayesian networks, reviewed in Section 9.5.

11.5.2   Examples
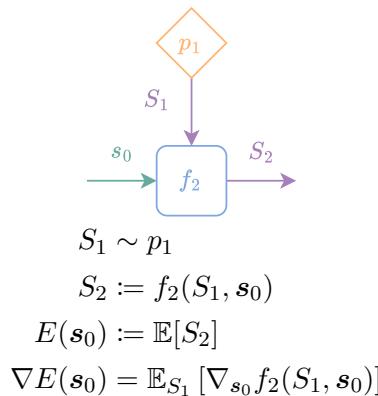
We now present several examples that illustrate our formalism. We use the legend below in the following illustrations.

Function □ Sampler ◇ → Deterministic variable → Stochastic variable

- Example 1 (SFE estimator):

$$S_1 \sim p_1(\cdot \mid \boldsymbol{s}_0)$$
$$S_2 := f_2(S_1)$$
$$E(\boldsymbol{s}_0) := \mathbb{E}[S_2]$$
$$\nabla E(\boldsymbol{s}_0) = \mathbb{E}_{S_1}[f_2(S_1)\nabla_{\boldsymbol{s}_0} \log p_1(S_1 \mid \boldsymbol{s}_0)]$$
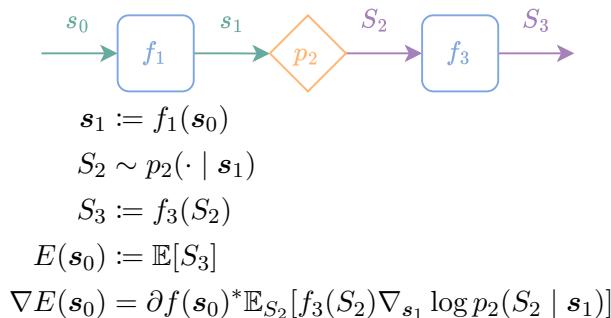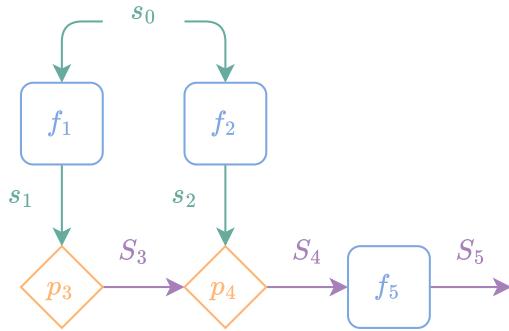
- Example 2 (Pathwise estimator):

$$S_1 \sim p_1$$
$$S_2 := f_2(S_1, \boldsymbol{s}_0)$$
$$E(\boldsymbol{s}_0) := \mathbb{E}[S_2]$$
$$\nabla E(\boldsymbol{s}_0) = \mathbb{E}_{S_1}\left[\nabla_{\boldsymbol{s}_0} f_2(S_1, \boldsymbol{s}_0)\right]$$

- Example 3 (SFE estimator + chain rule):

$$\boldsymbol{s}_1 := f_1(\boldsymbol{s}_0)$$
$$S_2 \sim p_2(\cdot \mid \boldsymbol{s}_1)$$
$$S_3 := f_3(S_2)$$
$$E(\boldsymbol{s}_0) := \mathbb{E}[S_3]$$
$$\nabla E(\boldsymbol{s}_0) = \partial f(\boldsymbol{s}_0)^* \mathbb{E}_{S_2}[f_3(S_2)\nabla_{\boldsymbol{s}_1} \log p_2(S_2 \mid \boldsymbol{s}_1)]$$

- Example 4:

$$s_1 := f_1(s_0)$$
$$s_2 := f_2(s_0)$$
$$S_3 \sim p_3(\cdot \mid s_1)$$
$$S_4 \sim p_4(\cdot \mid s_2, S_3)$$
$$S_5 := f_5(S_4)$$
$$E(s_0) := \mathbb{E}[S_5] = \mathbb{E}_{S_3} \left[\mathbb{E}_{S_4}[f_5(S_4)] \right]$$
$$\nabla E(s_0) = (\mathbb{E}_{S_3} \left[\nabla_{s_1} \log p(S_3 \mid s_1) \mathbb{E}_{S_4}[f_5(S_4)] \right],$$
$$\mathbb{E}_{S_3} \left[\mathbb{E}_{S_4} \left[f_5(S_4) \nabla_{s_2} \log p_4(S_4 | s_2, S_3) \right] \right])$$

As can be seen, the gradient expressions can quickly become quite complicated, demonstrating the merits of automatic differentiation in stochastic computation graphs.

11.5.3 Unbiased gradient estimators

The output of a stochastic program is a random variable

$$S_K := f(s_0).$$

It implicitly defines a probability distribution $p(\cdot|s_0)$ such that $S_K \sim p(\cdot|s_0)$. Executing the stochastic program once gives us an i.i.d. sample from $p(\cdot|s_0)$.

Since derivatives are defined for deterministic variables, we need a way to convert a random variable to a deterministic variable. One way

to do so is to consider the expected value (another way would be the mode)

$$E(\boldsymbol{s}_0) \coloneqq \mathbb{E}[S_K] = \mathbb{E}[f(\boldsymbol{s}_0)] \in \text{conv}(\mathcal{S}_K),$$

where the expectation is over $S_K \sim p(\cdot|\boldsymbol{s}_0)$ or equivalently over the intermediate random variables S_k

$$S_k \sim p_k(\cdot|\boldsymbol{s}_{\text{determ}(k)}, S_{\text{random}(k)}),$$

for $k \in \mathcal{V}_p$ (the distribution nodes). We then wish to compute the gradient or more generally the Jacobian of $E(\boldsymbol{s}_0)$.

If all nodes in the stochastic computation graph are function nodes, we can estimate the gradient of $E(\boldsymbol{s}_0)$ using the pathwise estimator a.k.a. reparametrization trick (Section 11.4). This is the approach taken by Kingma and Welling (2013) and Rezende *et al.* (2014).

If all nodes in the stochastic computation graph are distribution nodes, we can use the SFE estimator (Section 11.3). Schulman *et al.* (2015) propose a surrogate loss so that using autodiff on that loss produces an unbiased gradient of the expectation, using the SFE estimator. Foerster *et al.* (2018) extend the approach to support high-order differentiation. Krieken *et al.* (2021) further extend the approach by supporting different estimators per node, as well as control variates.

Converting distribution nodes into function nodes and vice-versa

Our formalism uses two types of nodes: distribution nodes with associated conditional distribution p_k and function nodes with associated function f_k. It is often possible to convert between node types.

Converting a distribution node into a function node is exactly the reparametrization trick studied in Section 11.4. We can use transformations such as the location-scale transform or the inverse transform.

Converting a function node into a distribution node can be done using the change-of-variables theorem, studied in Section 11.4.4, on a pushforward disstribution.

Because the pathwise estimator has lower variance than SFE, this is the method of choice when the f_k functions are available. The conversion from distribution node to function node and vice-versa is illustrated in Fig. 11.1.
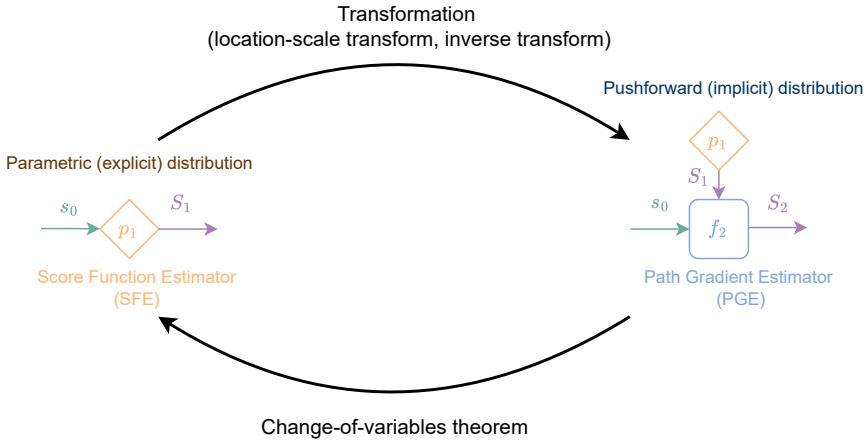
Figure 11.1: It is sometimes possible to convert a distribution node to a function node and vice-versa using a suitable transformation.

11.5.4 Local vs. global expectations

A stochastic computation graph can be seen as a **stochastic process**, a collection of random variables S_k, indexed by k, the position in the topological order. However, random variables are incompatible with autodiff. Replacing random variables by their expectation can be seen as a way to make them compatible with autodiff. Two strategies are then possible.

As we saw in the previous section, a strategy is to consider the expectation of the last output S_K. This strategy corresponds to a **global smoothing**. The two major advantages are that i) we do not need to assume that f_{k+1} is well-defined on $\text{conv}(\mathcal{S}_k)$ and ii) this induces a probability distribution over program executions. This is for instance useful to compute the variance of the program. The gradient of the program's expected value can be estimated by the reparametrization trick or by the SFE, depending on the type of nodes used.

A second strategy is to replace an intermediate random variable $S_k \in \mathcal{S}_k$, for $k \in \{1, \ldots, K\}$, by its expectation $\mathbb{E}[S_k] \in \text{conv}(\mathcal{S}_k)$. This strategy corresponds to a **local smoothing**. A potential drawback of this approach is that $\mathbb{E}[S_k]$ belongs to $\text{conv}(\mathcal{S}_k)$, the convex hull of $\mathcal{S}_k$.

Therefore, the function f_{k+1} in which $\mathbb{E}[S_k]$ is fed must be well-defined on $\mathrm{conv}(\mathcal{S}_k)$, which may not always be the case. In the case of control flows, another disadvantage is computational. We saw in Section 5.6 and Section 5.7 that using a soft comparison operator within a conditional statement induces a distribution on a binary or categorical random variable, corresponding to the branch to be selected. A conditional statement can then be locally smoothed out by replacing the random variable by its expectation i.e., a **convex combination** of all the branches. This means that, unless the distribution has sparse support, all branches must be evaluated.

11.6   Differential equations

11.6.1   Parameterized differential equations

From residual networks to neural ODEs

Starting from $s_0 \coloneqq x$, residual networks, reviewed in Section 4.5, iterate for $k \in \{1, \ldots, K\}$

$$s_k \coloneqq s_{k-1} + h_k(s_{k-1}, w_k).$$

A residual network can be seen as parameterizing incremental discrete-time input changes (hence the name "residual")

$$s_k - s_{k-1} = h_k(s_k, w_k).$$

Chen *et al.* (2018) proposed to parameterize continuous-time (instantaneous) changes instead. They considered the evolution $s(t)$ of the inputs in continuous time driven by a function $h(t, s, w)$ parameterized by w, starting from x. Formally, the evolution $s(t)$ is the solution of the **ordinary differential equation** (ODE)

$$
\begin{aligned}
s(0) &= x \\
s'(t) &= h(t, s(t), w) \quad t \in [0, T]
\end{aligned}
\tag{11.7}
$$

Here, $s'(t)$ is the vector of derivatives of s as defined in Remark 2.3, and T denotes a final time for the trajectory. The output of such a **neural ODE** (Chen *et al.*, 2018) is then $f(x, w) \coloneqq s(T)$. Alternatively, the

output can be seen as the solution of an **integration** problem

$$f(\boldsymbol{x}, \boldsymbol{w}) = \boldsymbol{s}(T) = \boldsymbol{x} + \int_0^T h(t, \boldsymbol{s}(t), \boldsymbol{w})dt. \tag{11.8}$$

Differential equations like Eq. (11.7) arise in many contexts beyond neural ODEs, ranging from modeling physical systems to pandemics (Braun and Golubitsky, 1983). Moreover, the differential equation presented in Eq. (11.7) is just an example of an ordinary differential equation, while controlled differential equations or stochastic differential equations can also be considered.

Existence of a solution

First and foremost, the question is whether $\boldsymbol{s}(t)$ is well-defined. Fortunately, the answer is positive under mild conditions, as shown by Picard-Lindelöf's theorem recalled below (Butcher, 2016, Theorem 16).

Theorem 11.1 (Exsistence and uniqueness of ODE solutions)**.** If $h : [0, T] \times \mathcal{S} \to \mathcal{S}$ is continuous in its first variable and Lipschitz-continuous in its second variable, then there exists a unique differentiable map $\boldsymbol{s} : [0, T] \to \mathcal{S}$ satisfying

$$\boldsymbol{s}(0) = \boldsymbol{s}_0$$
$$\boldsymbol{s}'(t) = h(t, \boldsymbol{s}(t)) \quad t \in [0, T],$$

for some given $\boldsymbol{s}_0 \in \mathcal{S}$.

For time-independent linear functions $h(t, \boldsymbol{s}) = \boldsymbol{A}\boldsymbol{s}$, the integral in Eq. (11.8) can be computed in closed form as

$$\boldsymbol{s}_t = \exp(t\boldsymbol{A})(\boldsymbol{s}_0),$$

where $\exp(\boldsymbol{A})$ is the matrix exponential. Hence, the output $\boldsymbol{s}(T)$ can be expressed as a simple function of the parameters ($\boldsymbol{A}$ in this case). However, generally, we do not have access to such analytical solutions, and, just as for solving optimization problems in Chapter 10, we need to resort to some iterative algorithms.

Integration methods

To numerically solve an ODE, we can use **integration methods**, whose goal is to build a sequence $\boldsymbol{s}_k$ that approximates the solution $\boldsymbol{s}(t)$ at times t_k. The simplest integration method is the **explicit Euler method**, that approximates the solutions between times t_{k-1} and t_k as

$$\boldsymbol{s}(t_{k-1}) - \boldsymbol{s}(t_k) = \int_{t_{k-1}}^{t_k} h(t, \boldsymbol{s}(t), \boldsymbol{w}) dt$$
$$\approx \delta_k h(t_{k-1}, \boldsymbol{s}(t_{k-1}), \boldsymbol{w}),$$

for a time-step

$$\delta_k := t_k - t_{k-1}.$$

The resulting integration scheme consists in computing starting from $\boldsymbol{s}_0 = \boldsymbol{x}$, for $k \in \{1, \ldots, K\}$,

$$\boldsymbol{s}_k := \boldsymbol{s}_{k-1} + \delta_k h(t_{k-1}, \boldsymbol{s}_{k-1}, \boldsymbol{w}).$$

Assimilating $\delta_k h(t_{k-1}, \boldsymbol{s}_{k-1}, \boldsymbol{w})$ with $h_k(\boldsymbol{s}_{k-1}, \boldsymbol{w}_k)$, we find that residual networks are essentially the discretization of a neural ODE by an explicit Euler method; more precisely, a non-autonomous neural ODEs, see e.g. (Davis *et al.*, 2020).

Euler's forward method is only one integration method among many. To cite a few, there are implicit Euler methods, semi-implicit methods, Runge-Kutta methods, linear multistep methods, etc. See, e.g., Gautschi (2011) for a detailed review. The quality of an integration method is measured by its consistency and its stability (Gautschi, 2011). These concepts naturally influence the development of evaluation and differentiation techniques for ODEs. We briefly summarize them below.

Given a fixed time interval $\delta_k = \delta$ and $K = \lceil T/\delta \rceil$ points, an integration method is **consistent of order** k if $\|\boldsymbol{s}_k - \boldsymbol{s}(k\delta)\| = O(\delta^k)$ as $\delta \to 0$ and therefore $k \to +\infty$. The higher the order k, the fewer points we need to reach an approximation error ε on the points considered. The term $\|\boldsymbol{s}_k - \boldsymbol{s}(k\delta)\| = O(\delta^k)$ is reminiscent of the error encountered in finite differences (Chapter 6) and is called the **truncation error**.

The (absolute) **stability** of a method is defined by the set of time-steps such that the integration method can integrate $s'(t) = \lambda s(t)$ for some $\lambda \in \mathbb{C}$ without blowing up as $t \to +\infty$.

11.6.2 Continuous adjoint method

Since different parameters $\boldsymbol{w}$ induce different trajectories associated to $h(t, \boldsymbol{s}, \boldsymbol{w})$ in Eq. (11.7), we may want to select one of these trajectories by minimizing some criterion. For example, we may consider selecting $\boldsymbol{w} \in \mathcal{W}$ by minimizing a loss L on the final point of the trajectory,

$$\min_{\boldsymbol{w} \in \mathcal{W}} L(f(\boldsymbol{x}, \boldsymbol{w}), \boldsymbol{y}), \tag{11.9}$$

where

$$f(\boldsymbol{x}, \boldsymbol{w}) \coloneqq \boldsymbol{s}(T) = \boldsymbol{x} + \int_0^T h(t, \boldsymbol{s}(t), \boldsymbol{w}) dt.$$

To solve such problems, we need to access gradients of ℓ composed with f through VJPs of the solution of the ODE. The VJPs can actually be characterized as solutions of an ODE themselves thanks to the **continuous time adjoint method** (Pontryagin, 1985), presented below, and whose proof is postponed to Section 11.6.6.

Proposition 11.7 (Continuous-time adjoint method). Consider a function $h : [0, T] \times \mathcal{S} \times \mathcal{W} \to \mathcal{S}$, continuous in its first variable, Lipschitz-continuous and continuously differentiable in its second variable. Assume that $\partial_3 h(t, \boldsymbol{s}, \boldsymbol{w})$ exists for any $t, \boldsymbol{s}, \boldsymbol{w}$, and is also continuous in its first variable, Lipschitz-continuous in its second variable. Denote $\boldsymbol{s} : \mathcal{S} \to \mathcal{S}$ the solution of the ODE

$$\begin{aligned} \boldsymbol{s}(0) &= \boldsymbol{x} \\ \boldsymbol{s}'(t) &= h(t, \boldsymbol{s}(t), \boldsymbol{w}) \quad t \in [0, T], \end{aligned}$$

and $f(\boldsymbol{x}, \boldsymbol{w}) = \boldsymbol{s}(T)$ the final state of the ODE at time T.

Then, the function f is differentiable, and for an output direction $\boldsymbol{u} \in \mathcal{S}$, its VJP along $\boldsymbol{u}$ is given by

$$\partial f(\boldsymbol{x}, \boldsymbol{w})^* \boldsymbol{u} = (\boldsymbol{r}(0), \boldsymbol{g})$$

for

$$\boldsymbol{g} = \int_0^T \partial_3 h(t, \boldsymbol{s}(t), \boldsymbol{w})^* \boldsymbol{r}(t) dt$$

and for $\boldsymbol{r}$ solving the **adjoint** (backward) ODE

$$\boldsymbol{r}'(t) = -\partial_2 h(t, \boldsymbol{s}(t), \boldsymbol{w})^* \boldsymbol{r}(t)$$
$$\boldsymbol{r}(T) = \boldsymbol{u}.$$

In particular, the gradient $\nabla(L \circ f)(\boldsymbol{x}, \boldsymbol{w})$ for $L : \mathcal{S} \to \mathbb{R}$ a differentiable loss is obtained by solving the adjoint ODE with $\boldsymbol{r}(T) = \nabla L(\boldsymbol{s}(T))$.

11.6.3   Gradients via the continuous adjoint method

Proposition 11.7 gives a formal definition of the gradient. However, just as computing the mapping $f(\boldsymbol{x}, \boldsymbol{w})$ itself, computing its VJP or the gradient of $L \circ f$ requires solving an integration problem. Note that the integration of $\boldsymbol{r}(t)$ in Proposition 11.7 requires also values of $\boldsymbol{s}(t)$. Therefore, we need to integrate both $\boldsymbol{r}(t)$ and $\boldsymbol{s}(t)$. Such an approach is generally referred as **optimize-then-discretize** because we first formulate the gradient in continuous time (the "optimize part") and then discretize the resulting ODE.

Simple discretization scheme

A first approach consists in defining a backward discretization scheme that can approximate $\boldsymbol{s}(t)$ backward in time. Namely, by defining $\boldsymbol{\sigma}(t) = \boldsymbol{s}(T - t), \boldsymbol{\rho}(t) = \boldsymbol{r}(T - t)$, and $\boldsymbol{\gamma}(t) = \int_t^T \partial_3 h(\tau, \boldsymbol{s}(\tau), \boldsymbol{w})^* \boldsymbol{r}(\tau) d\tau$, the derivative of $L \circ f$ is given by $(\boldsymbol{\rho}(T), \boldsymbol{\gamma}(T))$. The functions $\boldsymbol{\sigma}, \boldsymbol{\rho}, \boldsymbol{\gamma}$ are solutions of a standard ODE

$$\begin{aligned}
\boldsymbol{\sigma}(0) &= \boldsymbol{s}(T), & \boldsymbol{\sigma}'(t) &= -h(T - t, \boldsymbol{\sigma}(t), \boldsymbol{w}), \\
\boldsymbol{\rho}(0) &= \nabla L(\boldsymbol{s}(T)), & \boldsymbol{\rho}'(t) &= \partial_2 h(T - t, \boldsymbol{\sigma}(t), \boldsymbol{w})^* \boldsymbol{\rho}(t), \\
\boldsymbol{\gamma}(0) &= 0, & \boldsymbol{\gamma}'(t) &= \partial_3 h(T - t, \boldsymbol{\sigma}(t), \boldsymbol{w})^* \boldsymbol{\rho}(t).
\end{aligned}$$

The above ODE can then be solved by any integration method. Note, however, that it requires first computing $\boldsymbol{s}(T)$ and $\nabla L(\boldsymbol{s}(T))$ by an integration method. The overall computation of the gradient using an explicit Euler method to solve forward and backward ODEs is summarized in Algorithm 11.2.

Algorithm 11.2 Gradient computation via continuous adjoint method with Euler explicit discretization

---

1: **Functions:** $h : [0, T] \times \mathcal{S} \times \mathcal{W} \to \mathbb{R}$, $L : \mathcal{S} \to \mathbb{R}$
2: **Inputs:** input $\boldsymbol{x}$, parameters $\boldsymbol{w}$, number of discretization steps K.
3: Set discretization step $\delta = T/K$, denote $h_k(\boldsymbol{s}, \boldsymbol{w}) = h(k\delta, \boldsymbol{s}, \boldsymbol{w})$.
4: Set $\boldsymbol{s}_0 \coloneqq \boldsymbol{x}$
5: **for** $k \coloneqq 1, \ldots, K$ **do**   ▷ Forward discretization
6:      Compute $\boldsymbol{s}_k \coloneqq \boldsymbol{s}_{k-1} + \delta h_{k-1}(\boldsymbol{s}_{k-1}, \boldsymbol{w})$.
7: Compute $\boldsymbol{u} \coloneqq \nabla L(\boldsymbol{s}_K)$.
8: Initialize $\boldsymbol{r}_K \coloneqq \boldsymbol{u}$, $\hat{\boldsymbol{s}}_K = \boldsymbol{s}_K$, $\boldsymbol{g}_K = \boldsymbol{0}$
9: **for** $k \coloneqq K, \ldots, 1$ **do**   ▷ Backward discretization
10:      Compute $\hat{\boldsymbol{s}}_{k-1} \coloneqq \hat{\boldsymbol{s}}_k - \delta h_k(\hat{\boldsymbol{s}}_k, \boldsymbol{w})$
11:      Compute $\boldsymbol{r}_{k-1} \coloneqq \boldsymbol{r}_k + \delta \partial_2 h_k(\hat{\boldsymbol{s}}_k, \boldsymbol{w})^* \boldsymbol{r}_k$
12:      Compute $\boldsymbol{g}_{k-1} \coloneqq \boldsymbol{g}_k + \delta \partial_3 h_k(\hat{\boldsymbol{s}}_k, \boldsymbol{w})^* \boldsymbol{r}_k$
13: **Output:** $(\boldsymbol{r}_0, \boldsymbol{g}_0) \approx \nabla (L \circ f)(\boldsymbol{x}, \boldsymbol{w})$

Algorithm 11.2 naturally looks like the reverse mode of autodiff for a residual neural networks with **shared weights**. A striking difference is that the intermediate computations $\boldsymbol{s}_k$ are not kept in memory and, instead, new variables $\hat{\boldsymbol{s}}_k$ are computed along the backward ODE. One may believe that by switching to continuous time, we solved the memory issues encountered in reverse-mode autodiff. Unfortunately, this comes at the cost of numerical stability. As we use a discretization scheme to recompute the intermediate states backward in time through $\hat{\boldsymbol{s}}_k$ in Algorithm 11.2, we accumulate some truncation errors.

To understand the issue here, consider applying Algorithm 11.2 repeatedly on the same parameters but using $\hat{\boldsymbol{s}}_0$ instead of $\boldsymbol{s}_0 = \boldsymbol{x}$ each time. In the continuous realm, $\sigma(T) = \boldsymbol{s}(0)$. But after discretization, $\hat{\boldsymbol{s}}_0 \approx \sigma(T)$ does not match $\boldsymbol{s}_0$. Therefore, by applying Algorithm 11.2 with $\boldsymbol{s}_0 = \hat{\boldsymbol{s}}_0$, we would not get the same output even if in continuous time we naturally should have. This thought exercise illustrates that Algorithm 11.2 induces some noise in the estimation of the gradient.

Multiple shooting scheme

An alternative approach consists in integrating both the forward and backward ODEs jointly. Namely, we may solve an ODE with boundary values

$$\boldsymbol{s}'(t) = h(t, \boldsymbol{s}(t), \boldsymbol{w}), \quad \boldsymbol{s}(0) = \boldsymbol{x},$$
$$\boldsymbol{r}'(t) = -\partial_2 h(t, \boldsymbol{s}(t), \boldsymbol{w})^* \boldsymbol{r}(t), \quad \boldsymbol{r}(T) = \nabla L(\boldsymbol{s}(T))$$
$$\boldsymbol{g}'(t) = -\partial_3 h(t, \boldsymbol{s}(t), \boldsymbol{w})^* \boldsymbol{r}(t), \quad \boldsymbol{g}(T) = 0,$$

by means of a multiple shooting method or a collocation method (Stoer *et al.*, 1980). This approach still requires $\nabla L(\boldsymbol{s}(T))$ to be approximated first.

11.6.4   Gradients via reverse-mode on discretization

A simpler approach consists in replacing the objective in Eq. (11.9) by its version discretized using some numerical method, such as an Euler forward discretization scheme. That is, we seek to solve

$$\min_{\boldsymbol{w} \in \mathcal{W}} \quad L(\boldsymbol{s}_K) \quad \text{where} \quad \boldsymbol{s}_k = \boldsymbol{s}_{k-1} + \delta h(k\delta, \boldsymbol{s}_{k-1}, \boldsymbol{w}) \ k \in \{1, \ldots, K\},$$

with $\boldsymbol{s}_0 = \boldsymbol{0}$ and δ some discretization step. Gradients of the objective can be computed by automatic differentiation. That approach is often referred to as **discretize-then-optimize**. At first glance, this approach may suffer from very high memory requirements. Indeed, to get an accurate solution of the ODE, a numerical integration method may require K to be very large. Since a naive implementation of reverse-mode automatic differentiation has a memory that scales linearly with K, computing the gradient by a discretize-then-optimize method could be prohibitive. However, the memory requirements may easily be amortized using checkpointing, as explained in Section 7.5; see also (Gholaminejad *et al.*, 2019).

As for the **optimize-then-discretize** method, we still accumulate some truncation errors in the forward discretization process. This discretization error occurs when computing the gradient in reverse-mode too. The discretize-then-optimize method can be seen as computing gradients of a surrogate objective. For that objective, the gradients are

correct and well-defined. However, they may not match the gradients of the true ODE formulation.

To compare the discretize-then-optimize and optimize-then-discretize approaches, Gholaminejad *et al.* (2019) compared their performance on an ODE whose solution can be computed analytically by selecting h to be linear in s. The authors observed that discretize-then-optimize generally outperformed optimize-then-discretize. A middle ground can actually be found by using reversible differentiation schemes.

11.6.5   Reversible discretization schemes

Our exposition of the optimize-then-discretize or discretize-then-optimize approaches used a simple Euler explicit discretization scheme. However, for both approaches, we could have used other discretization schemes instead, such as reversible discretization schemes.

A reversible discretization scheme is a discretization scheme such that we have access to a closed-form formula for the inverse of its discretization step. Formally, a discretization method $\mathcal{M}$ builds an approximation $(s_k)_{k=1}^K$ of the solution of an ODE $s'(t) = h(t, s(t))$ on an interval $[0, T]$ by computing for $k \in (1, \ldots, K)$

$$t_k, s_k, c_k = \mathcal{M}(t_{k-1}, s_{k-1}, c_{k-1}; h, \delta), \tag{11.10}$$

where $\delta > 0$ is some fixed discretization step, t_k is the time step (typically $t_k = t_{k-1} + \delta$), s_k is the approximation of $s(t_k)$, and c_k is some additional context variables used by the discretization method to build the iterates. An explicit Euler method does not have a context, but just as an optimization method may update some internal states, a discretization method can update some context variable. The discretization scheme in Eq. (11.10) is a forward discretization scheme as we took a positive discretization step. By taking a negative discretization step, we obtain the corresponding backward discretization scheme, for $k \in (K, \ldots, 1)$,

$$t_{k-1}, s_{k-1}, c_{k-1} = \mathcal{M}(t_k, s_k, c_k; h, -\delta).$$

A discretization method is **reversible** if we have access to $\mathcal{M}^{-1}$ to recompute the inputs of the discretization step from its outputs,

$$t_{k-1}, s_{k-1}, c_k = \mathcal{M}^{-1}(t_k, s_k, c_k; h, \delta).$$

A reversible discretization method is **symmetric** if the backward discretization scheme is exactly the inverse of the forward discretization scheme, i.e.,

$$\mathcal{M}(t_k, \boldsymbol{s}_k, \boldsymbol{c}_k; h, -\delta) = \mathcal{M}^{-1}(t_k, \boldsymbol{s}_k, \boldsymbol{c}_k; h, \delta).$$

The explicit Euler method is clearly not symmetric and a priori not reversible, unless we can solve for $\boldsymbol{y}_{k-1}$, the equation $\boldsymbol{y}_k = \boldsymbol{y}_{k-1} - \delta f(\boldsymbol{y}_{k-1})$.

Leapfrog method

The (asynchronous) **leapfrog method** (Zhuang *et al.*, 2021; Mutze, 2013) on the other hand is an example of symmetric reversible discretization method. For a constant discretization step δ, given $t_{k-1}, \boldsymbol{s}_{k-1}, \boldsymbol{c}_{k-1}$ and a function h, it computes

$$\bar{t}_{k-1} := t_{k-1} + \frac{\delta}{2}$$
$$\bar{\boldsymbol{s}}_{k-1} := \boldsymbol{s}_{k-1} + \frac{\delta}{2}\boldsymbol{c}_{k-1}$$
$$\bar{\boldsymbol{c}}_{k-1} := h(\bar{t}_{k-1}, \bar{\boldsymbol{s}}_{k-1})$$
$$t_k := \bar{t}_{k-1} + \frac{\delta}{2}$$
$$\boldsymbol{s}_k := \bar{\boldsymbol{s}}_{k-1} + \frac{\delta}{2}\bar{\boldsymbol{c}}_{k-1}$$
$$\boldsymbol{c}_k := 2\bar{\boldsymbol{c}}_{k-1} - \boldsymbol{c}_{k-1}$$
$$\mathcal{M}(t_{k-1}, \boldsymbol{s}_{k-1}, \boldsymbol{c}_{k-1}; h, \delta) := (t_k, \boldsymbol{s}_k, \boldsymbol{c}_k).$$

One can verify that we indeed have $\mathcal{M}(t_k, \boldsymbol{s}_k, \boldsymbol{c}_k; h, -\delta) = (t_{k-1}, \boldsymbol{s}_k, \boldsymbol{c}_k)$.

By using a reversible symmetric discretization scheme in the optimize-then-discretize approach, we ensure that, at the end of the backward discretization pass, we recover exactly the original input. Therefore, by repeating forward and backward discretization schemes we always get the same gradient, which was not the case for an Euler explicit scheme.

By using a reversible discretization scheme in the discretize-then-optimize method, we address the memory issues of reverse mode autodiff. As explained in Section 7.6, we can recompute intermediate values during the backward pass rather than storing them.

Momentum residual networks

In the leapfrog method, the additional variables c_k may actually be interpreted as velocities of a system whose acceleration is driven by the given function, that is, $s''(t) = h(t, s(t), w)$. Such an interpretation suggests alternatives to the usual neural ODE paradygm. For instance, **momentum neural networks** (Sander *et al.*, 2021b), can be interpreted as the discretization of a **second-order ordinary differential equations**, which are naturally amenable to reversible differentiation schemes with a low memory footprint.

11.6.6 Proof of the continuous adjoint method

In the following, we denote $s(t, x, w)$ the solution of the ODE at time t given the input x and the parameters w. We focus here on the formulation of the VJP. The proof relies on the existence of partial derivatives of $s(t, x, w)$, which we do not cover here and refer to, e.g., Pontryagin (1985) for a complete proof of such facts given the assumptions.

We use the ODE constraint to introduce adjoint variables, this time in the form of a continuously differentiable function r. For any such a function r, we have

$$
\begin{aligned}
\langle f(x, w), u \rangle = {} & \langle s(T, x, w), u \rangle \\
& + \int_0^T \langle r(t), h(t, s(t, x, w), w) - \partial_t s(t, x, w) \rangle dt,
\end{aligned}
$$

using Leibniz notations such as $\partial_t s(t, x, w) = \partial_1 s(t, x, w)$. The VJPs

then decompose as

$$\partial_w f(x, w)^*[u]$$
$$= \partial_w s(T, x, w)^* u$$
$$+ \int_0^T (\partial_w s(t, x, w)^* \partial_s^* h(t, s(t, x, w), w)^* - \partial_{wt}^2 s(t, x, w)^*) r(t) dt$$
$$+ \int_0^T \partial_w h(t, s(t, x, w), w)^* r(t) dt,$$
$$\partial_x f(x, w)^*[u]$$
$$= \partial_x s(T, x, w)^* u$$
$$+ \int_0^T (\partial_x s(t, x, w)^* \partial_s^* h(t, s(t, x, w), w)^* - \partial_{xt}^2 s(t, x, w)^*) r(t) dt$$

Here the second derivative terms $\partial_{wt}^2 s(t, x, w)^* r, \partial_{xt}^2 s(t, x, w)^* r$ correspond to second derivatives of $\langle s(t, x, w), r \rangle$. Since the Hessian is symmetric (Schwartz's theorem presented in Proposition 2.10), we can swap the derivatives in t and w or x. Then, to express the gradient uniquely in terms of first derivatives of s, we use an integration by part to have for example

$$\int_0^T \partial_{wt}^2 s(t, x, w)^* r(t) dt = \int_0^T \partial_{tw}^2 s(t, x, w)^* r(t) dt$$
$$= (\partial_w s(T, x, w)^* r(T) - \partial_w s(0, x, w)^* r(0))$$
$$- \int_0^T \partial_w s(t, x, w)^* r(t)^* \partial_t r(t) dt.$$

Since $s(0) = x$, we have $\partial_w s(0, x, w)^* r(0) = 0$. The VJP w.r.t. w can then be written as

$$\partial_w f(x, w)^*[u]$$
$$= \partial_w s(T, x, w)^*[u - r(T)]$$
$$+ \int_0^T \partial_w s(t, x, w)^*[\partial_s h(t, s(t, x, w), w)^* r(t) + \partial_t r(t)] dt$$
$$+ \int_0^T \partial_w h(t, s(t, x, w), w)^* r(t) dt.$$

By choosing $r(t)$ to satisfy the adjoint ODE

$$\partial_t r(t) = -\partial_s h(t, s(t, x, w), w)^* r(t), \quad r(T) = u,$$

the expression of the VJP simplifies as

$$\partial_{\boldsymbol{w}} f(\boldsymbol{x}, \boldsymbol{w})^*[\boldsymbol{u}] = \int_0^T \partial_{\boldsymbol{w}} h(t, \boldsymbol{s}(t, \boldsymbol{x}, \boldsymbol{w}), \boldsymbol{w})^* \boldsymbol{r}(t) dt.$$

For the VJP w.r.t. to $\boldsymbol{x}$, we can proceed similarly. Using an integration by part, we have, this time, $\partial_{\boldsymbol{x}} \boldsymbol{s}(0, \boldsymbol{x}, \boldsymbol{w})^* \boldsymbol{r}(0) = \boldsymbol{r}(0)$ since $\boldsymbol{s}(0) = \boldsymbol{x}$. Choosing the same curve $\boldsymbol{r}(t)$ satisfying the adjoint ODE we get

$$\partial_{\boldsymbol{x}} f(\boldsymbol{x}, \boldsymbol{w})^*[\boldsymbol{u}] = \boldsymbol{r}(0).$$

The existence of a curve $\boldsymbol{r}$ solution of the backward ODE can easily be shown from Picard Lindelöf's theorem and the assumptions.

11.7 Summary

In this chapter, we studied how to differentiate integrals, with a focus on expectations and solutions of a differential equation.

For differentiating through expectations, we studied two main methods: the score function estimator (SFE, a.k.a. REINFORCE) and the path gradient estimator (PGE, a.k.a. reparametrization trick). The SFE is suitable when it is easy to sample from the distribution and its log-PDF is **explicitly** available. It is an unbiased estimator, but is known to suffer from high variance. The PGE is suitable for pushforward distributions, distributions that are **implicitly** defined through a transformation, or a sequence of them. These distributions can be easily sampled from, by injecting a source of randomness (such as noise) through the transformations. An unbiased, low-variance estimator of the gradient of their expectation is easily obtained, provided that we can interchange integration and differentiation.

If we have an explicit distribution, we can sometimes convert it to an implicit distribution, thanks to the **location-scale transformation** or the **inverse transformation**. Conversely, if we have an implicit distribution, we can convert it to an explicit distribution using the **change-of-variables theorem**. However, this formula requires to compute the determinant of an inverse Jacobian, and is computationally expensive in general. Normalizing flows use invertible transformations so that the inverse Jacobian is cheap to compute, by design. We saw

that **stochastic computation graphs** can use a mix of explicit and implicit distributions at each node.

For differentiating through the solution of a differential equation, two approaches can be considered. We can express the gradient as the solution of a differential equation thanks to the **continuous adjoint method**. We may then discretize backwards in time the differential equation that the gradient satisfies. This is the **optimize-then-discretize** approach. We can also first discretize the problem in such a way that the gradient can simply be computed by reverse mode auto-diff, applied on the discretization steps. This is the **discretize-then-optimize** approach. The optimize-then-discretize approach has no memory cost, but discrepancies between the forward and backward discretization passes often lead to numerical errors. The discretize-then-optimize introduces no such discrepancies but may come at a large memory cost. **Reversible discretization schemes** can circumvent the memory cost, as they enable the recomputation of intermediate discretization steps backwards in time.

Part IV

Smoothing programs

12

Smoothing by optimization

In this chapter, we review smoothing by **infimal convolution**.

12.1 Primal approach

We first review how to smooth functions in the **primal** space.

12.1.1 Infimal convolution

The infimal convolution, sometimes abbreviated inf-conv, is defined as follows.

> **Definition 12.1** (Infimal convolution). The infimal convolution between two functions $f \colon \mathbb{R}^M \to \mathbb{R}$ and $g \colon \mathbb{R}^M \to \mathbb{R}$ is defined by
>
> $$\begin{aligned} (f \square g)(\boldsymbol{\mu}) &:= \inf_{\boldsymbol{u} \in \mathbb{R}^M} f(\boldsymbol{u}) + g(\boldsymbol{\mu} - \boldsymbol{u}) \\ &:= \inf_{\boldsymbol{z} \in \mathbb{R}^M} f(\boldsymbol{\mu} + \boldsymbol{z}) + g(\boldsymbol{z}) \\ &= \inf_{\boldsymbol{u}, \boldsymbol{z} \in \mathbb{R}^M} f(\boldsymbol{u}) + g(\boldsymbol{z}) \text{ s.t. } \boldsymbol{u} = \boldsymbol{\mu} + \boldsymbol{z} \end{aligned}$$

Some examples are given in Table 12.1. As can be seen from the above, the infimal convolution, like the classical convolution, is **com-**

Table 12.1: Examples of infimal convolutions.

f_1	f_2	$f_1 \square f_2$
f	0	$\inf_{\boldsymbol{u} \in \mathbb{R}^M} f(\boldsymbol{u})$
$\iota_\mathcal{C}$	$\|\cdot\|_2$	$d_\mathcal{C} := \inf_{\boldsymbol{u} \in \mathcal{C}} \|\cdot -\boldsymbol{u}\|_2$
f	$\frac{1}{2}\|\cdot\|_2^2$	$M_f := \inf_{\boldsymbol{u} \in \mathbb{R}^M} \|\cdot -\boldsymbol{u}\|_2^2 + f(\boldsymbol{u})$
$\iota_\mathcal{C}$	$\iota_\mathcal{D}$	$\iota_{\mathcal{C}+\mathcal{D}}$
f	$\iota_{\{v\}}$	$f(\cdot - \boldsymbol{v})$
f	$\langle \cdot, \boldsymbol{v} \rangle$	$\langle \cdot, \boldsymbol{v} \rangle - f^*(\boldsymbol{v})$

mutative,

$$(f \square g)(\boldsymbol{\mu}) = (g \square f)(\boldsymbol{\mu}).$$

12.1.2 Moreau envelope

When $g(\boldsymbol{z})$ is set to a quadratic regularization $R(\boldsymbol{z}) := \frac{1}{2}\|\boldsymbol{z}\|_2^2$, the infimal convolution $f \square R$ gives the so-called **Moreau envelope** of f, also known as **Moreau-Yoshida** regularization of f.

> **Definition 12.2** (Moreau envelope). Given a function $f \colon \mathbb{R}^M \to \mathbb{R}$, its Moreau envelope is given by
>
> $$M_f(\boldsymbol{\mu}) := (f \square R)(\boldsymbol{\mu})$$
>
> $$= \inf_{\boldsymbol{u} \in \mathbb{R}^M} f(\boldsymbol{u}) + \frac{1}{2}\|\boldsymbol{\mu} - \boldsymbol{u}\|_2^2$$
>
> $$= \inf_{\boldsymbol{z} \in \mathbb{R}^M} f(\boldsymbol{\mu} + \boldsymbol{z}) + \frac{1}{2}\|\boldsymbol{z}\|_2^2.$$

Note that $\boldsymbol{\mu}$ and $\boldsymbol{u}$ belong to the same primal space. Intuitively, the Moreau envelope is the minimal value over $\boldsymbol{u} \in \mathbb{R}^M$ of a trade-off between staying close to the input $\boldsymbol{\mu}$ according to the **proximity term** $\frac{1}{2}\|\boldsymbol{\mu} - \boldsymbol{u}\|_2^2$ and $f(\boldsymbol{u})$. As a comparison, the **proximal operator**, reviewed in Definition 15.3, returns the solution, instead of the value:

$$\operatorname{prox}_f(\boldsymbol{\mu}) := \arg\min_{\boldsymbol{u} \in \mathbb{R}^M} \frac{1}{2}\|\boldsymbol{\mu} - \boldsymbol{u}\|_2^2 + f(\boldsymbol{u}).$$

That is, we have

$$M_f(\boldsymbol{\mu}) = \frac{1}{2}\|\boldsymbol{\mu} - \mathrm{prox}_f(\boldsymbol{\mu})\|_2^2 + f(\mathrm{prox}_f(\boldsymbol{\mu})). \qquad (12.1)$$

We now state useful properties of the Moreau envelope.

Proposition 12.1 (Properties of Moreau envelope). Let $f\colon \mathbb{R}^M \to \mathbb{R}$.

   1. Gradient:
$$\nabla M_f(\boldsymbol{\mu}) = \boldsymbol{\mu} - \mathrm{prox}_f(\boldsymbol{\mu}).$$

   If f is convex, then

$$\nabla M_{f^*}(\boldsymbol{\mu}) = \mathrm{prox}_f(\boldsymbol{\mu}),$$

   where f^* is the convex conjugate of f.

   2. Same minimum as original function:

$$\min_{\boldsymbol{\mu}\in\mathbb{R}^M} M_f(\boldsymbol{\mu}) = \min_{\boldsymbol{u}\in\mathbb{R}^M} f(\boldsymbol{u}).$$

Proof.

   1. The first claim follows from Danskin's theorem, reviewed in Section 10.2. The second claim is Moreau's decomposition.

   2. Provided that the Moreau envelope exists, we have

$$\begin{aligned}
\min_{\boldsymbol{\mu}\in\mathbb{R}^M} M_f(\boldsymbol{\mu}) &= \min_{\boldsymbol{\mu}\in\mathbb{R}^M} \min_{\boldsymbol{u}\in\mathbb{R}^M} \frac{1}{2}\|\boldsymbol{\mu} - \boldsymbol{u}\|_2^2 + f(\boldsymbol{u}) \\
&= \min_{\boldsymbol{u}\in\mathbb{R}^M} \min_{\boldsymbol{\mu}\in\mathbb{R}^M} \frac{1}{2}\|\boldsymbol{\mu} - \boldsymbol{u}\|_2^2 + f(\boldsymbol{u}) \\
&= \min_{\boldsymbol{u}\in\mathbb{R}^M} f(\boldsymbol{u}).
\end{aligned}$$

$\hfill\square$

To illustrate smoothing from the Moreau envelope perspective, we show how to smooth the 1-norm.

Example 12.1 (Smoothing the 1-norm via infimal convolution). We wish to smooth $f(\boldsymbol{u}) = \|\boldsymbol{u}\|_1$. The corresponding proximal operator is the soft-thresholding operator (see Section 15.4)

$$\operatorname{prox}_f(\boldsymbol{\mu}) = \underset{\boldsymbol{u} \in \mathbb{R}^M}{\arg\min} \frac{1}{2} \|\boldsymbol{\mu} - \boldsymbol{u}\|_2^2 + \|\boldsymbol{u}\|_1$$

$$= \operatorname{sign}(\boldsymbol{\mu}) \cdot \max(|\boldsymbol{\mu}| - 1, 0).$$

Using Eq. (12.1) and after some algebraic manipulations, we obtain

$$[M_f(\boldsymbol{\mu})]_j = \begin{cases} \frac{\mu_j^2}{2} & \text{if } |\mu_j| \le 1 \\ |\mu_j| - \frac{1}{2} & \text{if } |\mu_j| > 1 \end{cases}.$$

That is, we recover the **Huber loss**.

12.2 Legendre–Fenchel transforms, convex conjugates

12.2.1 Definition

Consider affine functions of the form

$$\boldsymbol{u} \mapsto \langle \boldsymbol{u}, \boldsymbol{v} \rangle - b.$$

These functions are parametrized by their slope $\boldsymbol{v} \in \mathbb{R}^D$ and their intercept $-b \in \mathbb{R}$. Now, suppose we fix $\boldsymbol{v}$. Given a function $f(\boldsymbol{u})$, affine lower bounds of $f(\boldsymbol{u})$ are all the functions of $\boldsymbol{u}$ such that b satisfies

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle - b \le f(\boldsymbol{u}) \Leftrightarrow \langle \boldsymbol{u}, \boldsymbol{v} \rangle - f(\boldsymbol{u}) \le b.$$

The **tightest** lower bound is then the function such that b is defined by

$$b := \sup_{\boldsymbol{u} \in \operatorname{dom}(f)} \langle \boldsymbol{u}, \boldsymbol{v} \rangle - f(\boldsymbol{u}),$$

where we recall that the domain of f is defined by

$$\operatorname{dom}(f) := \{\boldsymbol{u} \in \mathbb{R}^M : f(\boldsymbol{u}) < \infty\}.$$

This leads to the definition of **Legendre-Fenchel transform**, a.k.a. , **convex conjugate**.
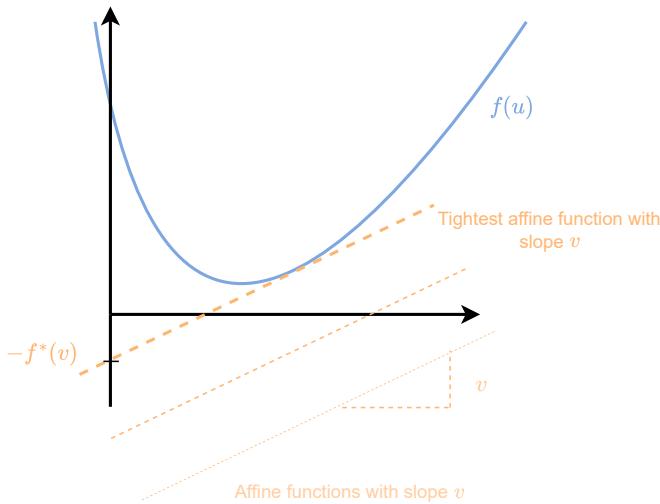
Figure 12.1: For a fixed slope v, the function $u \mapsto uv - f^*(v)$ is the tightest affine lower bound of f.

Definition 12.3 (Convex conjugate). Given a function $f \colon \mathbb{R}^M \to \mathbb{R} \cup \{\infty\}$, its convex conjugate is defined by

$$f^*(\boldsymbol{v}) := \sup_{\boldsymbol{u} \in \mathrm{dom}(f)} \langle \boldsymbol{u}, \boldsymbol{v} \rangle - f(\boldsymbol{u}).$$

We use a sup rather than a max to indicate that $f^*(\boldsymbol{v})$ is potentially ∞. Following the previous discussion, $-f^*(\boldsymbol{v})$ is the intercept of the tightest affine lower bound with slope $\boldsymbol{v}$ of $f(\boldsymbol{u})$. This is illustrated Fig. 12.1.

12.2.2   Closed-form examples

Computing $f^*(\boldsymbol{v})$ involves the resolution of a maximization problem, which could be difficult in general without assumption on f. In some cases, however, we can compute an analytical solution, as we now illustrate.

Example 12.2 (Analytical conjugate examples). When $f(\boldsymbol{u}) = \frac{1}{2}\|\boldsymbol{u}\|_2^2$, with $\mathrm{dom}(f) = \mathbb{R}^M$, the conjugate is

$$f^*(\boldsymbol{v}) = \max_{\boldsymbol{u} \in \mathbb{R}^M} \langle \boldsymbol{u}, \boldsymbol{v} \rangle - \frac{1}{2}\|\boldsymbol{u}\|_2^2.$$

Setting the gradient $\boldsymbol{u} \mapsto \langle \boldsymbol{u}, \boldsymbol{v} \rangle - \frac{1}{2}\|\boldsymbol{u}\|_2^2$ to zero, we obtain $\boldsymbol{u}^\star = \boldsymbol{v}$. Plugging $\boldsymbol{u}^\star$ back, we therefore obtain

$$f^*(\boldsymbol{v}) = \langle \boldsymbol{u}^\star, \boldsymbol{v} \rangle - \frac{1}{2}\|\boldsymbol{u}^\star\|_2^2 = \frac{1}{2}\|\boldsymbol{v}\|_2^2.$$

Therefore, $f = f^*$ in this case.

When $f(\boldsymbol{u}) = \langle \boldsymbol{u}, \log \boldsymbol{u} \rangle$, with $\mathrm{dom}(f) = \mathbb{R}_+^M$, the minimizer of $u \mapsto \langle \boldsymbol{u}, \boldsymbol{v} \rangle - \langle \boldsymbol{u}, \log \boldsymbol{u} \rangle$ is $\boldsymbol{u}^\star = \exp(\boldsymbol{v} - \mathbf{1})$ and the conjugate is

$$f^*(\boldsymbol{v}) = \sum_{j=1}^{M} \exp(v_j - 1).$$

See for instance Boyd and Vandenberghe (2004) or Beck (2017) for many more examples. We emphasize that the image of f can be the extended real line $\mathbb{R} \cup \{\infty\}$. This is useful for instance in order to incorporate constraints using an **indicator function**. Indeed, if

$$f(\boldsymbol{u}) = \iota_{\mathcal{C}}(\boldsymbol{u}) = \begin{cases} 0 & \text{if } \boldsymbol{u} \in \mathcal{C} \\ \infty & \text{otherwise} \end{cases},$$

so that $\mathrm{dom}(f) = \mathcal{C}$, then

$$\boldsymbol{f}^*(\boldsymbol{v}) = \sup_{\boldsymbol{u} \in \mathrm{dom}(f)} \langle \boldsymbol{u}, \boldsymbol{v} \rangle - f(\boldsymbol{u}) = \sup_{\boldsymbol{u} \in \mathcal{C}} \langle \boldsymbol{u}, \boldsymbol{v} \rangle,$$

which is known as the **support function** of the set $\mathcal{C}$, with maximizer known as **linear maximization oracle** (LMO).

12.2.3 Properties

The conjugate enjoys several useful properties, that we now summarize.

Proposition 12.2 (Convex conjugate properties).

1. **Convexity:** $f^*(v)$ is a **convex** function for **all** $f \colon \mathbb{R}^M \to \mathbb{R} \cup \{\infty\}$ (even if f is nonconvex).

2. **Fenchel-Young inequality:** for all $u, v \in \mathbb{R}^M$

$$f(u) + f^*(v) - \langle u, v \rangle \geq 0.$$

3. **Gradient:** if the supremum in Definition 12.3 is uniquely achieved, then $f^*(v)$ is differentiable at v and its gradient is

$$\nabla f^*(v) = \arg\max_{u \in \mathrm{dom}(f)} \langle u, v \rangle - f(u).$$

Otherwise, $f^*(v)$ is sub-differentiable at v and we get a sub-gradient instead.

4. **Maps:** If f and f^* are differentiable, then

$$v = \nabla f(u) \Leftrightarrow u = \nabla f^*(v) \Leftrightarrow f^*(v) + f(u) - \langle u, v \rangle = 0.$$

5. **Biconjugate:** $f = f^{**}$ if and only if f is convex and closed (i.e., its sublevel sets form a closed set), otherwise $f^{**} \leq f$.

Proof. We include proofs for each claim.

1. This follows from the fact that $v \mapsto \sup_{u \in \mathcal{C}} g(u, v)$ is convex if g is convex in v. Note that this is true even if g is nonconvex in u. Here, $g(u, v) = \langle u, v \rangle - f(u)$, which is affine in v and therefore convex in v.

2. This follows immediately from Definition 12.3.

3. This follows from Danskin's theorem, reviewed in Section 10.2. Another way to see this is by observing that

$$f^*(v) = \langle g, v \rangle - f(g)$$
$$f^*(v') \geq \langle g, v' \rangle - f(g),$$

where $\boldsymbol{g} \coloneqq \arg\max\limits_{\boldsymbol{u}\in\mathrm{dom}(f)} \langle \boldsymbol{u}, \boldsymbol{v} \rangle - f(\boldsymbol{u})$. Subtracting the two, we obtain

$$f^*(\boldsymbol{v}') \geq f^*(\boldsymbol{v}) + \langle \boldsymbol{g}, \boldsymbol{v}' - \boldsymbol{v} \rangle.$$

Now, using that f^* is convex and Definition 14.6, we obtain that $\boldsymbol{g} = \nabla f^*(\boldsymbol{v})$.

4. See, e.g., Bauschke and Combettes (2011, Proposition 16.10).

5. See Boyd and Vandenberghe (2004, Section 3.3).

$\square$

12.2.4   Conjugate calculus

While deriving a conjugate expression can be difficult in general, in some cases, it is possible to use simple rules to derive conjugates in terms of other conjugates.

Proposition 12.3 (Conjugate calculus rules)**.**

1. **Separable functions:** if $f(\boldsymbol{u}) = \sum_{j=1}^{M} f_j(u_j)$, then

$$f^*(\boldsymbol{v}) = \sum_{j=1}^{M} f_j^*(v_j).$$

2. **Scalar multiplication:** if $f(\boldsymbol{u}) = c \cdot g(\boldsymbol{u})$, for $c > 0$, then

$$f^*(\boldsymbol{v}) = c \cdot g^*(\boldsymbol{v}/c).$$

3. **Addition to an affine function and translation:** if $f(\boldsymbol{u}) = g(\boldsymbol{u}) + \langle \boldsymbol{\alpha}, \boldsymbol{u} \rangle + \beta$, then

$$f^*(\boldsymbol{v}) = g^*(\boldsymbol{v} - \boldsymbol{\alpha}) - \beta.$$

4. **Composition with an invertible linear map:** if $f(\boldsymbol{u}) = g(M\boldsymbol{u})$, where $x \mapsto M\boldsymbol{x}$ is an invertible linear map, then

$$f^*(\boldsymbol{v}) = g^*(M^{-T}\boldsymbol{v}).$$

12.2.5   Fast Legendre transform

When an analytical solution is not available, we can resort to numerical schemes to approximately compute the conjugate. When f is convex, because $-f$ is concave, the maximization in Definition 12.3 is that of a concave function. Therefore, the conjugate can be computed to arbitrary precision in polynomial time using algorithms such as projected gradient ascent or conditional gradient. Without convexity assumption on f, $f^*(\boldsymbol{v})$ can be approximated by

$$f^*(\boldsymbol{v}) \approx \sup_{\boldsymbol{u} \in \mathcal{U}} \langle \boldsymbol{u}, \boldsymbol{v} \rangle - f(\boldsymbol{u}),$$

where $\mathcal{U} \subseteq \mathrm{dom}(f)$ is a discrete grid of values. We can then compute $f^*(\boldsymbol{v})$ for $\boldsymbol{v} \in \mathcal{V}$ using the linear-time Legendre transform algorithm (Lucet, 1997), where $\mathcal{V} \subseteq \mathrm{dom}(f^*)$ is another discrete grid. The complexity is $O(|\mathcal{U}| \cdot |\mathcal{V}|)$, which is linear in the grid sizes. However, the grid sizes are typically $|\mathcal{U}| = |\mathcal{V}| = O(N^M)$, for N equally-distributed points in each of the M dimensions. Therefore, this approach is limited to small-dimensional settings, e.g., $M \in \{1, 2, 3\}$.

12.3   Dual approach

12.3.1   Duality between strong convexity and smoothness

We now state a well-known result that will underpin this whole chapter: smoothness and strong convexity are dual to each other (Hiriart-Urruty and Lemaréchal, 1993; Kakade *et al.*, 2009; Beck, 2017; Zhou, 2018). For a review of the notions of smoothness and strong convexity, see Section 14.4.

Proposition 12.4 (Duality between strong convexity and smoothness).
f is μ-smooth w.r.t. the norm $\|\cdot\|$ over $\mathrm{dom}(f)$ if and only if f^* is $\frac{1}{\mu}$-strongly convex w.r.t. the dual norm $\|\cdot\|_*$ over $\mathrm{dom}(f^*)$.

We give two examples in Table 12.2.

Table 12.2: Examples of strongly-convex and smooth conjugate pairs.

Function	Norm	Domain	Conjugate	Dual norm	Dual domain
$\frac{1}{2}\|\boldsymbol{u}\|_2^2$	$\|\cdot\|_2$	$\mathbb{R}^M$	$\frac{1}{2}\|\boldsymbol{v}\|_2^2$	$\|\cdot\|_2$	$\mathbb{R}^M$
$\langle \boldsymbol{u}, \log \boldsymbol{u} \rangle$	$\|\cdot\|_1$	$\triangle^M$	$\mathrm{logsumexp}(\boldsymbol{v})$	$\|\cdot\|_\infty$	$\mathbb{R}^M$

12.3.2 Smoothing by dual regularization

The duality between smoothness and strong convexity suggests a generic approach in order to smooth any function $f\colon \mathbb{R}^M \to \mathbb{R}$, by going through the **dual** space.

1. Compute the conjugate f^*:

$$f^*(\boldsymbol{v}) \coloneqq \sup_{\boldsymbol{u}\in\mathrm{dom}(f)} \langle \boldsymbol{u}, \boldsymbol{v} \rangle - f(\boldsymbol{u}).$$

2. Add strongly-convex regularization Ω to the conjugate:

$$f_\Omega^*(\boldsymbol{v}) \coloneqq f^*(\boldsymbol{v}) + \Omega(\boldsymbol{v}).$$

3. Compute the conjugate of f_Ω^*:

$$f_\Omega(\boldsymbol{u}) = f_\Omega^{**}(\boldsymbol{u}).$$

Note that $\boldsymbol{u}$ and $\boldsymbol{v}$ belong to different spaces, i.e., $\boldsymbol{u} \in \mathrm{dom}(f)$ and $\boldsymbol{v} \in \mathrm{dom}(f^*)$. Following Proposition 12.4, if Ω is μ-strongly convex, then $f_\Omega(\boldsymbol{u})$ is $\frac{1}{\mu}$-smooth. Furthermore, following Proposition 12.2, $f_\Omega(\boldsymbol{u})$ is convex, even if f is nonconvex. Therefore, $f_\Omega(\boldsymbol{u})$ is a **smooth convex relaxation** of $f(\boldsymbol{u})$.

Steps 1 and 3 are the most challenging, as they both require the derivation of a conjugate. While an analytical solution may not exist in general, in some simple cases, there is, as we now illustrate.

Example 12.3 (Smoothing the 1-norm via dual regularization)**.** We wish to smooth the 1-norm $f(\boldsymbol{u}) \coloneqq \|\boldsymbol{u}\|_1 = \sum_{j=1}^M |u_j|$.

1. **Compute the conjugate.** The conjugate of any norm $\|\cdot\|$ is the indicator function of the dual norm's unit ball $\{\boldsymbol{v} \in$

$\mathbb{R}^M \colon \|\boldsymbol{v}\|_* \leq 1\}$. The dual norm of $\|\boldsymbol{u}\|_1$ is $\|\boldsymbol{v}\|_\infty$. Moreover,

$$\{\boldsymbol{v} \in \mathbb{R}^M \colon \|\boldsymbol{v}\|_\infty \leq 1\} = [-1, 1]^M.$$

Recalling that $\iota_{\mathcal{C}}$ is the indicator function of $\mathcal{C}$, we obtain

$$f^*(\boldsymbol{v}) = \iota_{[-1,1]^M}(\boldsymbol{v}).$$

2. **Adding strongly-convex regularization.** We add quadratic regularization $\Omega(\boldsymbol{v}) \coloneqq \frac{1}{2}\|\boldsymbol{v}\|_2^2$ to define

$$f_\Omega^*(\boldsymbol{v}) \coloneqq \iota_{[-1,1]^M}(\boldsymbol{v}) + \Omega(\boldsymbol{v}).$$

3. **Computing the conjugate.**

$$f_\Omega(\boldsymbol{u}) = \langle \boldsymbol{u}, \boldsymbol{v}^\star \rangle - \Omega(\boldsymbol{v}^\star) = (H(u_i))_{i=1}^M,$$

where $\boldsymbol{v}^\star = \mathrm{clip}\,(\boldsymbol{u}) \coloneqq \max\,(\min\,(\boldsymbol{u}, 1), -1)$, and H, known as the Huber loss is

$$H(u) = \begin{cases} \frac{1}{2}u^2 & \text{if } |u| \leq 1 \\ |u| - \frac{1}{2} & \text{otherwise} \end{cases}.$$

ReLU functions can be smoothed out in a similar way, as we see in more details in Section 12.4.1.

Remark 12.1 (Regularization scaling). The conjugate of a 1-strongly convex regularizer Ω gives a 1-smooth approximation of the original function. To control the smoothness of the approximation, it suffices to smooth with $\varepsilon\Omega$ for $\varepsilon > 0$, leading to a $1/\varepsilon$-smooth approximation. This is easily achieved by using

$$f_{\varepsilon\Omega}(\boldsymbol{v}) = \varepsilon f_\Omega(\boldsymbol{v}/\varepsilon)$$
$$\nabla f_{\varepsilon\Omega}(\boldsymbol{v}) = \nabla f_\Omega(\boldsymbol{v}/\varepsilon).$$

Therefore, if we know how to compute f_Ω, we can also compute $f_{\varepsilon\Omega}$ and its gradient easily.

12.3.3 Equivalence between primal and dual regularizations

We call $R\colon \operatorname{dom}(f) \to \mathbb{R}$ the primal regularization to distinguish it from the dual regularization $\Omega\colon \operatorname{dom}(f^*) \to \mathbb{R}$. It turns out that both regularizations are equivalent.

Proposition 12.5 (Equivalence between primal and dual regularizations). Let $f\colon \mathbb{R}^M \to \mathbb{R}$ and $R\colon \mathbb{R}^M \to \mathbb{R}$. Then, $f_\Omega = (f \square R)$ with $\Omega = R^*$.

Proof. We have

$$f_\Omega(\boldsymbol{u}) = (f^* + \Omega)^*(\boldsymbol{u}) = \sup_{\boldsymbol{v} \in \operatorname{dom}(\boldsymbol{f}^*)} \langle \boldsymbol{u}, \boldsymbol{v} \rangle - f^*(\boldsymbol{v}) - \Omega(\boldsymbol{v}).$$

If h_1 and h_2 are convex, we have $(h_1 + h_2)^* = h_1^* \square h_2^*$ (Beck, 2017, Theorem 4.17). Using $h_1 = f^*$ and $h_2 = \Omega = R^*$ gives the desired result (note that f^* and R^* are convex even if f and R are not). $\qquad\square$

In particular, with $R(\boldsymbol{u}) = \frac{1}{2}\|\boldsymbol{u}\|_2^2$, this shows that

$$M_f = f_R = f_{R^*}.$$

Given the equivalence between primal and dual regularizations, using one way or the other is mainly a matter of mathematical or algorithmic convenience, depending on the case.

Remark 12.2 (Regularization scaling). Following Definition 12.2, if we use dual regularization $\varepsilon\Omega$, where $\varepsilon > 0$ controls the regularization strength, the corresponding primal regularization is $R = \varepsilon\Omega^*(\cdot/\varepsilon)$. That is, we have

$$f_{\varepsilon\Omega} = f \square \varepsilon\Omega^*(\cdot/\varepsilon).$$

For applications of smoothing techniques to non-smooth optimization, see (Nesterov, 2005; Beck and Teboulle, 2012).

12.4 Examples

12.4.1 Smoothed ReLU functions

The ReLU function is defined by

$$\operatorname{relu}(u) := \begin{cases} u & \text{if } u \geq 0 \\ 0 & \text{otherwise} \end{cases} = \max(u, 0).$$

Its conjugate is

$$\text{relu}^*(v) = \iota_{[0,1]}(v).$$

To notice why, we observe that since the objective is linear

$$\max_{v\in[0,1]} uv = \max_{v\in\{0,1\}} uv = \begin{cases} 1 & \text{if } u \geq 0 \\ 0 & \text{otherwise} \end{cases}. \qquad (12.2)$$

If we use the regularizer $\Omega(v) = v\log v + (1-v)\log(1-v)$, we obtain

$$\text{relu}_\Omega(u) = \text{softplus}(u) = \log(1 + \exp(u)).$$

If we use the regularizer $\Omega(v) = v(v-1)$, we obtain

$$\text{relu}_\Omega(u) = \text{sparseplus}(u) = \begin{cases} 0, & u \leq -1 \\ \frac{1}{4}(u+1)^2, & -1 < u < 1 \ . \\ u, & u \geq 1 \end{cases}$$

12.4.2 Smoothed max operators

With a slight notation overloading, let us define the maximum operator as

$$\max(\boldsymbol{u}) := \max_{j\in[M]} u_j.$$

Its conjugate is

$$\max{}^*(\boldsymbol{v}) = \iota_{\triangle^M}(\boldsymbol{v}).$$

To notice why, we observe that the vertices of the probability simplex $\triangle^M$ are the standard basis vectors $\boldsymbol{e}_1, \ldots, \boldsymbol{e}_M$. Since the objective is linear, we then have

$$\max(\boldsymbol{u}) = \max_{\boldsymbol{v}\in\triangle^M} \langle \boldsymbol{u}, \boldsymbol{v} \rangle = \max_{\boldsymbol{v}\in\{\boldsymbol{e}_1,\ldots,\boldsymbol{e}_M\}} \langle \boldsymbol{u}, \boldsymbol{v} \rangle.$$

We can therefore define the max operator smoothed by a strongly convex regularizer Ω as

$$\max{}_\Omega(\boldsymbol{u}) := \max_{\boldsymbol{v}\in\triangle^M} \langle \boldsymbol{u}, \boldsymbol{v} \rangle - \Omega(\boldsymbol{v}).$$

This smoothed max operator can be useful in a neural network, for example as a smoothed max pooling layer.

Besides strong convexity, two useful assumptions about Ω are

A.1. $\Omega(\boldsymbol{v}) = 0$ for all $\boldsymbol{v} \in \{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_M\}$,

A.2. $\Omega(P\boldsymbol{v}) = \Omega(\boldsymbol{v})$ for any permutation matrix P.

Using Jensen's inequality, these assumptions imply that $-\Omega$ is an "entropy function": it is maximized at $\boldsymbol{v} = \frac{1}{M}\,\mathbf{1}$ (the uniform distribution) and minimized at any $\boldsymbol{v} \in \{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_M\}$ (a delta distribution) (Blondel *et al.*, 2020, Proposition 4). We give two examples of Ω below satisfying A.1 and A.2.

When $\Omega(\boldsymbol{v}) = \langle \boldsymbol{v}, \log \boldsymbol{v} \rangle$ (**Shannon's negative entropy**), we obtain

$$\max_{\Omega}(\boldsymbol{u}) = \mathrm{logsumexp}(\boldsymbol{u}) = \log \sum_{j=1}^{M} e^{u_j}.$$

Alternatively, we can use $\Omega(\boldsymbol{v}) = \frac{1}{2}\langle \boldsymbol{v}, \boldsymbol{v} - \mathbf{1} \rangle$ (**Gini's negative entropy**), which is up to a constant equal to quadratic regularization. For this choice, we therefore obtain

$$\max_{\Omega}(\boldsymbol{u}) = \mathrm{sparsemax}(\boldsymbol{u}) \coloneqq \max_{\boldsymbol{v} \in \triangle^M} \langle \boldsymbol{u}, \boldsymbol{v} \rangle - \frac{1}{2}\langle \boldsymbol{v}, \boldsymbol{v} - \mathbf{1} \rangle.$$

We discuss how to compute $\boldsymbol{v}^{\star} = \mathrm{sparseargmax}(\boldsymbol{u})$ in the sequel.

The properties of the smoothed max operator $\max_{\Omega}$ have been studied in (Mensch and Blondel, 2018, Lemma 1).

Using the vector $\boldsymbol{u} = [u, 0] \in \mathbb{R}^2$ as input, the smoothed max operator recovers the smoothed ReLU:

$$\max_{\Omega}([u, 0]) = \mathrm{relu}_{\Psi}(u),$$

where we defined $\Psi(u) \coloneqq \Omega([u, 1 - u])$. With $\Omega([v, 1 - v])$, we recover $v \log v + (1 - v) \log(1 - v)$; with $\Omega([v, 1 - v])$, we recover $v(v - 1)$, that we used to smooth the ReLU.

Smoothed min

Given a smoothed max operator $\max_{\Omega}$, we can easily define a smoothed min operator as

$$\min_{\Omega}(\boldsymbol{u}) \coloneqq -\max_{\Omega}(-\boldsymbol{u}).$$

12.4.3   Relaxed step functions (sigmoids)

The binary step function, a.k.a. Heaviside step function, is defined by

$$\text{step}(u) := \begin{cases} 1 & \text{if } u \geq 0 \\ 0 & \text{otherwise} \end{cases}.$$

From Eq. (12.2), its variational form is

$$\text{step}(u) = \arg\max_{v \in [0,1]} uv.$$

We can therefore define the relaxation

$$\text{step}_\Omega(u) := \arg\max_{v \in [0,1]} uv - \Omega(v).$$

Notice that, unlike the case of the smoothed ReLU, it is a regularized argmax, not a regularized max. Strongly convex regularization Ω ensures that $\text{step}_\Omega(u)$ is a Lipschitz continuous function of u, unlike $\text{step}(u)$. If we use the regularizer $\Omega(v) = v \log v + (1 - v) \log(1 - v)$, we obtain the closed form

$$\text{step}_\Omega(u) = \text{logistic}(u) := \frac{1}{1 + e^{-u}} = \frac{e^u}{1 + e^u}.$$

This function is differentiable everywhere. As an alternative, if we use $\Omega(v) = v(v - 1)$, we obtain a piecewise linear sigmoid,

$$\text{step}_\Omega(u) = \text{sparsesigmoid}(u) := \begin{cases} 0, & u \leq -1 \\ \frac{1}{2}(u + 1), & -1 < u < 1 \\ 1, & u \geq 1 \end{cases}.$$

Unlike the logistic function, it can reach the exact values 0 or 1. However, the function has two kinks, where the function is non-differentiable.

It turns out that the three sigmoids we presented above (step, logistic, sparsesigmoid) are all equal to the derivative of their corresponding non-linearity:

$$\text{step}(u) = \text{relu}'(u)$$
$$\text{logistic}(u) = \text{softplus}'(u)$$
$$\text{sparsesigmoid}(u) = \text{sparseplus}'(u)$$
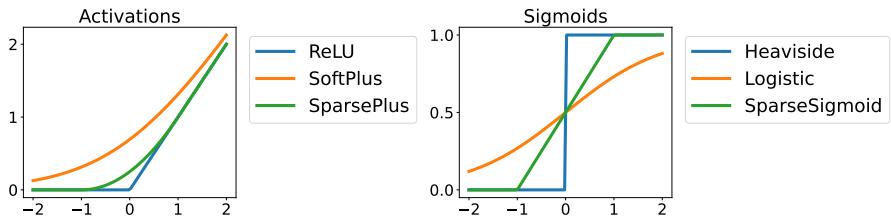
Figure 12.2: Some ReLU functions and sigmoids. Differentiating the left functions give the right functions.

and more generally

$$\text{relu}'_\Omega(u) = \text{step}_\Omega(u).$$

This is again a consequence of Danskin's theorem; see Example 10.2.

We illustrate the smoothed ReLu functions and relaxed step functions (sigmoids) in Fig. 12.2.

12.4.4   Relaxed argmax operators

With a slight notation overloading, let us now define

$$\text{argmax}(\boldsymbol{u}) := \phi(\arg\max_{j\in[M]} u_j),$$

where $\phi(j) = \text{onehot}(j) = \boldsymbol{e}_j$ is used to embed any integer $j \in [M]$ into $\mathbb{R}^M$. Following the previous paragraph, we have the variational form

$$\text{argmax}(\boldsymbol{u}) = \arg\max_{\boldsymbol{v}\in\triangle^M}\langle\boldsymbol{u}, \boldsymbol{v}\rangle = \arg\max_{\boldsymbol{v}\in\{\boldsymbol{e}_1,\dots,\boldsymbol{e}_M\}}\langle\boldsymbol{u}, \boldsymbol{v}\rangle,$$

where the second equality uses that a linear function is maximized at one vertex of the simplex. This variational form suggests to define the relaxation

$$\text{argmax}_\Omega(\boldsymbol{u}) := \arg\max_{\boldsymbol{v}\in\triangle^M}\langle\boldsymbol{u}, \boldsymbol{v}\rangle - \Omega(\boldsymbol{v}).$$

When $\Omega(\boldsymbol{v}) = \langle\boldsymbol{v}, \log\boldsymbol{v}\rangle$, we obtain

$$\text{argmax}_\Omega(\boldsymbol{u}) = \text{softargmax}(\boldsymbol{u}) = \frac{\exp(\boldsymbol{u})}{\sum_{j=1}^{M}\exp(u_j)},$$

which is differentiable everywhere.

When $\Omega(\boldsymbol{v}) = \frac{1}{2}\langle \boldsymbol{v}, \boldsymbol{v} - \mathbf{1} \rangle$, which is up to a constant equal to $\frac{1}{2}\|\boldsymbol{v}\|_2^2$, we obtain the sparseargmax (Martins and Astudillo, 2016)

$$
\begin{aligned}
\mathrm{argmax}_\Omega(\boldsymbol{u}) &= \mathrm{sparseargmax}(\boldsymbol{u}) \\
&\coloneqq \underset{\boldsymbol{v} \in \triangle^M}{\arg\max} \langle \boldsymbol{u}, \boldsymbol{v} \rangle - \langle \boldsymbol{v}, \boldsymbol{v} - \mathbf{1} \rangle \\
&= \underset{\boldsymbol{v} \in \triangle^M}{\arg\min} \|\boldsymbol{u} - \boldsymbol{v}\|_2^2,
\end{aligned}
$$

which is nothing but the Euclidean projection onto the probability simplex, discussed in Section 15.3. At its name indicates, sparseargmax is **sparse** but it is only differentiable almost everywhere.

Similarly to sigmoids, it turns out that these mappings are equal to the gradient of their corresponding non-linearities:

$$
\mathrm{argmax}_\Omega(\boldsymbol{u}) = \nabla\mathrm{max}_\Omega(\boldsymbol{u}).
$$

Relaxed argmin operators

Given a smoothed max operator max_Ω, we can easily define a relaxed argmin

$$
\mathrm{argmin}_\Omega(\boldsymbol{u}) \coloneqq \nabla\mathrm{min}_\Omega(\boldsymbol{u}) = \nabla\mathrm{max}_\Omega(-\boldsymbol{u}).
$$

12.5   Summary

We reviewed how to smooth a function by infimal convolution between the function and primal regularization. The Moreau envelope is a special case, obtained by using quadratic regularization.

The Legendre-Fenchel transformation, a.k.a. convex conjugate, can be seen as a dual representation of a function: instead of representing f by its graph $(\boldsymbol{u}, f(\boldsymbol{u}))$ for $\boldsymbol{u} \in \mathrm{dom}(f)$, we can represent it by the set of tangents with slope $\boldsymbol{v}$ and intercept $-f^*(\boldsymbol{v})$ for $\boldsymbol{v} \in \mathrm{dom}(f^*)$ As its name indicates, it is convex, even if the original function is not.

Infimal convolution can equivalently be obtained by going to this dual space, applying dual regularization there and coming back. We showed how to apply these techniques to create smoothed ReLU and max functions. We also showed that taking their gradients allowed us to obtain generalized sigmoids and argmax functions.

13

Smoothing by integration

In this chapter, we review smoothing techniques based on **convolution**.

13.1 Convolution

13.1.1 Convolution operators

The convolution between two functions f and g produces another function, denoted $f * g$. It is defined by

$$(f * g)(\mu) := \int_{-\infty}^{\infty} f(u)g(\mu - u)\, du, \qquad (13.1)$$

assuming that the integral is well defined. It is therefore the integral of the product of f and g after g is reflected about the y-axis and shifted. It can be seen as a generalization of the **moving average**. Using the change of variable $z := \mu - u$, we can also write

$$(f * g)(\mu) = \int_{-\infty}^{\infty} f(\mu - z)g(z)\, dz = (g * f)(\mu). \qquad (13.2)$$

The convolution operator is therefore **commutative**.

13.1.2   Convolution with a kernel

The convolution is frequently used together with a **kernel** κ to create a smooth approximation $f * \kappa$ of f. The most frequently used kernel is the **Gaussian kernel** with width σ, defined by

$$\kappa_\sigma(z) := \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}(\frac{z}{\sigma})^2}.$$

This is the probability density function (PDF) of the normal distribution with zero mean and variance σ^2. The term $\frac{1}{\sqrt{2\pi}\sigma}$ is a normalization constant, ensuring that the kernel sums to 1 for all σ. We therefore say that κ_σ is a **normalized kernel**.

Averaging perspective

Applying the definition of the convolution in Eq. (13.1), we obtain

$$(f * \kappa_\sigma)(\mu) := \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\infty} f(u) e^{-\frac{1}{2}(\frac{\mu-u}{\sigma})^2} du$$

$$= \mathbb{E}_{U \sim p_{\mu,\sigma}}[f(U)],$$

where

$$p_{\mu,\sigma}(u) := \kappa_\sigma(\mu - u) = \kappa_\sigma(z) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}(\frac{\mu-u}{\sigma})^2}$$

is the PDF of the Gaussian distribution with mean μ and variance σ^2. Therefore, we can see $f * \kappa_\sigma$ as the **expectation** of $f(u)$ over a Gaussian **centered around** μ. This property is true for all translation-invariant kernels, that correspond to a location-scale family distribution (e.g., the Laplace distribution). The convolution therefore performs an averaging with all points, with points nearby μ given more weight by the distribution. The parameter σ controls the importance we want to give to farther points. We call this viewpoint averaging, as we replace $f(\boldsymbol{u})$ by $\mathbb{E}[f(U)]$.

Perturbation perspective

Conversely, using the alternative definition of the convolution operator in Eq. (13.2), which stems from the commutativity of the convolution,

we have

$$(f * \kappa_\sigma)(\mu) := \int_{-\infty}^{\infty} f(\mu - z)e^{-\frac{1}{2}\left(\frac{z}{\sigma}\right)^2} dz$$
$$= \mathbb{E}_{Z \sim p_{0,\sigma}}[f(\mu - Z)]$$
$$= \mathbb{E}_{Z \sim p_{0,\sigma}}[f(\mu + Z)],$$

where, in the third line, we used that $p_{0,\sigma}$ is sign invariant, i.e., $p_{0,\sigma}(z) = p_{0,\sigma}(-z)$. This viewpoint shows that smoothing by convolution with a Gaussian kernel can also be seen as injecting Gaussian **noise** or **perturbations** to the function's input.

Limit case

When $\sigma \to 0$, the kernel κ_σ converges to a Dirac delta function,

$$\lim_{\sigma \to 0} \kappa_\sigma(z) = \delta(z).$$

Since the Dirac delta is the multiplicative identity of the convolution algebra (this is also known as the sifting property), when $\sigma \to 0$, $f * \kappa_\sigma$ converges to f, i.e.,

$$\lim_{\sigma \to 0}(f * \kappa_\sigma)(u) = f(u).$$

13.1.3   Discrete convolution

Many times, we work with functions whose convolution does not have an analytical form. In these cases, we can use a discrete convolution on a grid of values. For two functions f and g defined over $\mathbb{Z}$, the discrete convolution is defined by

$$(f * g)[i] := \sum_{j=-\infty}^{\infty} f[j]g[i - j].$$

As for its continuous counterpart, the discrete convolution is commutative, namely,

$$(f * g)[i] = \sum_{j=-\infty}^{\infty} f[i - j]g[j] = (g * f)[i].$$
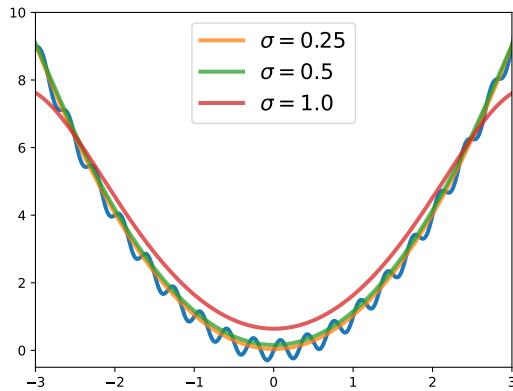
Figure 13.1: Smoothing of the signal $f[t] := t^2 + 0.3\sin(6\pi t)$ with a sampled and renormalized Gaussian kernel.

When g has finite support over the set $S := \{-M, -M+1, \ldots, 0, \ldots, M-1, M\}$, meaning that $g[i] = 0$ for all $i \notin S$, a finite summation may be used instead, i.e.,

$$(f * g)[i] = \sum_{j=-M}^{M} f[i-j]g[j] = (g * f)[i].$$

In practice, convolution between a discrete signal $f \colon \mathbb{Z} \to \mathbb{R}$ and a continuous kernel $\kappa \colon \mathbb{R} \to \mathbb{R}$ is implemented by discretizing the kernel. One of the simplest approaches consists in sampling points on an interval, evaluating the kernel at these points and renormalizing the obtained values, so that the sampled kernel sums to 1. This is illustrated with the Gaussian kernel in Fig. 13.1. Since the Gaussian kernel decays exponentially fast, we can choose a small interval around 0. For a survey of other possible discretizations of the Gaussian kernel, see Getreuer (2013).

13.1.4 Differentiation

Remarkably, provided that the two functions are integrable with integrable derivatives, the derivative of the convolution satisfies

$$(f * g)' = (f' * g) = (f * g'),$$

which simply stems from switching derivative and integral in the definition of the convolution. Moreover, we have the following proposition.

> **Proposition 13.1** (Differentiability of the convolution)**.** If g is n-times differentiable with compact support over $\mathbb{R}$ and f is locally integrable over $\mathbb{R}$, then $f * g$ is n-times differentiable over $\mathbb{R}$.

13.1.5 Multidimensional convolution

So far, we studied the convolution of one-dimensional functions. The definition can be naturally extended to multidimensional functions $f\colon \mathbb{R}^M \to \mathbb{R}$ and $g\colon \mathbb{R}^M \to \mathbb{R}$ as

$$(f * g)(\boldsymbol{\mu}) := \int_{\mathbb{R}^M} f(\boldsymbol{u})g(\boldsymbol{\mu} - \boldsymbol{u})\, d\boldsymbol{u},$$

assuming again that the integral exists. Typically, a Gaussian kernel with diagonal covariance matrix is used

$$\kappa_\sigma(\boldsymbol{z}) := \prod_{j=1}^{M} \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{1}{2}(\frac{z_j}{\sigma_j})^2} = \frac{1}{\sqrt{2\pi}^M \sigma^M} e^{-\frac{1}{2}\frac{\|z\|_2^2}{\sigma^2}},$$

where, in the second equality, we assumed $\sigma_1 = \cdots = \sigma_M$. In an image processing context, where $M = 2$, it is approximated using a discrete convolution and it is called a **Gaussian blur**.

13.1.6 Link between convolution and infimal convolution

Recall the definition of infimal convolution (Section 12.1):

$$h(\mu) := (f\square g)(\mu) := \inf_{u\in\mathbb{R}} f(u) + g(\mu - u).$$

If we replace the minimum with a soft minimum (Section 12.4.2), we then obtain

$$h_\varepsilon(\mu) := (f\square g)_\varepsilon(\mu) := -\varepsilon \log \int e^{-\frac{1}{\varepsilon}(f(u)+g(\mu-u))}\, du.$$

By using the exponential change of variable (sometimes referred to as **Cole-Hopf transformation** in a partial differential equation context)

$$\mathcal{C}_\varepsilon\{f\}(u) := e^{-\frac{1}{\varepsilon}f(u)}$$
$$\mathcal{C}_\varepsilon^{-1}\{F\}(v) = -\varepsilon \log F(v),$$

we can define each function in the exponential domain,

$$F_\varepsilon := \mathcal{C}_\varepsilon\{f\}, \ \ G_\varepsilon := \mathcal{C}_\varepsilon\{g\}, \ \ H_\varepsilon := \mathcal{C}_\varepsilon\{h_\varepsilon\}.$$

We then obtain

$$H_\varepsilon(\mu) = (F_\varepsilon * G_\varepsilon)(\mu).$$

In the exponential domain, the convolution is therefore the counterpart of the infimal convolution, if we replace the **min-plus algebra** with the **sum-product algebra**. Back to log domain, we obtain

$$h_\varepsilon(\mu) = \mathcal{C}_\varepsilon^{-1}\{H_\varepsilon\}(\mu).$$

Combining the transformation and its inverse, we can write

$$h_\varepsilon(\mu) = \mathcal{C}_\varepsilon^{-1}\{\mathcal{C}_\varepsilon\{f\} * \mathcal{C}_\varepsilon\{g\}\}(\mu).$$

As an example, when $g(z) = \frac{1}{2}z^2$, in which case $f \square g$ is the Moreau envelope (see Section 12.1), we obtain $G_\varepsilon(z) = \exp(-\frac{1}{2\varepsilon}z^2)$, the (unnormalized) Gaussian kernel.

13.2   Fourier and Laplace transforms

Let us define the **Fourier transform** of f by

$$F(s) := \mathcal{F}\{f\}(s) := \int_{-\infty}^{\infty} f(t)e^{-i2\pi st}\,dt, \quad s \in \mathbb{R}.$$

Note that $\mathcal{F}\{f\}$ is a function transformation: it transforms f into another function F.

13.2.1   Convolution theorem

Now, consider the convolution

$$h(t) := (f * g)(t).$$

If we define the three transformations

$$F := \mathcal{F}\{f\}, \; G := \mathcal{F}\{g\}, \; H := \mathcal{F}\{h\},$$

the **convolution theorem** states that

$$H(s) = \mathcal{F}\{h\}(s) = F(s) \cdot G(s), \quad s \in \mathbb{R}.$$

Written differently, we have

$$\mathcal{F}\{f * g\} = \mathcal{F}\{f\} \cdot \mathcal{F}\{g\}.$$

In words, in the Fourier domain, the convolution operation becomes a multiplication. Conversely,

$$h(t) = (f * g)(t) = \mathcal{F}^{-1}\{F \cdot G\}(t), \quad t \in \mathbb{R}.$$

The convolution theorem also holds if we replace the Fourier transform with the Laplace transform or with the two-sided (bilateral) Laplace transform.

13.2.2   Link between Fourier and Legendre transforms

In Section 12.2, we studied another function transformation: the convex conjugate, also known as Legendre-Fenchel transform. We recap the analogies between these transforms in Table 13.1. In particular, the counterpart of

$$\mathcal{F}\{f * g\} = \mathcal{F}\{f\} \cdot \mathcal{F}\{g\}.$$

for the infimal convolution is

$$(f \Box g)^* = f^* + g^*.$$

In words, the Legendre-Fenchel transform is to the infimal convolution what the Fourier transform is to the convolution.

13.2.3   The soft Legendre-Fenchel transform

Let $f \colon \mathbb{R}^M \to \mathbb{R}$. The convex conjugate of f (see Section 12.2) is

$$f^*(\boldsymbol{v}) := \max_{\boldsymbol{u} \in \mathbb{R}^M} \; \langle \boldsymbol{u}, \boldsymbol{v} \rangle - f(\boldsymbol{u}).$$

If necessary, we can support constraints by including an indicator function in the definition of f. The conjugate can be smoothed out using a log-sum-exp, which plays the role of a soft maximum (Section 12.4.2).

Table 13.1: Analogy between Fourier and Legendre transforms. See Proposition 12.3 for more conjugate calculus rules.

	Fourier $\mathcal{F}\{f\}$	Legendre f^*
Semiring	$(+, \cdot)$	$(\min, +)$
Scaling $(a > 0)$	$f(t) = g(t/a)$	$f(t) = ag(t/a)$
	$\mathcal{F}\{f\}(t) = a\mathcal{F}\{g\}(as)$	$f^*(s) = ag^*(s)$
Translation	$f(t) = g(t - t_0)$	$f(t) = g(t - t_0)$
	$\mathcal{F}\{f\}(s) = e^{-i2\pi t_0 s}\mathcal{F}\{g\}(s)$	$f^*(s) = g^*(s) + t_0$
Convolution	$h = f * g$	$h = f \square g$
	$\mathcal{F}\{h\} = \mathcal{F}\{f\} \cdot \mathcal{F}\{g\}$	$h^* = f^* + g^*$
Gaussian / quadratic	$f(t) = e^{-at^2}$	$f(t) = \frac{a}{2}t^2$
	$\mathcal{F}\{f\}(s) = \sqrt{\frac{\pi}{a}}e^{-\pi^2 s^2/a}$	$f^*(s) = \frac{1}{2a}s^2$
Smoothing	$f * \kappa_\sigma$	$f \square \frac{1}{2\varepsilon}\|\cdot\|_2^2$

Definition 13.1 (Soft convex conjugate).

$$f_\varepsilon^*(\boldsymbol{v}) := \varepsilon \log \int \exp\left(\frac{1}{\varepsilon}\left[\langle \boldsymbol{u}, \boldsymbol{v}\rangle - f(\boldsymbol{u})\right]\right) d\boldsymbol{u}.$$

In the limit $\varepsilon \to 0$, we recover the convex conjugate. We now show that this smoothed conjugate can be rewritten using a convolution if we apply a bijective transformation to f.

Proposition 13.2 (Smoothed convex conjugate as convolution). The smoothed conjugate can be rewritten as

$$f_\varepsilon^*(\boldsymbol{v}) = \mathcal{Q}_\varepsilon^{-1}\left\{\frac{1}{\mathcal{Q}_\varepsilon\{f\} * G_\varepsilon}\right\}(\boldsymbol{v})$$

where

$$G_\varepsilon := \mathcal{C}\left\{\frac{1}{2}\|\cdot\|_2^2\right\} = \exp\left(-\frac{1}{2}\frac{\|\cdot\|_2^2}{\varepsilon}\right)$$

$$\mathcal{Q}_\varepsilon\{f\} := \mathcal{C}\left\{f(\cdot) - \frac{1}{2}\|\cdot\|_2^2\right\} = \exp\left(\frac{1}{2\varepsilon}\|\cdot\|_2^2 - \frac{1}{\varepsilon}f(\cdot)\right)$$

$$\mathcal{Q}_\varepsilon^{-1}\{F\} := \frac{1}{2}\|\cdot\|_2^2 - \varepsilon\log(F(\cdot)).$$

This insight was tweeted by Gabriel Peyré in April 2020.

Proof.

$$f_\varepsilon(\boldsymbol{v}) := \varepsilon\log\int\exp\left(\frac{1}{\varepsilon}\langle\boldsymbol{u},\boldsymbol{v}\rangle - \frac{1}{\varepsilon}f(\boldsymbol{u}))\right)d\boldsymbol{u}$$

$$= \varepsilon\log\int\exp\left(-\frac{1}{2\varepsilon}\|\boldsymbol{u}-\boldsymbol{v}\|_2^2 + \frac{1}{2\varepsilon}\|\boldsymbol{u}\|_2^2 + \frac{1}{2\varepsilon}\|\boldsymbol{v}\|_2^2 - \frac{1}{\varepsilon}f(\boldsymbol{u}))\right)d\boldsymbol{u}$$

$$= \varepsilon\log\int\exp\left(-\frac{1}{2\varepsilon}\|\boldsymbol{u}-\boldsymbol{v}\|_2^2 + \frac{1}{2\varepsilon}\|\boldsymbol{u}\|_2^2 - \frac{1}{\varepsilon}f(\boldsymbol{u}))\right)d\boldsymbol{u} + \frac{1}{2}\|\boldsymbol{v}\|_2^2$$

$$= \varepsilon\log\int G_\varepsilon(\boldsymbol{v}-\boldsymbol{u})\mathcal{Q}_\varepsilon\{f\}(\boldsymbol{u})d\boldsymbol{u} + \frac{1}{2}\|\boldsymbol{v}\|_2^2$$

$$= \varepsilon\log(\mathcal{Q}_\varepsilon\{f\} * G_\varepsilon)(\boldsymbol{v}) + \frac{1}{2}\|\boldsymbol{v}\|^2$$

$$= \frac{1}{2}\|\boldsymbol{v}\|^2 - \varepsilon\log\left(\frac{1}{\mathcal{Q}_\varepsilon\{f\} * G_\varepsilon}\right)(\boldsymbol{v})$$

$$= \mathcal{Q}_\varepsilon^{-1}\left\{\frac{1}{\mathcal{Q}_\varepsilon\{f\} * G_\varepsilon}\right\}(\boldsymbol{v})$$

$$\square$$

What did we gain from this viewpoint? The convex conjugate can often be difficult to compute in closed form. If we replace $\mathbb{R}^M$ with a discrete set $\mathcal{S}$ (i.e., a grid), we can then approximate the smoothed convex conjugate in $O(n\log n)$, where $n = |\mathcal{S}|$, using a discrete convolution,

$$(\mathcal{Q}_\varepsilon\{f\} * G_\varepsilon)(\boldsymbol{v}) \approx \sum_{\boldsymbol{u}\in\mathcal{S}} G_\varepsilon(\boldsymbol{v}-\boldsymbol{u})\mathcal{Q}_\varepsilon\{f\}(\boldsymbol{u})$$

$$= \boldsymbol{K}\boldsymbol{q},$$

where $\boldsymbol{K}$ is the $n\times n$ Gaussian kernel matrix whose entries correspond to $\exp(-\frac{1}{2\varepsilon}\|\boldsymbol{u}-\boldsymbol{u}'\|_2^2)$ for $\boldsymbol{u},\boldsymbol{u}' \in \mathcal{S}$ and $\boldsymbol{q}$ is the n-dimensional vector whose
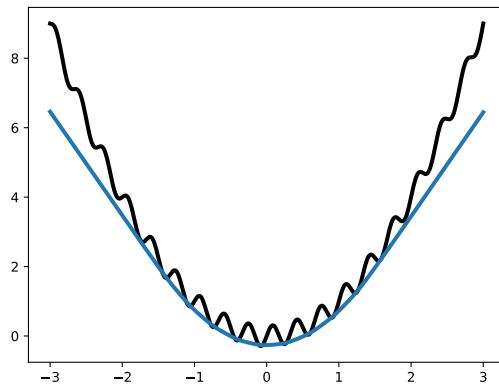
Figure 13.2: Applying the smoothed conjugate twice gives a smoothed biconjugate (convex envelope) of the function.

entries correspond to $\exp(\frac{1}{\varepsilon}(\frac{1}{2}\|\boldsymbol{v}\|_2^2 - f(\boldsymbol{u}))$ for $\boldsymbol{u} \in \mathcal{S}$. This provides a GPU-friendly alternative to the fast Legendre transform algorithm, discussed in Section 12.2. Of course, due to the curse of dimensionality, the technique is limited to functions defined on low-dimensional sets. We illustrate in Fig. 13.2 the application of the technique to computing an approximate biconjugate (convex envelope) of a function.

Remark 13.1 (Link with the two-sided Laplace transform). For one-dimensional functions, instead of using a convolution, we can also write the soft convex conjugate as

$$f_\varepsilon^*(v) = \varepsilon \log \int_{-\infty}^{\infty} \exp\left(\frac{1}{\varepsilon}\left[uv - f(u)\right]\right) du$$

$$= \varepsilon \log \mathcal{B}\left\{e^{-\frac{f}{\varepsilon}}\right\}\left(-\frac{v}{\varepsilon}\right)$$

$$= -\mathcal{C}_\varepsilon^{-1}\left\{\mathcal{B}\left\{\mathcal{C}_\varepsilon\{f\}\right\}\right\}\left(-\frac{v}{\varepsilon}\right)$$

where we defined the two-sided (bilateral) Laplace transform

$$\mathcal{B}\{g\}(v) := \int_{-\infty}^{\infty} e^{-uv} g(u) du$$

and where we assumed that the integral exists.

13.3 Examples

In this section, we review practical examples for which the convolution with a Gaussian kernel enjoys an analytical solution.

13.3.1 Smoothed step function

Example 13.1 (Smoothed Heaviside). The Heaviside step function is defined by

$$\text{step}(u) := h(u) := \begin{cases} 1 & \text{if } u \geq 0 \\ 0 & \text{otherwise} \end{cases}.$$

With the Gaussian kernel, we therefore obtain

$$(h * \kappa_\sigma)(\mu) = \int_{-\infty}^{\mu} \kappa_\sigma(z) h(\mu - z) dz + \int_{\mu}^{\infty} \kappa_\sigma(z) h(\mu - z) dz$$

$$= \int_{-\infty}^{\mu} \kappa_\sigma(z) dz$$

$$= \Phi_\sigma(\mu)$$

$$= \frac{1}{2} \left[1 + \text{erf} \left(\frac{\mu}{\sqrt{2}\sigma} \right) \right],$$

where $\Phi_\sigma(\mu)$ is the CDF of the Gaussian distribution with zero mean and variance σ^2, and where we used the error function

$$\text{erf}(z) := \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt,$$

that we both already encountered in Chapter 3. Although there is no closed form for the error function, it is commonly available in numerical analysis software, such as SciPy.
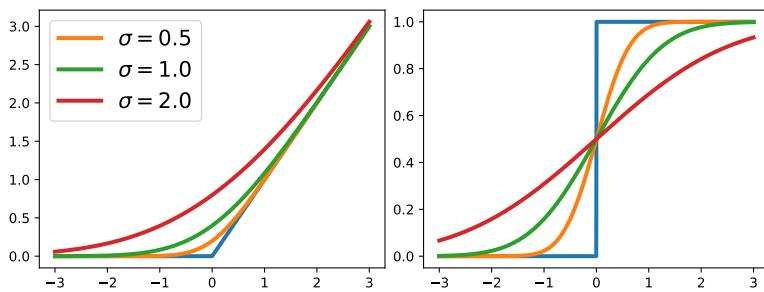
Figure 13.3: Smoothing of the ReLU and Heaviside functions by convolution with a Gaussian kernel, for three values of the width σ.

13.3.2 Smoothed ReLU function

Example 13.2 (Smoothed ReLU). The ReLU is defined by

$$r(u) := \begin{cases} u & \text{if } u \geq 0 \\ 0 & \text{otherwise} \end{cases} = u \cdot h(u).$$

Similarly to the previous example, we obtain

$$
\begin{aligned}
(r * \kappa_\sigma)(\mu) &= \int_{-\infty}^{\mu} \kappa_\sigma(z) r(\mu - z) dz \\
&= \int_{-\infty}^{\mu} \kappa_\sigma(z)(\mu - z) dz \\
&= \mu \int_{-\infty}^{\mu} \kappa_\sigma(z) z - \int_{-\infty}^{\mu} \kappa_\sigma(z) z dz \\
&= \mu \Phi_\sigma(\mu) + \sigma^2 \kappa_\sigma(\mu).
\end{aligned}
$$

In the second integral, setting $a := \frac{1}{2\sigma^2}$, we used

$$\int z e^{-az^2} dz = -\frac{1}{2a} \int e^t dt = -\frac{1}{2a} e^t + C = -\frac{1}{2a} e^{-az^2} + C$$

and $t := -az^2 \Rightarrow z dz = -\frac{1}{2a} dt$.

To illustrate differentiation of the convolution, we show how to differentiate the smoothed ReLu.

Example 13.3 (Differentiating the smoothed ReLU). Differentiating the smoothed ReLU from Example 13.2, we obtain

$$(r * \kappa_\sigma)' = (r' * \kappa_\sigma) = h * \kappa_\sigma = \Phi_\sigma.$$

Therefore, unsurprisingly, the derivative of the smoothed ReLU is the smoothed Heaviside step function. Differentiating once again, we obtain,

$$(r * \kappa_\sigma)'' = (h * \kappa_\sigma)' = (h' * \kappa_\sigma) = \delta * \kappa_\sigma = \kappa_\sigma,$$

where the derivative h' is well-defined almost everywhere. We can arrive at the same result by using that $h * \kappa_\sigma = \Phi_\sigma$ and $\Phi_\sigma' = \kappa_\sigma$, since Φ_σ and κ_σ are the CDF and PDF of the Gaussian with zero mean and σ^2 variance.

13.4 Perturbation of blackbox functions

In this section, we review how to approximately compute a convolution with a kernel and its gradient using Monte-Carlo estimation.

13.4.1 Expectation in a location-scale family

A rather intuitive approach to smooth a function $f : \mathbb{R}^M \to \mathbb{R}$ is to average its values on an input $\boldsymbol{\mu}$, perturbed by some additive noise $Z \sim p$, for some noise distribution p. This defines the surrogate

$$f_\sigma(\boldsymbol{\mu}) := \mathbb{E}_{Z \sim p}[f(\boldsymbol{\mu} + \sigma Z)].$$

The parameter σ controls the perturbation strength: as $\sigma \to 0$, we naturally recover f. An equivalent viewpoint is obtained by defining the transformation (change of variables)

$$U := \boldsymbol{\mu} + \sigma Z.$$

We then have

$$U \sim p_{\boldsymbol{\mu},\sigma},$$

where $p_{\boldsymbol{\mu},\sigma}$ is the **location-family distribution** generated by the noise distribution p. It is the pushforward distribution of Z through the

transformation (see Section 11.4.3). In this notation, the initial noise distribution p is then simply $p = p_{\mathbf{0},1}$. The perturbed function can then be expressed from these two perspectives as

$$f_\sigma(\boldsymbol{\mu}) = \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[f(\boldsymbol{\mu} + \sigma \cdot Z)]$$
$$= \mathbb{E}_{U \sim p_{\boldsymbol{\mu},\sigma}}[f(U)]. \tag{13.3}$$

Writing the expectation as the integral of a p.d.f, we naturally recover the smoothing by convolution presented earlier,

$$f_\sigma(\boldsymbol{\mu}) = \int f(\boldsymbol{\mu} + \sigma \boldsymbol{z}) p_{\mathbf{0},1}(\boldsymbol{z}) d\boldsymbol{z}$$
$$= f * \kappa_\sigma(\boldsymbol{\mu}),$$

where we defined the kernel

$$\kappa_\sigma(\boldsymbol{z}) := p_{\mathbf{0},\sigma}(-\boldsymbol{z}).$$

In the sequel, we assume that the noise distribution decomposes as

$$p_{\mathbf{0},1}(\boldsymbol{z}) := \exp(-\nu(\boldsymbol{z}))/C,$$

where $\nu(\boldsymbol{z})$ is the **log-density** of the noise distribution and C is a normalization constant. For instance, the Gaussian distribution with diagonal covariance matrix and the corresponding **Gaussian kernel** are obtained with $\nu(\boldsymbol{z}) = \frac{1}{2}\|\boldsymbol{z}\|_2^2$ and $C = \sqrt{2\pi}^M$.

Approximation by Monte-Carlo estimation

Instead of approximating the integral above (continuous convolution) with a discrete convolution on a grid, as we did in Section 13.1.3, the expectation perspective suggests that we can estimate $f_\sigma(\boldsymbol{\mu})$ by Monte-Carlo estimation: we simply draw samples from the distribution, evaluate the function at these samples and average.

13.4.2 Gradient estimation by reparametrization

If f is differentiable with finite expectation and Leibniz's integration rule holds, we have

$$\nabla f_\sigma(\boldsymbol{\mu}) = \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[\nabla f(\boldsymbol{\mu} + \sigma \cdot Z)]. \tag{13.4}$$

If f is differentiable almost everywhere, the formula may still hold, see Section 11.1. For example, if f is the ReLU, then ∇f is the Heaviside step function, and we obtain the correct gradient of f_σ using the formula above; see Example 13.1. However, if f is not absolutely continuous, the formula may not hold. For example, if f is the Heaviside function, the right-hand side of (13.4) is 0 which does not match the gradient of f_σ; see Example 13.1.

From the second expression of f_σ in (13.3), we can see the formula of the gradient in (13.4) as a reparametrization trick $U = \boldsymbol{\mu} + \sigma Z$; see Section 11.4. Namely, we have

$$
\begin{aligned}
\nabla f_\sigma(\boldsymbol{\mu}) &= \nabla_{\boldsymbol{\mu}} \mathbb{E}_{U \sim p_{\boldsymbol{\mu},\sigma}}[f(U)] \\
&= \nabla_{\boldsymbol{\mu}} \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[f(\boldsymbol{\mu} + \sigma \cdot Z)] \\
&= \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[\nabla_{\boldsymbol{\mu}} f(\boldsymbol{\mu} + \sigma \cdot Z)] \\
&= \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[\nabla f(\boldsymbol{\mu} + \sigma \cdot Z)].
\end{aligned}
\tag{13.5}
$$

13.4.3 Gradient estimation by SFE, Stein's lemma

In some cases, we may not have access to ∇f or f may not be absolutely continuous and therefore the formula in (13.4) cannot apply. For these cases, we can use the score function estimator (SFE) from Section 11.3. Here, for $f_\sigma(\boldsymbol{\mu}) = \mathbb{E}_{U \sim p_{\boldsymbol{\mu},\sigma}}[f(U)]$, we botain

$$
\nabla f_\sigma(\boldsymbol{\mu}) = \mathbb{E}_{U \sim p_{\boldsymbol{\mu},\sigma}}[f(U) \nabla_{\boldsymbol{\mu}} \log p_{\boldsymbol{\mu},\sigma}(U)].
$$

Since the PDF can be written as

$$
p_{\boldsymbol{\mu},\sigma}(\boldsymbol{u}) = \frac{1}{\sigma} p_{\mathbf{0},1}((\boldsymbol{u} - \boldsymbol{\mu})/\sigma),
$$

where

$$
p_{\mathbf{0},1}(\boldsymbol{z}) := \exp(-\nu(\boldsymbol{z}))/C,
$$

we obtain

$$
\nabla_{\boldsymbol{\mu}} \log p_{\boldsymbol{\mu},\sigma}(\boldsymbol{u}) = \nabla \nu((\boldsymbol{u} - \boldsymbol{\mu})/\sigma)/\sigma.
$$

To summarize, we have shown that

$$
\begin{aligned}
\nabla f_\sigma(\boldsymbol{\mu}) &= \mathbb{E}_{U \sim p_{\boldsymbol{\mu},\sigma}}[f(U) \nabla \nu((U - \boldsymbol{\mu})/\sigma)/\sigma] \\
&= \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[f(\boldsymbol{\mu} + \sigma \cdot Z) \nabla \nu(Z)/\sigma],
\end{aligned}
\tag{13.6}
$$

where we used the change of variable $Z = (U - \boldsymbol{\mu})/\sigma$. The same technique can also be used if we want to estimate the gradient w.r.t. $\boldsymbol{\theta} = (\boldsymbol{\mu}, \sigma)$ or if we want to estimate the Jacobian of the expectation of a vector-valued function.

In the particular case of Gaussian noise, since $\nabla \nu(\boldsymbol{z}) = \boldsymbol{z}$, we obtain

$$\nabla f_\sigma(\boldsymbol{\mu}) = \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[f(\boldsymbol{\mu} + \sigma \cdot Z)Z/\sigma].$$

This is known as **Stein's lemma**. It should be noted that the above is an unbiased estimator of the gradient of the smoothed function f_σ, but a biased estimator of the gradient of the original function f (assuming that it exists). However, smoothing is usually a good thing, as it can accelerate the convergence of gradient-based algorithms.

13.4.4   Link between reparametrization and SFE

Using the log-derivative identity, we have for any distribution with differentiable density p

$$\mathbb{E}_{Z \sim p}[h(Z)\nabla \log p(Z)] = \int_{\mathbb{R}^M} h(\boldsymbol{z}) \left(\frac{\nabla p(\boldsymbol{z})}{p(\boldsymbol{z})} \right) p(\boldsymbol{z}) d\boldsymbol{z}$$
$$= \int_{\mathbb{R}^M} h(\boldsymbol{z}) \nabla p(\boldsymbol{z}) d\boldsymbol{z}.$$

Using **integration by parts** and assuming that $h(\boldsymbol{z})p(\boldsymbol{z})$ goes to zero when $\|\boldsymbol{z}\| \to \infty$, we have

$$\int_{\mathbb{R}^M} h(\boldsymbol{z}) \nabla p(\boldsymbol{z}) d\boldsymbol{z} = - \int_{\mathbb{R}^M} p(\boldsymbol{z}) \nabla h(\boldsymbol{z}) d\boldsymbol{z}.$$

We have therefore the identity

$$\mathbb{E}_{Z \sim p}[h(Z)\nabla \log p(Z)] = -\mathbb{E}_{Z \sim p}[\nabla h(Z)].$$

Importantly, contrary to the SFE estimator from Section 11.3, this identity uses gradients with respect to $\boldsymbol{z}$, not with respect to the parameters of the distribution. Nevertheless, using the reparametrization

$h(\boldsymbol{z}) \coloneqq f(\boldsymbol{\mu} + \sigma \cdot \boldsymbol{z})$, we have $\nabla h(\boldsymbol{z}) = \nabla f(\boldsymbol{\mu} + \sigma \cdot \boldsymbol{z}) \cdot \sigma$ so that

$$
\begin{aligned}
\nabla f_\sigma(\boldsymbol{\mu}) &= \nabla_{\boldsymbol{\mu}} \mathbb{E}_{U \sim p_{\boldsymbol{\mu}, \sigma}}[f(U)] \\
&= \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[\nabla f(\boldsymbol{\mu} + \sigma \cdot Z)] \quad \text{(reparametrization trick)} \\
&= -\mathbb{E}_{Z \sim p_{\mathbf{0},1}}[h(Z) \nabla \log p(Z)/\sigma] \\
&= \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[h(Z) \nabla \nu(Z)/\sigma] \\
&= \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[f(\boldsymbol{\mu} + \sigma \cdot Z) \nabla \nu(Z)/\sigma] \quad \text{(score function estimator)}
\end{aligned}
$$

Essentially, integration by parts allowed us to convert the reparametrization trick estimator into the SFE estimator. For more applications of integration by parts in machine learning, see Francis Bach's excellent blog post.

13.4.5 Variance reduction and evolution strategies

As discussed in Chapter 11, the SFE suffers from high variance. We now apply variance reduction techniques to it. To do so, we assume that $\nabla \nu(Z)$ has zero mean for $Z \sim p_{\mathbf{0},1}$. This assumption for example holds for Gaussian or centered Gumbel noise distributions. This assumption implies that

$$
\mathbb{E}_{Z \sim p_{\mathbf{0},1}}[f(\boldsymbol{\mu}) \nabla \nu(Z)/\sigma] = f(\boldsymbol{\mu}) \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[\nabla \nu(Z)/\sigma] = \mathbf{0}
$$

and therefore

$$
\nabla f_\sigma(\boldsymbol{\mu}) = \mathbb{E}_{Z \sim p_{\mathbf{0},1}}\left[(f(\boldsymbol{\mu} + \sigma \cdot Z) - f(\boldsymbol{\mu})) \nabla \nu(Z)/\sigma\right]. \qquad (13.7)
$$

This is an example of **control variate** discussed in Section 11.3. This can be interpreted as using a **finite difference** for computing a directional derivative in the **random direction** Z (see "limit case" below). Inspired by a **central finite difference**, we can also use

$$
\nabla f_\sigma(\boldsymbol{\mu}) = \mathbb{E}_{Z \sim p_{\mathbf{0},1}}\left[(f(\boldsymbol{\mu} + \sigma \cdot Z) - f(\boldsymbol{\mu} - \sigma \cdot Z)) \nabla \nu(Z)/(2\sigma)\right].
$$

These estimators have been used as part of blackbox (zero-order) optimization algorithms, such as **evolution strategies** (Salimans *et al.*, 2017) or **random gradient-free optimization** (Nesterov and Spokoiny, 2017). For quadratic functions, it is easy to show that the second estimator achieves lower variance (Recht and Frostig, 2017). The

idea of sampling both Z and $-Z$ simultaneously is called antithetic (Geweke, 1988) or mirrored sampling (Brockhoff *et al.*, 2010). Evolution strategies have also been used to obtain unbiased gradient estimators of partially unrolled computational graphs (Vicol *et al.*, 2021).

13.4.6 Zero-temperature limit

We now discuss the limit case $\sigma \to 0$. That is, we assume that we do **not** want to perform smoothing and that ∇f exists. We recall that the directional derivative of f at $\boldsymbol{\mu}$ in the direction $\boldsymbol{z}$ is

$$\begin{aligned} \partial f(\boldsymbol{\mu})[\boldsymbol{z}] &= \langle \nabla f(\boldsymbol{\mu}), \boldsymbol{z} \rangle \\ &= \lim_{\sigma \to 0} \left[f(\boldsymbol{\mu} + \sigma \cdot \boldsymbol{z}) - f(\boldsymbol{\mu}) \right] / \sigma. \end{aligned}$$

When $\sigma \to 0$ and Z follows the standard Gaussian distribution, meaning that $\nabla \nu(\boldsymbol{z}) = \boldsymbol{z}$, Eq. (13.7) therefore becomes

$$\begin{aligned} \nabla f_\sigma(\boldsymbol{\mu}) &= \mathbb{E}_{Z \sim p_{\mathbf{0},1}} \left[\partial f(\boldsymbol{\mu})[Z] \nabla \nu(Z) \right] \\ &= \mathbb{E}_{Z \sim p_{\mathbf{0},1}} \left[\partial f(\boldsymbol{\mu})[Z] Z \right] \\ &= \mathbb{E}_{Z \sim p_{\mathbf{0},1}} \left[\langle \nabla f(\boldsymbol{\mu}), Z \rangle Z \right] \\ &= \mathbb{E}_{Z \sim p_{\mathbf{0},1}} \left[\nabla f(\boldsymbol{\mu}) Z Z^\top \right] \\ &= \nabla f(\boldsymbol{\mu}). \end{aligned}$$

This should not be too surprising, as we already know from the convolution perspective that $f_\sigma(\boldsymbol{\mu}) = (f * \kappa_\sigma)(\boldsymbol{\mu}) \to f(\boldsymbol{\mu})$ when $\sigma \to 0$. This recovers the randomized forward-mode estimator already presented in Section 7.7.

13.5 Gumbel tricks

13.5.1 The Gumbel distribution

The Gumbel distribution is a distribution frequently used in extreme value theory. It arises naturally as the distribution of the logarithm of a negative exponential family. We consider its centered version with PDF

$$p(z) = \exp(-\nu(z)),$$

where

$$\nu(z) = z + \gamma + \exp(-(z + \gamma)),$$

and where $\gamma \approx 0.577$ is Euler's constant. We extend it to a multivariate distribution by taking M independent centered Gumbel distributions $Z = (Z_1, \ldots, Z_m)$ with associated location-scale family

$$\boldsymbol{\mu} + \sigma Z \sim p_{\boldsymbol{\mu}, \sigma},$$

and $p_{\mathbf{0}, 1} = p$. As $\mathbb{E}_{Z \sim p_{\mathbf{0}, 1}}[\nabla \nu(Z)] = \mathbf{0}$, we can use the Gumbel noise as an alternative to the Gaussian noise used in Section 13.4. Thankfully, in particular cases, we can compute closed-form expressions of the expectation.

> **Remark 13.2** (Sampling Gumbel noise). If $U \sim \mathrm{Uniform}(0, 1)$, then $Z := -\log(-\log(U))$ satisfies $Z \sim \mathrm{Gumbel}(0, 1)$.

> **Remark 13.3** (Link between Gumbel and exponential distribution). A random variable Z is distributed as a $p_{\mu, 1}$ Gumbel distribution if and only if $\exp(-Z)$ is distributed as an exponential distribution $\mathrm{Exp}(\exp(\mu - \gamma))$. To see this, one can simply compute the CDF of $\exp(-Z)$ and recognize the CDF of $\mathrm{Exp}(\exp(\mu - \gamma))$. Therefore, when comparing Gumbel distributions we can use standard properties of the exponential distribution.

13.5.2 Perturbed comparison

To start with, the Gumbel distribution can be used to smooth a binary comparison like the greater than or equal operators. Recall that the latter is defined for any $\mu_1, \mu_2 \in \mathbb{R}$ as

$$\mathrm{gt}(\mu_1, \mu_2) := \begin{cases} 1 & \text{if } \mu_1 \geq \mu_2 \\ 0 & \text{if } \mu_1 < \mu_2 \end{cases} = \mathrm{step}(\mu_1 - \mu_2),$$

where step is the Heaviside function. As shown below, by perturbing each variable with Gumbel noise, we recover $\mathrm{logistic}(a - b) = 1/(1 + e^{-(a-b)})$ as an approximation of $\mathrm{step}(a - b)$.

Proposition 13.3 (Gumbel trick for binary variables). Let $Z_1, Z_2 \sim \mathrm{Gumbel}(0, 1)$ be independent random variables. The difference of their location-scale transform (Section 11.4.1) is distributed according to a logistic distribution (Remark 3.1), i.e.,

$$\mu_1 + \sigma Z_1 - (\mu_2 + \sigma Z_2) \sim \mathrm{Logistic}(\mu_2 - \mu_1, \sigma),$$

for $\mu_1, \mu_2 \in \mathbb{R}$ and $\sigma > 0$. In particular, we have

$$\mathbb{E}[\mathrm{gt}(\mu_1 + \sigma Z_1, \mu_2 + \sigma Z_2)] = \frac{1}{1 + e^{-(\mu_1 - \mu_2)/\sigma}}.$$

Proof. We first derive the CDF of $\mu_1 + \sigma Z_1 - (\mu_2 + \sigma Z_2)$ as

$$\mathbb{P}(\mu_1 + \sigma Z_1 - (\mu_2 + \sigma Z_2) \le t) = \mathbb{P}\left(\mu_1/\sigma + Z_1 \le (\mu_2 + t)/\sigma + Z_2\right)$$

$$= \mathbb{P}\left(e^{-(\mu_1/\sigma + Z_1)} \ge e^{-((\mu_2 + t)/\sigma + Z_2)}\right).$$

By Remark 13.3, $e^{-(\mu_1/\sigma + Z_1)} \sim \mathrm{Exp}(\exp(\mu_1/\sigma - \gamma))$, and similarly for $e^{-(\mu_2 + t)/\sigma + Z_2}$. Now one easily shows that if $U \sim \mathrm{Exp}(u), V \sim \mathrm{Exp}(v)$ independent, then $\mathbb{P}(U \le V) = u/(u + v)$. Hence, we get

$$\mathbb{P}(\mu_1 + \sigma Z_1 - (\mu_2 + \sigma Z_2) \le t) = \frac{e^{(\mu_2 + t)/\sigma - \gamma}}{e^{(\mu_2 + t)/\sigma - \gamma} + e^{\mu_1/\sigma - \gamma}}$$

$$= \frac{1}{1 + e^{-(t - (\mu_2 - \mu_1))/\sigma}}.$$

We recognize the CDF of the logistic distribution with mean $\mu_2 - \mu_1$ and scale σ, denoted $\mathrm{Logistic}(\mu_2 - \mu_1, \sigma)$. For the last claim, we simply have that

$$\mathbb{E}[\mathrm{gt}(\mu_1 + \sigma Z_1, \mu_2 + \sigma Z_2)] = \mathbb{E}\left[\mathrm{step}(\mu_1 + \sigma Z_1 - (\mu_2 + \sigma Z_2)\right]$$

$$= \mathbb{P}(\mu_1 + \sigma Z_1 - (\mu_2 + \sigma Z_2) \ge 0)$$

$$= \frac{1}{1 + e^{-(\mu_1 - \mu_2)/\sigma}}.$$

$$\square$$

13.5.3 Perturbed argmax

Suppose we want to smooth

$$\boldsymbol{y}(\boldsymbol{u}) := \underset{\boldsymbol{y} \in \{\boldsymbol{e}_1, \dots, \boldsymbol{e}_M\}}{\arg\max} \langle \boldsymbol{y}, \boldsymbol{u} \rangle = \phi(i(\boldsymbol{u})),$$

where

$$i(\boldsymbol{u}) := \arg\max_{i \in [M]} u_i$$

$$\phi(i) := \boldsymbol{e}_i$$

with $\phi(i)$ is the one-hot encoding of $i \in [M]$. It turns out that the function $\boldsymbol{y}(\boldsymbol{u})$ perturbed using Gumbel noise enjoys a closed form expectation, which is nothing else than the softargmax.

Proposition 13.4 (Gumbel trick for categorical variables). Given M independent Gumbel random variables $Z \sim p_{\boldsymbol{0},1}$, define

$$Y := i(\boldsymbol{\mu} + \sigma \cdot Z) \in [M],$$

for $\boldsymbol{\mu} \in \mathbb{R}^M$ and $\sigma > 0$. Then, Y is distributed according to

$$q_{\boldsymbol{\mu},\sigma} := \mathrm{Categorical}(\mathrm{softargmax}(\boldsymbol{\mu}/\sigma)).$$

Moreover, we have

$$\begin{aligned}
\boldsymbol{y}_\sigma(\boldsymbol{\mu}) &= \mathbb{E}_{Z \sim p_{\boldsymbol{0},1}}[\boldsymbol{y}(\boldsymbol{\mu} + \sigma \cdot Z)] \\
&= \mathbb{E}_{Y \sim q_{\boldsymbol{\mu},\sigma}}[\phi(Y)] \\
&= \mathrm{softargmax}(\boldsymbol{\mu}/\sigma).
\end{aligned}$$

Proof. For $k \in [M]$, we have that

$$\begin{aligned}
\mathbb{P}(Y = k) &= \mathbb{P}\left(\arg\max_{i \in [M]}\{\mu_i + \sigma Z_i\} = k\right) \\
&= \mathbb{P}\left(\arg\min_{i \in [M]}\{e^{-\mu_i/\sigma - Z_i}\} = k\right)
\end{aligned}$$

By Remark 13.3, we have that $e^{-\mu_i/\sigma - Z_i} \sim \mathrm{Exp}(\exp(\mu_i/\sigma - \gamma))$. One easily verifies as an exercise, that, for $U_1, \ldots, U_M$ independent exponential variables with parameters $u_1, \ldots, u_m$, we have $\mathbb{P}(\arg\min_{i \in [M]}\{U_i\} = k) = u_k/\sum_{i=1}^M u_i$. Hence, we get

$$\mathbb{P}(Y = k) = \frac{\exp(\mu_k/\sigma)}{\sum_{i=1}^M \exp(\mu_i/\sigma)},$$

that is,
$$Y \sim \text{Categorical}(\text{softargmax}(\boldsymbol{\mu}/\sigma)).$$
The last claim follows from the distribution of Y and the definition of ϕ. □

13.5.4 Perturbed max

A similar result holds if we now wish to perturb the max instead of the argmax.

> **Proposition 13.5** (Link to log-sum-exp). Given M independent Gumbel random variables $Z \sim p_{\mathbf{0},1}$, and,
>
> $$f(\boldsymbol{u}) := \max_{i \in [M]} u_i,$$
>
> the random variable
>
> $$V := f(\boldsymbol{\mu} + \sigma \cdot Z).$$
>
> is distributed according to
>
> $$q_{\boldsymbol{\mu},\sigma} := p_{\sigma \text{LSE}(\boldsymbol{\mu}/\sigma),\sigma}.$$
>
> Moreover, we have
>
> $$f_\sigma(\boldsymbol{\mu}) = \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[f(U + \sigma \cdot Z)] = \mathbb{E}_{V \sim q_{\boldsymbol{\mu},\sigma}}[V] = \sigma \cdot \text{LSE}(\boldsymbol{\theta}/\sigma).$$

Proof. We derive the CDF of $f(\boldsymbol{\mu} + \sigma \cdot Z)$ as

$$\mathbb{P}(\max_{i \in [M]}\{\mu_i + \sigma Z_i\} \le t) = \mathbb{P}\left(\min_{i \in [M]}\{e^{-(\mu_i/\sigma - Z_i)}\} \ge e^{-t/\sigma}\right)$$

We have $e^{-(\mu_i/\sigma - Z_i)} \sim \text{Exp}(\exp(\mu_i/\sigma_i) - \gamma)$ and for $U_1, \ldots, U_M$ independent exponential random variables with parameters u_i, $\min_{i \in [M]} U_i \sim \text{Exp}(\sum_{i=1}^M u_i)$. Hence,

$$\mathbb{P}\left(\max_{i \in [M]}\{\mu_i + \sigma Z_i\} \le t\right) = \exp\left(-\sum_{i=1}^M (\exp(\mu_i/\sigma - \gamma))\exp(-t/\sigma)\right)$$

$$= \exp(-\exp(-(t - \sigma\text{LSE}(\boldsymbol{\mu}/\sigma))/\sigma - \gamma)).$$

We recognize the CDF of the centered Gumbel distribution with location-scale parameters $\sigma \mathrm{LSE}(\boldsymbol{\mu}/\sigma)$, σ. $\qquad\square$

For further reading on the Gumbel trick, see Tim Vieira's great blog.

13.5.5 Gumbel trick for sampling

The Gumbel trick is also useful in its own right for **sampling** without computing the normalization constant of the softargmax. Indeed, Proposition 13.4 ensures that if Z is Gumbel noise, then Y is distributed according to Categorical(softargmax($\boldsymbol{\mu}/\sigma$)). Computing the arg-maximum, as required to compute Y, can be done in one pass. Therefore, we obtain a one-pass algorithm to sample directly from the logits $\boldsymbol{\mu}$, without explicitly computing the probabilities softargmax($\boldsymbol{\mu}/\sigma$).

One may wonder whether such trick could also be used with the normal distribution. Unfortunately, there is no closed form in this case because it would require integrating the CDF of the maximum of $M-1$ Gaussian distributions. However, other tricks can be defined such as using Weibull distributions, see Balog *et al.* (2017).

13.5.6 Perturb-and-MAP

Previously, we discussed the Gumbel trick in the classification setting, where $\mathcal{Y} = [M]$. In the structured prediction setting, outputs are typically embedded in $\mathbb{R}^M$ but the output space is very large. That is, $\mathcal{Y} \subseteq \mathbb{R}^M$ but $|\mathcal{Y}| \gg M$. Structured outputs are then decoded using a maximum a-posteriori (MAP) oracle

$$f(\boldsymbol{u}) := \max_{\boldsymbol{y} \in \mathcal{Y}} \langle \boldsymbol{y}, \boldsymbol{u} \rangle$$

$$\boldsymbol{y}(\boldsymbol{u}) := \arg\max_{\boldsymbol{y} \in \mathcal{Y}} \langle \boldsymbol{y}, \boldsymbol{u} \rangle.$$

For this setting, the perturbed versions of f and $\boldsymbol{y}$,

$$f_\sigma(\boldsymbol{\mu}) := \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[f(\boldsymbol{\mu} + \sigma \cdot Z)]$$

$$\boldsymbol{y}_\sigma(\boldsymbol{\mu}) := \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[\boldsymbol{y}(\boldsymbol{\mu} + \sigma \cdot Z)],$$

no longer enjoy a closed form in general. However, we can approximate them using Monte-carlo estimation. For the gradient of $\nabla f_\sigma(\boldsymbol{\mu})$, two estimators exist (Abernethy *et al.*, 2016; Berthet *et al.*, 2020).

Proposition 13.6 (Gradient of perturbed max). Let $\mathcal{Y} \subseteq \mathbb{R}^M$ and $p_{\mathbf{0},1}$ be a noise distribution with density

$$p_{\mathbf{0},1}(\boldsymbol{z}) := \exp(-\nu(\boldsymbol{z}))/C.$$

Then, $f_\sigma(\boldsymbol{\mu})$ is smooth, and its gradient is given by

$$\begin{aligned}
\nabla f_\sigma(\boldsymbol{\mu}) &= \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[\boldsymbol{y}(\boldsymbol{\mu} + \sigma \cdot Z)] \\
&= \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[f(\boldsymbol{\mu} + \sigma \cdot Z)\nabla\nu(Z)\sigma] \\
&\in \mathrm{conv}(\mathcal{Y}).
\end{aligned}$$

We therefore have $\nabla f_\sigma(\boldsymbol{\mu}) = \boldsymbol{y}_\sigma(\boldsymbol{\mu})$.

The first estimator is simply a consequence of the reparametrization trick seen in Eq. (13.5) and of $\boldsymbol{y} = \nabla f$, which follows from Danskin's theorem (see Section 10.2). The second estimator is just SFE seen in Eq. (13.6). The first estimator usually has lower variance, as it uses more information, namely that $\boldsymbol{y} = \nabla f$.

The Jacobian of $\boldsymbol{y}_\sigma(\boldsymbol{\mu})$ also has two estimators (Abernethy *et al.*, 2016; Berthet *et al.*, 2020).

Proposition 13.7 (Jacobian of perturbed argmax). Under the same notation as in Proposition 13.6, we have

$$\begin{aligned}
\partial \boldsymbol{y}_\sigma(\boldsymbol{\mu}) &= \mathbb{E}_{Z \sim p_{\mathbf{0},1}}\left[\boldsymbol{y}(\boldsymbol{\mu} + \sigma Z)\nabla\nu(Z)^\top/\sigma\right] \\
&= \mathbb{E}_{Z \sim p_{\mathbf{0},1}}\left[f(\boldsymbol{\mu} + \sigma Z)\left(\nabla\nu(Z)\nabla\nu(Z)^\top - \nabla^2\nu(Z)\right)/\sigma^2\right].
\end{aligned}$$

The first estimator uses SFE. The second estimator is obtained by differentiating through

$$\boldsymbol{y}_\sigma(\boldsymbol{\mu}) = \nabla f_\sigma(\boldsymbol{\mu}) = \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[f(\boldsymbol{\mu} + \sigma \cdot Z)\nabla\nu(Z)/\sigma].$$

The first estimator usually has lower variance. Note that we cannot use the reparametrization trick this time, since $\boldsymbol{y}$ is discontinuous, contrary to f.

Link between perturbation and regularization

As shown in (Berthet *et al.*, 2020, Proposition 2.2), assuming $\mathcal{Y}$ is a convex polytope with non-empty interior and p has a strictly positive density, the function

$$f_\sigma(\boldsymbol{\mu}) \coloneqq \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[f(\boldsymbol{\mu} + \sigma \cdot Z)] = \mathbb{E}_{Z \sim p_{\mathbf{0},1}}[\max_{\boldsymbol{y} \in \mathcal{Y}}\langle \boldsymbol{\mu} + \sigma \cdot Z, \boldsymbol{y}\rangle]$$

is strictly convex and its convex conjugate $f_\sigma^*(\boldsymbol{y})$ is Legendre-type. We can therefore rewrite $f_\sigma(\boldsymbol{\mu})$ from the regularization perspective as

$$f_\sigma(\boldsymbol{\mu}) = \max_{\boldsymbol{y} \in \mathcal{Y}}\langle \boldsymbol{\mu}, \boldsymbol{y}\rangle - f_\sigma^*(\boldsymbol{y}).$$

and $\nabla f_\sigma(\boldsymbol{\mu}) = \boldsymbol{y}_\sigma(\boldsymbol{\mu})$ is a **mirror map**, a one-to-one mapping from $\mathbb{R}^M$ to the interior of $\mathcal{Y}$. Unfortunately, $f_\sigma^*(\boldsymbol{y})$ does not enjoy a closed form in general. Conversely, does any regularization has a corresponding noise distribution? The reciprocal is not true.

13.5.7 Gumbel-softmax

Suppose we want to smooth out the **composition** $h(\boldsymbol{u}) \coloneqq g(\boldsymbol{y}(\boldsymbol{u}))$ by

$$h_\sigma(\boldsymbol{\mu}) \coloneqq \mathbb{E}_{Z \sim p_{\mathbf{0},1}}\left[g(\boldsymbol{y}(\boldsymbol{\mu} + \sigma Z))\right]$$

where

$$\boldsymbol{y}(\boldsymbol{u}) \coloneqq \arg\max_{\boldsymbol{y} \in \{e_1,\ldots,e_M\}} \langle \boldsymbol{y}, \boldsymbol{u}\rangle.$$

This is useful to compute the expectation of a loss (instead of the loss of an expectation). To compute the gradient of $h_\sigma(\boldsymbol{\mu})$, we can readily use SFE. However, we saw that it suffers from high variance. Unfortunately, we cannot use the reparametrization trick here, since $\boldsymbol{y}(\boldsymbol{u})$ is a discontinuous function.

The key idea of the Gumbel-sofmax (Jang *et al.*, 2016; Maddison *et al.*, 2016) is to replace $\boldsymbol{y}(\boldsymbol{u})$ with a softargmax (with temperature parameter τ) to define

$$h_{\sigma,\tau}(\boldsymbol{\mu}) \coloneqq \mathbb{E}_{Z \sim p_{\mathbf{0},1}}\left[g(\text{softargmax}_\tau(\boldsymbol{\mu} + \sigma Z))\right].$$

Since the softargmax is a regularized argmax, we can see the Gumbel-softmax approach as using **both** regularization and perturbation. The

key benefit is that we can now use the reparametrization trick to get an unbiased estimator of $\nabla h_{\sigma,\tau}(\boldsymbol{\mu})$. However, this will be a **biased** estimator of $\nabla h_\sigma(\boldsymbol{\mu})$, the amount of bias being controlled by the temperature τ. In particular, in the limit case $\tau \to 0$, we have $h_{\sigma,\tau}(\boldsymbol{\mu}) \to h_\sigma(\boldsymbol{\mu})$. One caveat, however, is that the function g needs to be well defined on $\triangle^M$, instead of $\{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_M\}$.

The use of the softargmax transformation defines a continuous distribution (Jang *et al.*, 2016; Maddison *et al.*, 2016), that we now explain with $\sigma = 1$.

Proposition 13.8 (Gumbel-softargmax / Concrete distributions). Let us define the **continuous** random variable

$$T \coloneqq \operatorname{softargmax}_\tau(\boldsymbol{\mu} + Z) \in \triangle^M,$$

where $Z \sim p_{\mathbf{0},1}$ is a Gumbel random variable. Then T is distributed according to a distribution with density

$$p_{\boldsymbol{\mu},\tau}(\boldsymbol{t}) \coloneqq \Gamma(M)\tau^{M-1}\left(\sum_{i=1}^M \frac{\pi_i}{t_i^\tau}\right)^{-M}\prod_{i=1}^M \frac{\pi_i}{t_i^{\tau+1}},$$

where $\boldsymbol{\pi} \coloneqq \operatorname{softargmax}(\boldsymbol{\mu})$.

We can extend the Gumbel softargmax to the structured setting by replacing

$$\boldsymbol{y}(\boldsymbol{u}) \coloneqq \arg\max_{\boldsymbol{y} \in \mathcal{Y}}\langle \boldsymbol{y}, \boldsymbol{u}\rangle,$$

with its regularized variant (Paulus *et al.*, 2020). Similarly as before, one caveat is that g needs to be well defined on $\operatorname{conv}(\mathcal{Y})$ instead of $\mathcal{Y}$. Moreover, regularizing $\boldsymbol{y}$ is not always easy computationally.

13.6   Summary

We studied smoothing techniques based on function convolution with a kernel. Due to the commutativity of the convolution, we can alternatively see these as the expectation of the function, perturbed with noise, assuming the kernel corresponds to the PDF of some noise distribution. Their gradients can be estimated using the path gradient estimator

(PGE) or score function estimator (SFE), depending on whether the gradient of the original function is available or not. We saw that Stein's lemma is a special case of SFE used with Gaussian noise. The so-called "evolution strategies" are just a variant of that with variance reduction and can be interpreted as randomized finite difference. When using Gumbel noise, we were able to derive closed-form expressions for the expectation in specific cases: perturbed comparison, perturbed argmax and perturbed max.

We also studied the connections between smoothing by optimization and smoothing by integration. Infimal convolution is the counterpart of convolution, and the Legendre-Fenchel transform is the counterpart of Fourier and Laplace's transforms. Infimal convolution uses a min-plus algebra in the log domain, while the convolution uses a sum-product algebra in the exponential domain.

Part V

Optimizing differentiable programs

14

Optimization basics

14.1 Objective functions

Consider a function L, for example evaluating the error or "loss" $L(\boldsymbol{w})$ achieved by a model with parameters $\boldsymbol{w} \in \mathcal{W}$, where $\mathcal{W} = \mathbb{R}^P$. To find the best possible model parameterization, we seek to minimize $L(\boldsymbol{w})$, that is, to compute approximately

$$L^\star := \inf_{\boldsymbol{w} \in \mathcal{W}} L(\boldsymbol{w}),$$

assuming that the infimum exists (i.e., $L(\boldsymbol{w})$ is lower bounded). We will denote a solution, if it exists, by

$$\boldsymbol{w}^\star \in \arg\min_{\boldsymbol{w} \in \mathcal{W}} L(\boldsymbol{w}) := \left\{ \boldsymbol{w} \in \mathcal{W} : L(\boldsymbol{w}) = \min_{\boldsymbol{w}' \in \mathcal{W}} L(\boldsymbol{w}') \right\}.$$

In general, an analytical solution is not available and computing such a minimum approximately requires an optimization algorithm. An optimization algorithm is an iterative procedure, which, starting from an initial point $\boldsymbol{w}^0$, outputs after t iterations a point $\boldsymbol{w}^t$ that approximates the minimum of L up to some accuracy ε, i.e.,

$$L(\boldsymbol{w}^t) - L^\star \leq \varepsilon. \tag{14.1}$$

14.2   Oracles

To produce iterates $\boldsymbol{w}^1, \boldsymbol{w}^2, \ldots$ that converge to a minimum, the algorithm naturally needs to have access to information about L. For example, the algorithm needs a priori to be able to evaluate L to know if it decreased its value or not. Such information about the function is formalized by the notion of **oracles** (Nemirovski and Yudin, 1983). Formally, oracles are procedures that an algorithm can call to access information about the objective $L(\boldsymbol{w})$ at any given point $\boldsymbol{w} \in \mathcal{W}$. We usually mainly consider the following three oracles.

- **Zero-order oracle:** evaluating the function $L(\boldsymbol{w}) \in \mathbb{R}$.
- **First-order oracle:** evaluating the gradient $\nabla L(\boldsymbol{w}) \in \mathcal{W}$ for L differentiable.
- **Second-order oracle:** evaluating the Hessian matrix $\nabla^2 L(\boldsymbol{w})$, or evaluating the Hessian-vector product (HVP) $\nabla^2 L(\boldsymbol{w})\boldsymbol{v} \in \mathcal{W}$, for L twice differentiable and any vector $\boldsymbol{v} \in \mathcal{W}$.

Given an oracle $\mathcal{O}$ for a function L, we can formally define an optimization algorithm as a procedure which computes the next iterate as a function of all past and current information. Formally, an algorithm $\mathcal{A}$ builds a sequence $\boldsymbol{w}^1, \ldots, \boldsymbol{w}^t$ from a starting point $\boldsymbol{w}^0$ as

$$\boldsymbol{w}^{t+1} := \mathcal{A}(\boldsymbol{w}^0, \ldots, \boldsymbol{w}^t, \mathcal{O}(\boldsymbol{w}^0), \ldots, \mathcal{O}(\boldsymbol{w}^t), \boldsymbol{\lambda}),$$

where $\boldsymbol{\lambda} \in \Lambda \subseteq \mathbb{R}^Q$ encapsulates some hyperparameters of the algorithm, such as the stepsize. Oftentimes, algorithms build the next iterate simply from the information collected at the current iterate, without using all past iterates. That is, they take the form $\boldsymbol{w}^{t+1} = \mathcal{A}(\boldsymbol{w}^t, \mathcal{O}(\boldsymbol{w}^t), \boldsymbol{\lambda})$. A classical example is the gradient descent algorithm, that uses a first-order oracle to compute iterates of the form

$$\boldsymbol{w}^{t+1} := \boldsymbol{w}^t - \gamma \nabla L(\boldsymbol{w}^t),$$

where the stepsize γ is a hyperparameter of the algorithm. The notion of oracle therefore delineates different classes of algorithms. For instance, we may consider zero-order algorithms or first-order algorithms.

14.3   Variational perspective of optimization algorithms

One of the most basic optimization algorithms is the **proximal point method**, which produces $\boldsymbol{w}^{t+1}$ from $\boldsymbol{w}^t$ by

$$\boldsymbol{w}^{t+1} := \arg\min_{\boldsymbol{w}\in\mathcal{W}} L(\boldsymbol{w}) + \frac{1}{2\gamma}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2.$$

In words, the next iterate is produces by solving a trade-off between minimizing the function L and staying close to $\boldsymbol{w}^t$. Unfortunately, the optimization problem involved in performing this parameter update is as difficult as the original optimization problem, making the proximal point method impractical.

As we shall see in Chapter 15 and Chapter 16, many optimization algorithms can be seen as an approximation of the proximal point method, in the sense that they solve

$$\boldsymbol{w}^{t+1} := \arg\min_{\boldsymbol{w}\in\mathcal{W}} \tilde{L}(\boldsymbol{w}, \boldsymbol{w}^t) + \frac{1}{2\gamma}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2.$$

or more generally

$$\boldsymbol{w}^{t+1} := \arg\min_{\boldsymbol{w}\in\mathcal{W}} \tilde{L}(\boldsymbol{w}, \boldsymbol{w}^t) + \frac{1}{\gamma}d(\boldsymbol{w}, \boldsymbol{w}^t),$$

where $\tilde{L}(\boldsymbol{w}, \boldsymbol{w}^t)$ is an approximation of $L(\boldsymbol{w})$ around $\boldsymbol{w}^t$ and $d(\boldsymbol{w}, \boldsymbol{w}')$ is some form of distance between $\boldsymbol{w}$ and $\boldsymbol{w}'$. Different choices of $\tilde{L}$ and d lead to different optimization algorithms, and to different trade-offs.

14.4   Classes of functions

When studying algorithms theoretically, stronger results can often be stated by restricting to certain classes of functions. We already covered continuous and differentiable functions in Chapter 2. We review a few important other classes in this section.

14.4.1   Lipschitz functions

Lipschitz continuity is a stronger form of continuity. Intuitively, a Lipschitz continuous function is limited in how fast it can change.

Definition 14.1 (Lipschitz-continuous functions). A function $g \colon \mathcal{W} \to \mathcal{F}$ is β-**Lipschitz continuous** if for all $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{W}$

$$\|g(\boldsymbol{w}) - g(\boldsymbol{v})\|_2 \leq \beta \|\boldsymbol{w} - \boldsymbol{v}\|_2.$$

Note that the definition is valid even for vector-valued functions.

With respect to arbitrary norms

Thanks to dual norms reviewed in Section 17.1, we can state a more general definition of Lipschitz continuity based on arbitrary norms, instead of the 2-norm. Moreover, we may consider Lipschitz-continuity over a subset of the input domain.

Definition 14.2 (Lipschitz continuous functions w.r.t. a norm). A function $g \colon \mathcal{W} \to \mathcal{F}$ is said to be β-Lipschitz w.r.t. a norm $\| \cdot \|$ over a set $\mathcal{C} \subseteq \mathcal{W}$ if for all $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{C}$

$$\|g(\boldsymbol{w}) - g(\boldsymbol{v})\|_* \leq \beta \|\boldsymbol{w} - \boldsymbol{v}\|.$$

When $\| \cdot \| = \| \cdot \|_2$, we recover Definition 14.1, since the 2-norm is dual to itself.

14.4.2   Smooth functions

A differentiable function L is said to be β-smooth if its gradients are β-Lipschitz continuous. Setting $g(\boldsymbol{w}) = \nabla L(\boldsymbol{w})$ in Definition 14.1, we obtain the following definition.

Definition 14.3 (Smooth functions). A differentiable function $L \colon \mathcal{W} \to \mathbb{R}$ is β-**smooth** for $\beta > 0$ if for all $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{W}$

$$\|\nabla L(\boldsymbol{w}) - \nabla L(\boldsymbol{v})\|_2 \leq \beta \|\boldsymbol{w} - \boldsymbol{v}\|_2.$$

Smoothness ensures that the information provided by the gradient at some $\boldsymbol{w}$ is meaningful in a neighborhood of $\boldsymbol{w}$, since its variations are upper-bounded. If the variations were not bounded, the gradient at $\boldsymbol{v}$

arbitrarily close to $\boldsymbol{w}$ could drastically change, rendering the information provided by a first-order oracle potentially useless.

Smoothness of a function can be interpreted as having a quadratic upper bound on the function as formalized below.

Proposition 14.1 (Smooth functions). If a differentiable function $L : \mathcal{W} \to \mathbb{R}$ is β-smooth then for all $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{W}$,

$$|L(\boldsymbol{w}) - L(\boldsymbol{v}) + \langle \nabla L(\boldsymbol{v}), \boldsymbol{w} - \boldsymbol{v} \rangle| \leq \frac{\beta}{2} \|\boldsymbol{w} - \boldsymbol{v}\|_2^2.$$

In particular, we have

$$L(\boldsymbol{w}) \leq L(\boldsymbol{v}) + \langle \nabla L(\boldsymbol{v}), \boldsymbol{w} - \boldsymbol{v} \rangle + \frac{\beta}{2} \|\boldsymbol{w} - \boldsymbol{v}\|_2^2.$$

Proof. This is shown by bounding $|L(\boldsymbol{v}) - L(\boldsymbol{w}) - \langle \nabla L(\boldsymbol{w}), \boldsymbol{v} - \boldsymbol{w} \rangle|$ using the integral representation of the objective along $\boldsymbol{w} - \boldsymbol{v}$, i.e., $|L(\boldsymbol{v}) - L(\boldsymbol{w}) - \langle \nabla L(\boldsymbol{w}), \boldsymbol{v} - \boldsymbol{w} \rangle| = |\int_0^1 \langle \nabla L(\boldsymbol{w} + s(\boldsymbol{v} - \boldsymbol{w})), \boldsymbol{v} - \boldsymbol{w} \rangle ds - \langle \nabla L(\boldsymbol{w}), \boldsymbol{v} - \boldsymbol{w} \rangle)| \leq \int_0^1 \|\nabla L(\boldsymbol{w} + s(\boldsymbol{v} - \boldsymbol{w})) ds - \nabla L(\boldsymbol{w})\|_2 \|\boldsymbol{v} - \boldsymbol{w}\|_2 \leq L \|\boldsymbol{w} - \boldsymbol{v}\|_2^2/2$, where the last inequality follows from the smoothness assumption and standard integration. $\square$

In other words, $L(\boldsymbol{w})$ is upper-bounded and lower-bounded around $\boldsymbol{v}$ by a quadratic function of $\boldsymbol{w}$. We will see in Section 15.1 that this characterization gives rise to a variational perspective on gradient descent.

With respect to arbitrary norms

We can generalize the definition of smoothness in Definition 14.3 to arbitrary norms.

Definition 14.4 (Smooth functions w.r.t. a norm). A function $L : \mathcal{W} \to \mathbb{R}$ is β-smooth w.r.t. a norm $\| \cdot \|$ over a set $\mathcal{C}$ if for all $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{C}$

$$\|\nabla L(\boldsymbol{w}) - \nabla L(\boldsymbol{v})\|_* \leq \frac{\beta}{2} \|\boldsymbol{w} - \boldsymbol{v}\|.$$

An equivalent characterization, generalizing Proposition 14.1 to arbitrary norms, is given below (see, e.g. Beck (2017, Theorem 5.8)).

Proposition 14.2 (Smooth functions w.r.t. a norm). If a differentiable function $L : \mathcal{W} \to \mathbb{R}$ is β-smooth w.r.t. a norm $\| \cdot \|$ over a set $\mathcal{C}$, then for all $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{C}$

$$| \underbrace{L(\boldsymbol{w}) - L(\boldsymbol{v}) - \langle \nabla L(\boldsymbol{v}), \boldsymbol{w} - \boldsymbol{v} \rangle}_{B_L(\boldsymbol{w},\boldsymbol{v})} | \leq \frac{\beta}{2} \|\boldsymbol{w} - \boldsymbol{v}\|^2,$$

where B_f is the Bregman divergence generated by f (Definition 17.2).

14.4.3 Convex functions

A convex function is a function such that its value on the average of two or more points is smaller than the average of the values of the functions at these points. This is illustrated in Figure 14.1 and formalized below.

Definition 14.5 (Convex functions). A function $L : \mathcal{W} \to \mathbb{R}$ is said to be **convex** if for all $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{W}$ and $\tau \in [0, 1]$

$$L(\tau \boldsymbol{w} + (1 - \tau)\boldsymbol{v}) \leq \tau L(\boldsymbol{w}) + (1 - \tau)L(\boldsymbol{v}).$$

The function L is **strictly convex** if the above inequality is strict for all $\boldsymbol{w} \neq \boldsymbol{v}$.

The above characterization can easily be generalized to multiple points. Namely, for $\boldsymbol{w}_1, \dots, \boldsymbol{w}_n \in \mathcal{W}$ and $\tau_1, \dots \tau_n \geq 0$ such that $\sum_{i=1}^{n} \tau_i = 1$ (that is, $\tau_1, \dots, \tau_n$ defines a probability distribution over $[n]$), we have if L is convex that

$$L \left(\sum_{i=1}^{n} \tau_i \boldsymbol{w}_i \right) \leq \sum_{i=1}^{n} \tau_i L(\boldsymbol{w}_i).$$

The point $\sum_{i=1}^{n} \tau_i \boldsymbol{w}_i$ is called a convex combination. This can be seen as comparing the function at the average point to the average of the values at theses points and can further be generalized to any random variable.

Proposition 14.3 (Jensen's inequality). A function $L\colon \mathcal{W} \to \mathbb{R}$ is convex if it satisfies **Jensen's inequality**, that is, for any random variable W on $\mathcal{W}$,

$$L(\mathbb{E}[W]) \leq \mathbb{E}[L(W)],$$

provided that the expectations are well-defined.

If the function considered is differentiable, an alternative characterization of convexity is to observe how linear approximations of the function lower bound the function. This is illustrated in Figure 14.1 and formalized below.

Definition 14.6 (Convex differentiable functions). A differentiable function $L : \mathcal{W} \to \mathbb{R}$ is convex if and only if for all $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{W}$

$$L(\boldsymbol{v}) \geq L(\boldsymbol{w}) + \langle \nabla L(\boldsymbol{w}), \boldsymbol{v} - \boldsymbol{w} \rangle.$$

The function L is strictly convex if and only if the above inequality is strict for any $\boldsymbol{w} \neq \boldsymbol{v}$.

The above characterization pinpoints the relevance of convex function in optimization: if we can find a point $\hat{\boldsymbol{w}}$ with null gradient, then we know that we have found the minimum as we have

$$\nabla L(\hat{\boldsymbol{w}}) = \boldsymbol{0} \implies \forall \boldsymbol{v} \in \mathbb{R}^P, \ L(\boldsymbol{v}) \geq L(\hat{\boldsymbol{w}}) \implies L(\hat{\boldsymbol{w}}) = L^\star.$$

This means that by having access to the gradient of the function or an approximation thereof, we have access to a sufficient criterion to know whether we found a global minimum. In the case of a gradient descent on a smooth function, convexity ensures convergence to a minimum at a sublinear rate as detailed below.

Finally, if the function is twice differentiable, convexity of a function can be characterized in terms of the Hessian of the function.

Proposition 14.4 (Convex twice differentiable functions). A twice differentiable function $L : \mathcal{W} \to \mathbb{R}$ is convex if and only if its Hessian is positive semi-definite,

$$\forall \boldsymbol{w} \in \mathcal{W}, \ \nabla^2 L(\boldsymbol{w}) \succeq 0, \text{ i.e., } \forall \boldsymbol{w}, \boldsymbol{v} \in \mathcal{W}, \ \langle \boldsymbol{v}, \nabla^2 L(\boldsymbol{w})\boldsymbol{v} \rangle \geq 0.$$

The function L is strictly convex if and only if the Hessian is positive-definite, $\forall \boldsymbol{w} \in \mathcal{W}$, $\nabla^2 L(\boldsymbol{w}) \succ 0$, i.e., $\forall \boldsymbol{w}, \boldsymbol{v} \in \mathcal{W}$, $\langle \boldsymbol{v}, \nabla^2 L(\boldsymbol{w})\boldsymbol{v} \rangle > 0$.

14.4.4 Strongly-convex functions

Convexity can also be strengthened by considering μ-strongly convex functions.

Definition 14.7 (Strongly-convex functions). A function $L : \mathcal{W} \to \mathbb{R}$ is μ-**strongly convex** for $\mu > 0$ if for all $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{W}$ and $\tau \in [0, 1]$

$$L(\tau \boldsymbol{w} + (1 - \tau)\boldsymbol{v}) \leq \tau L(\boldsymbol{w}) + (1 - \tau)L(\boldsymbol{v}) - \frac{\mu}{2}\tau(1 - \tau)\|\boldsymbol{w} - \boldsymbol{v}\|_2^2.$$

A differentiable function L is μ-strongly convex if and only if for all $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{W}$

$$L(\boldsymbol{v}) \geq L(\boldsymbol{w}) + \langle \nabla L(\boldsymbol{w}), \boldsymbol{w} - \boldsymbol{v} \rangle + \frac{\mu}{2}\|\boldsymbol{w} - \boldsymbol{v}\|_2^2.$$

A twice differentiable function is μ-strongly convex if and only if its Hessian satisfies

$$\forall \boldsymbol{w} \in \mathcal{W}, \ \nabla^2 L(\boldsymbol{w}) \succeq \mu \, \mathrm{I}, \text{ i.e., } \forall \boldsymbol{w}, \boldsymbol{v} \in \mathcal{W}, \ \langle \boldsymbol{v}, \nabla^2 L(\boldsymbol{w})\boldsymbol{v} \rangle \geq \mu\|\boldsymbol{v}\|_2^2.$$

The characterization of strong convexity for differentiable functions states that $L(\boldsymbol{w})$ is lower-bounded by a quadratic. This enables the design of linearly convergent algorithms as explained later. We naturally have the implications

$$L \text{ strongly convex} \implies L \text{ strictly convex} \implies L \text{ convex}.$$

With respect to arbitrary norms

A function can be strongly convex w.r.t. an arbitrary norm, simply by replacing the 2-norm in Definition 14.7 with that norm. For differentiable strongly convex functions, we have the following alternative characterization, generalizing Definition 14.7 to arbitrary norms.

> **Proposition 14.5** (Differentiable strongly-convex functions). If a differentiable function $L : \mathcal{W} \to \mathbb{R}$ is μ-strongly convex w.r.t. a norm $\|\cdot\|$ over a set $\mathcal{C}$, then for all $\boldsymbol{w}, \boldsymbol{v} \in \mathcal{C}$
>
> $$\frac{\mu}{2}\|\boldsymbol{w} - \boldsymbol{v}\|^2 \leq \underbrace{L(\boldsymbol{w}) - L(\boldsymbol{v}) - \langle \nabla L(\boldsymbol{v}), \boldsymbol{w} - \boldsymbol{v} \rangle}_{B_L(\boldsymbol{w}, \boldsymbol{v})}.$$

Obviously, if a function L is μ-strongly convex, then, λL is $(\mu\lambda)$-strongly convex. Because all norms are equivalent, if a function is strongly convex w.r.t. a norm, it is also strongly-convex w.r.t. another norm. However, stating the norm w.r.t. which strong convexity holds can lead to better constant μ (the higher, the better in terms of convergence rates of, e.g., a gradient descent). We also emphasize that it is important to mention over which set strong convexity holds. We give examples below.

> **Example 14.1** (Strongly convex functions). The function $f(\boldsymbol{u}) = \frac{1}{2}\|\boldsymbol{u}\|_2^2$ is 1-strongly convex w.r.t. $\|\cdot\|_2$ over $\mathbb{R}^M$.
>
> The function $f(\boldsymbol{u}) = \langle \boldsymbol{u}, \log \boldsymbol{u} \rangle$ is 1-strongly convex w.r.t. $\|\cdot\|_1$ over $\triangle^M$. More generally, $f(\boldsymbol{u})$ is $\frac{1}{\mu}$-strongly convex w.r.t. $\|\cdot\|_1$ over any bounded set $\mathcal{C} \subset \mathbb{R}_+^M$ such that $\mu = \sup_{\boldsymbol{u} \in \mathcal{C}} \|\boldsymbol{u}\|_1$ (Blondel, 2019). However, it is not strongly convex over $\mathbb{R}_+^M$, as it is not bounded.

14.4.5 Nonconvex functions

In general, the minimum of a function necessarily has a null gradient, that is,

$$\boldsymbol{w}^\star \in \arg\min_{\boldsymbol{w} \in \mathcal{W}} L(\boldsymbol{w}) \implies \nabla L(\boldsymbol{w}^\star) = 0.$$

To see this, consider the function $F : t \to L(\boldsymbol{w}^\star - t\nabla L(\boldsymbol{w}^*))$. If $\nabla L(\boldsymbol{w}^\star) \neq 0$, then $F'(0) = -\|\nabla L(\boldsymbol{w}^\star)\|_2^2 \neq 0$. Therefore, there exists a small $t > 0$ such that $F(t) < F(0)$, i.e., $L(\boldsymbol{w}^\star)$ is not the minimum. However, if the function is not convex, the converse is a priori not true: finding a point that has a null gradient does not ensure that we have found a global minimum as illustrated in Figure 14.2.
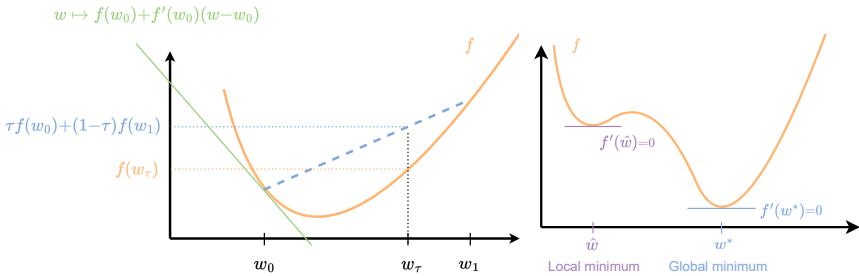
Figure 14.1: Convex function: any secant is above the function, any tangent is below the function, a point with zero gradient is a minimum.

Figure 14.2: Non-convex function: a point with zero gradient is not necessarily the global minimum.

For non-convex functions, a point with null gradient is called a **stationary point**. A stationary point may define a **local maximum** or a **local minimum**. Formally, $\hat{\boldsymbol{w}}$ is a local minimum if

$$\exists r > 0, \text{ s.t. } \forall \boldsymbol{v} \in \mathcal{W} \text{ satisfying } \|\boldsymbol{v} - \hat{\boldsymbol{w}}\| \le r, \text{ we have } L(\boldsymbol{v}) \ge L(\hat{\boldsymbol{w}}).$$

A local maximum is defined similarly, except that $L(\boldsymbol{v}) \le L(\hat{\boldsymbol{w}})$ in a neighborhood of $\hat{\boldsymbol{w}}$. For non-convex functions, convergence rates are therefore generally expressed in terms of convergence of the norm of the gradient $\|\nabla f(\boldsymbol{w}^t)\|_2$ towards 0. Such theoretical results do not ensure convergence to the global minimum but rather convergence to a point where no further progress may a priori be possible with just gradient information.

14.5   Performance guarantees

For a given class of functions, we can define the performance of an algorithm as the number of iterations the algorithm would need to find an ε-accurate solution as in Eq. (14.1). This is called the **computational complexity** of the algorithm, denoted

$$t = T(\varepsilon).$$

Alternatively, the performance of an algorithm can be stated in terms of **convergence rate**, i.e., the accuracy that the algorithm reaches

after t iterations,

$$\varepsilon = R(t),$$

where R is a decreasing positive function vanishing as $t \to +\infty$. Usually, R incorporates properties of the function minimized, such as its smoothness constant β and information on the initial point, such as its function value. The corresponding computational complexity $T(\varepsilon)$ is then given as the minimum number of iterations t such that $R(t) \leq \varepsilon$.

Convergence rates can generally be classified by considering the progress ratio on iteration t, defined by

$$\rho_t := \frac{L(\boldsymbol{w}^t) - L^\star}{L(\boldsymbol{w}^{t-1}) - L^\star}.$$

The asymptotic convergence rate is then defined by

$$\rho_\infty := \lim_{t \to +\infty} \rho_t.$$

We can classify the rates as follows.

1. **Sublinear convergence rates, $\rho_\infty = 1$:** the longer the algorithm runs, the slower it makes progress. That is, the relative progress eventually tends to stall as $t \to +\infty$. Examples of $R(t)$ in this category include $O(1/t), O(1/t^2)$ or more generally $O(1/t^\alpha)$ for some $\alpha > 0$. This is equivalent to $T(\varepsilon) = O(\varepsilon^{-1/\alpha})$.

2. **Linear convergence rates, $\rho_\infty = c \in (0,1)$:** the algorithm eventually reaches a state of constant relative progress at each iteration, leading to an overall rate $R(t) = O(\exp(-ct))$ for c depending on the properties of the objective. This corresponds to $T(\varepsilon) = O(c^{-1} \ln \varepsilon^{-1})$.

3. **Superlinear convergence rates, $\rho_\infty = 0$:** the relative progress is better at each new iteration. This can happen for, e.g., $R(t) = O(\exp(-t^2))$, leading to $T(\varepsilon) = O(\sqrt{\ln \varepsilon^{-1}})$ or $R(t) = O(\exp(-\exp(t)))$, also called a quadratic rate, leading to $T(\varepsilon) = O(\ln \ln \varepsilon^{-1})$.

The term linear may be misleading as the rates are in fact exponential. They are coined "linear" because of their behavior in log-scale.

Upper and lower bounds

The best performance of a class of algorithms equipped with a given oracle (e.g. first-order oracle) can be upper-bounded or lower-bounded. This allows to show that an algorithm with access limited to a certain type of oracle cannot theoretically do better than a certain number. For example, the computational complexity to minimize β-smooth functions restricted on $[0,1]^P$ with first-order oracles is lower bounded by $\frac{c}{\varepsilon^P}$ (Nemirovski and Yudin, 1983, p. 1.1.7). For example, with $P = 10$ and $\varepsilon = 10^{-3}$, this gives 10^{30} iterations. Note that these results are pessimistic by construction. The actual performance of an algorithm on a specific instance of this function class may be much better than this worst-case scenario, as it is the case with popular algorithms such as quasi-Newton methods. Better computational complexities can be achieved by further restricting the class of functions to the set of convex functions, which play a central role in optimization and many other fields.

Zero-order vs. first-order

For the class of smooth strongly convex functions, the computational complexity of the best first-order algorithm is (up to constant and logarithmic factors) P times better than that of the best zero-order algorithm (Nesterov, 2018; Nesterov and Spokoiny, 2017). This theoretical comparison shows that, while zero-order optimization algorithms may perform on par with first-order optimization algorithms for problems with a low dimension P, they can be much slower for high dimensional problems, i.e., $P \gg 1$.

In different settings, for example with stochastic oracles (Duchi *et al.*, 2015) or for different classes of functions, slightly different comparisons may be achieved, such as a $\sqrt{P}$ factor instead of P. However, the same conclusion holds in the current frameworks considered: first-order optimization algorithms can provide fast rates that are dimension independent while the rates of zero-order optimization algorithms generally depend on the dimension of the problem, making them unfit for high-dimensional problems.

This explains the immense success of first-order algorithms for training neural networks. Fortunately, using reverse-mode autodiff, as studied in Chapter 7, it can be shown that computing a gradient has roughly the same complexity as evaluating the function itself Section 7.3.3

14.6 Summary

The information available to us on a function can be formalized by the notion of **oracle**. Zero-order oracles can only evaluate the function; first-order oracles can also compute the gradient; second-order oracles can also compute the Hessian or the Hessian-vector product (HVP).

Most optimization algorithms reviewed in this book can be viewed from a **variational perspective**, in which the next iteration is produced by solving a trade-off between an approximation of the function and a proximity term. Different approximations and different proximity terms lead to different algorithms.

We also reviewed different classes of functions, and performance guarantees.

15

First-order optimization

15.1 Gradient descent

Gradient descent is one of the simplest algorithms in our toolbox to minimize a function. At each iteration, it moves along the negative gradient direction, scaled by a stepsize γ:

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \gamma \nabla L(\boldsymbol{w}^t). \tag{15.1}$$

15.1.1 Variational perspective

Consider the linear approximation of $L(\boldsymbol{w})$ around $\boldsymbol{w}^t$,

$$L(\boldsymbol{w}) \approx L(\boldsymbol{w}^t) + \langle \nabla L(\boldsymbol{w}^t), \boldsymbol{w} - \boldsymbol{w}^t \rangle.$$

One can easily check that the gradient descent update in Eq. (15.1) can be rewritten as the solution of a minimization problem, namely,

$$\boldsymbol{w}^{t+1} = \arg\min_{\boldsymbol{w} \in \mathcal{W}} L(\boldsymbol{w}^t) + \langle \nabla L(\boldsymbol{w}^t), \boldsymbol{w} - \boldsymbol{w}^t \rangle + \frac{1}{2\gamma} \|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2. \tag{15.2}$$

In words, a gradient descent update optimizes a trade-off between staying close to the current $\boldsymbol{w}^t$, thanks to the proximity term $\frac{1}{2\gamma}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2$, and minimizing the linearization of L around $\boldsymbol{w}^t$. Intuitively, by choosing γ

sufficiently small, we ensure that the minimizer of the regularized linear approximation stays in a neighborhood where the linear approximation is valid. This viewpoint is useful to motivate gradient descent extensions.

15.1.2 Convergence for smooth functions

As long as $\nabla L(\boldsymbol{w}^t) \neq \boldsymbol{0}$, the function $L_t(\gamma) \coloneqq L(\boldsymbol{w}^t - \gamma \nabla L(\boldsymbol{w}^t))$ has a negative derivative at 0, i.e., $L_t'(0) = -\|\nabla L(\boldsymbol{w}^t)\|_2^2$. Hence, as long as $\nabla L(\boldsymbol{w}^t) \neq \boldsymbol{0}$, there exists a stepsize ensuring a decrease in objective values at each iterate. However, without further assumptions, such a stepsize may depend on each iterate and may be infinitesimally small. To quantify the convergence of gradient descent with a constant stepsize, we restrict to the class of smooth functions. By applying Proposition 14.1 on the iterate of gradient descent, we obtain that

$$L(\boldsymbol{w}^{t+1}) \leq L(\boldsymbol{w}^t) - \gamma\|\nabla L(\boldsymbol{w}^t)\|_2^2 + \frac{\beta\gamma^2}{2}\|\nabla L(\boldsymbol{w}^t)\|_2^2.$$

Therefore, for β-smooth functions, by selecting $\gamma \leq \frac{1}{\beta}$, we get that

$$L(\boldsymbol{w}^{t+1}) - L(\boldsymbol{w}^t) \leq -\frac{\gamma}{2}\|\nabla L(\boldsymbol{w}^t)\|_2^2,$$

which illustrates the main mechanism behind gradient descent: each iteration decreases the objective by a constant times the norm of the gradient of the current iterate. This equation can further be summed over all iterates up to T. This telescopes the objective values, leading to

$$\begin{aligned}
\min_{t \in \{0,\ldots,T-1\}} \|\nabla L(\boldsymbol{w}^t)\|_2^2 &\leq \frac{1}{T}\sum_{t=0}^{T-1}\|\nabla L(\boldsymbol{w}^t)\|_2^2 \\
&\leq \frac{2}{\gamma T}\left(L(\boldsymbol{w}^0) - L(\boldsymbol{w}^T)\right) \\
&\leq \frac{2}{\gamma T}\left(L(\boldsymbol{w}^0) - L^\star\right),
\end{aligned}$$

where we recall that $L^\star$ is the infimum of L. Therefore, after sufficiently many iterations, gradient descent finds a point whose gradient norm is arbitrarily small.

Non-convex case

Without further assumptions, i.e., in the non-convex case, the above result (i.e., convergence to a stationary point, measured by the gradient norm) is the best we may get in theory. Denoting $T_s(\varepsilon)$ the number of iterations needed for a gradient descent to output a point that is ε-stationary, i.e., $\|\nabla L(\hat{\boldsymbol{w}})\|_2 \leq \varepsilon$, we have $T_s(\varepsilon) \leq O(\varepsilon^{-2})$.

Convex case

By adding a convexity assumption on the objective, we can use the lower bound provided by the convexity assumption to ensure convergence to a minimum. Namely, for a β-smooth and convex function f, and with stepsize $\gamma \leq 1/\beta$, we have that (Nesterov, 2018)

$$L(\boldsymbol{w}^T) - L^\star \leq \frac{1}{\gamma T}\|\boldsymbol{w}^0 - \boldsymbol{w}^\star\|_2^2.$$

That is, we get a sublinear convergence rate, and the associated computational complexity to find a minimum is $T(\varepsilon) = O(1/\varepsilon)$.

Strongly convex case

If we further strengthen the assumptions by considering β-smooth, μ-strongly convex functions, the convergence rate of a gradient descent can be shown to be (Nesterov, 2018), for any stepsize $\gamma \leq 1/\beta$,

$$\begin{aligned} L(\boldsymbol{w}^T) - L^\star &\leq (1 - \gamma\mu)^T \left(L(\boldsymbol{w}^0) - L^\star\right) \\ &\leq \exp\left(-\gamma\mu T\right)\left(L(\boldsymbol{w}^0) - L^\star\right). \end{aligned}$$

That is, we obtain a linear convergence rate and the associated computational complexity is $T(\varepsilon) = O(\ln \varepsilon^{-1})$. The above convergence rates may be further refined (Nesterov, 2018); we focused above on the simplest result for clarity.

Strong convexity can also be replaced by a weaker assumption, gradient-dominating property (Polyak, 1963), i.e., $\|\nabla L(\boldsymbol{v})\|_2^2 \geq c(L(\boldsymbol{v}) - L^\star)$ for some constant c and any $\boldsymbol{v} \in \mathcal{W}$. A convex, gradient-dominating function can also be minimized at a linear rate.

15.1.3   Momentum and accelerated variants

We started with gradient descent as a simple example of first-order optimization algorithm. However, different optimization algorithms can be designed from the access to first-order oracles and the knowledge of the class of functions considered. For example, consider quadratic convex functions $\boldsymbol{w} \mapsto \frac{1}{2}\boldsymbol{w}^\top \boldsymbol{A}\boldsymbol{w} + \boldsymbol{b}^\top \boldsymbol{w}$, that are a basic example of smooth strongly convex functions if $\boldsymbol{A}$ is positive definite. An optimal method in this case is the heavy-ball method of Polyak (1964), that can be written as

$$\boldsymbol{v}^{t+1} := \nu\boldsymbol{v}^t - \gamma\nabla L(\boldsymbol{w}^t)$$
$$\boldsymbol{w}^{t+1} := \boldsymbol{w}^t + \boldsymbol{v}^{t+1}.$$

The heavy-ball method uses an additional variable $\boldsymbol{v}^t$, that can be interpreted as the velocity of a ball driven by the negative gradient to converge towards a minimum. For $\nu = 0$, we recover usual gradient descent. For $\nu > 0$, the velocities accumulate a form of an inertia momentum, where ν is interpreted as the "mass" of the ball. In terms of convergence rates, the heavy-ball method can be shown to converge linearly similarly to gradient descent, but with a rate $O(\exp(-T\sqrt{\mu/\beta}))$ for appropriate choices of ν, γ. In comparison, by choosing an optimal stepsize for the gradient descent, its convergence rate is $O(\exp(-T\mu/\beta))$ which is provably worse, as we always have $\mu/\beta \leq 1$.

Beyond the case of quadratic functions, accelerated variants of gradient descent for convex or strongly convex functions have been developed by Nesterov (2018). Such variants have inspired the design of optimization algorithms in stochastic settings presented below.

15.2   Stochastic gradient descent

In machine learning, we are usually interested in minimizing the **expected loss** of the model over the data distribution ρ:

$$\min_{\boldsymbol{w}\in\mathcal{W}}\; L(\boldsymbol{w}) := \mathbb{E}_{S\sim\rho}\left[L(\boldsymbol{w}; S)\right].$$

For example, L is often set to $L(\boldsymbol{w}; S) := \ell(Y, f(X, \boldsymbol{w}))$, where ℓ is a loss function, f is a neural network and $S = (X, Y)$ is a random pair,

composed of an input X and an associated target Y, sampled from ρ. In this setting, since the data distribution ρ is generally unknown and may be infinite, we cannot exactly evaluate the expected loss $L(\boldsymbol{w})$ or its gradient $\nabla L(\boldsymbol{w})$.

In practice, we are often given a fixed dataset of n pairs $\boldsymbol{s}_i = (\boldsymbol{x}_i, \boldsymbol{y}_i)$. This is a special case of the expected loss setting, since this can be seen as a empirical distribution $\rho = \rho_n$

$$L(\boldsymbol{w}) = \mathbb{E}_{S \sim \rho_n}\left[L(\boldsymbol{w}; S)\right] = \frac{1}{n}\sum_{i=1}^{n} L(\boldsymbol{w}; (X_i, Y_i)).$$

The gradient of $L(\boldsymbol{w})$ is then

$$\nabla L(\boldsymbol{w}) := \frac{1}{n}\sum_{i=1}^{n} \nabla L(\boldsymbol{w}; (\boldsymbol{x}_i, \boldsymbol{y}_i)).$$

In this case, we see that the **full** gradient $\nabla L(\boldsymbol{w})$, as needed by gradient descent, is the average of the **individual** gradients. That is, the cost of computing $\nabla L(\boldsymbol{w})$ is proportional to the number of training points n. For n very large, that is a very large amount of samples, this computational cost can be prohibitive. Stochastic gradients circumvent this issue.

15.2.1   Stochastic gradients

Usually, even if we do not know ρ, we can sample from it, i.e., we have access to samples $S \sim \rho$ from ρ. We can then use a **stochastic gradient** of the form $\nabla L(\boldsymbol{w}; S)$ as a random estimate of $\nabla L(\boldsymbol{w})$. This may look like a rough estimate but, on average, this is a valid approximation since

$$\mathbb{E}_{S \sim p}\left[\nabla L(\boldsymbol{w}; S)\right] = \nabla L(\boldsymbol{w}).$$

We say that $\nabla L(\boldsymbol{w}; S)$ is an **unbiased estimator** of $\nabla L(\boldsymbol{w})$. To further improve the approximation, we may also consider **mini-batch** estimates by sampling $m \ll n$ data points $S_i := (X_i, Y_i)$ and using $\frac{1}{m}\sum_{i=1}^{m} \nabla L(\boldsymbol{w}; S_i)$, whose expectation still matches $\nabla L(\boldsymbol{w})$, while potentially reducing the approximation error by averaging multiple stochastic gradients. Computationally, the main advantage is that the cost is now proportional to m instead of n.

In whole generality, one can consider stochastic first-order oracles defined below.

> **Definition 15.1** (Stochastic first-order oracles). A **stochastic first-order oracle** of an expected objective $L(\boldsymbol{w})$ is a random estimate $g(\boldsymbol{w}; S)$ of $\nabla L(\boldsymbol{w})$ with S sampled according to some distribution q. A stochastic gradient is said to be an **unbiased estimator** if
>
> $$\mathbb{E}_{S \sim q}[g(\boldsymbol{w}; S)] = \nabla L(\boldsymbol{w}).$$
>
> The **variance** of a stochastic gradient is
>
> $$\mathbb{E}_{S \sim q}\left[\|g(\boldsymbol{w}; S) - \nabla L(\boldsymbol{w})\|_2^2\right].$$

When $q = \rho$, we recover stochastic gradients. When q is the product of m independent samples according to p, we recover mini-batch stochastic gradients. First-order stochastic optimization algorithms build upon stochastic first-order oracles to approximately find the minimum of the expected objective. In such a setting, the iterates of the algorithm are by definition random. Convergence rates therefore need to be expressed in probabilistic terms by considering for example the expected objective value according to the randomness of the oracles.

15.2.2 Vanilla SGD

Equipped with a stochastic first-order oracle, such as (mini-batch) stochastic gradients, we can define **stochastic gradient descent** as

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \gamma g(\boldsymbol{w}^t; S^t) \quad \text{where } S^t \sim q.$$

We assume that S^t is independent of $\boldsymbol{w}^t$. Compared to the usual gradient descent, the main impediment of the stochastic setting is the additional noise induced by the stochastic estimates: their variance.

For example, consider applying a stochastic gradient descent on the expectation of β-smooth convex functions $L(\boldsymbol{w}; \boldsymbol{s})$ with unbiased oracles. To harness the randomness of the iterates, consider after T iterations outputting the average of the first T iterates, that is $\bar{\boldsymbol{w}}^T := \frac{1}{T}\sum_{t=1}^{T} \boldsymbol{w}^t$. Moreover, suppose that the variance of the stochastic first-order oracles is bounded by σ^2 for all minimizers $\boldsymbol{w}^\star$ of L. Denoting by $\mathbb{E}_{S_0,\ldots,S_{T-1}}$ the randomness associated to the stochastic oracles, we have then that

for a stepsize $\gamma \leq 1/(4\beta)$, (Lan, 2012),

$$\mathbb{E}_{S_0,\ldots,S_{T-1}}[L(\bar{\boldsymbol{w}}^T)] - L^\star \leq \frac{1}{\gamma T}\|\boldsymbol{w}_0 - \boldsymbol{w}^\star\|_2^2 + 2\gamma\sigma^2.$$

The resulting convergence rate illustrates that a stochastic gradient descent converges to the minimum of the expected objective up to a constant term depending on the variance of the oracle and the stepsize. One can diminish the variance by considering mini-batches: if the variance of a single stochastic gradient is σ_1^2, considering a mini-batch of m gradients reduces the variance of the corresponding oracle to $\sigma_m = \sigma_1^2/m$. To decrease the additional term, one may also decrease the stepsizes over the iterations. For example, by choosing a decreasing stepsize like $\gamma^t = t^{-1/2}$, the convergence rate is then of the order $O((\|\boldsymbol{w}_0 - \boldsymbol{w}^\star\|_2^2 + \sigma^2 \ln t)/\sqrt(t))$. The stepsize can also be selected as a constant γ_0 that decreases the average objective for the first T_0 iterations and reduced by a multiplicative factor at regular intervals like $\gamma_j = \rho\gamma_{j-1}$ for $\rho \in (0,1)$ to handle iterations between T_j, T_{j+1}. Alternative stepsize schedules such as a cosine decay (Loshchilov and Hutter, 2016) have recently become popular.

The literature on alternative optimization schemes for stochastic optimization is still rapidly evolving, with new heuristics regularly proposed. We present below two popular techniques.

15.2.3 Momentum variants

Accelerated optimization algorithms developed in the deterministic setting may be extended to the stochastic setting. For example, the heavy-ball method can be adapted to the stochastic setting, leading to stochastic gradient descent with **momentum** (Sutskever *et al.*, 2013) generally implemented as

$$\boldsymbol{v}^{t+1} := \nu\boldsymbol{v}^t + \boldsymbol{g}(\boldsymbol{w}^t; S^t)$$
$$\boldsymbol{w}^{t+1} := \boldsymbol{w}^t - \gamma\boldsymbol{v}^{t+1}.$$

As mentioned earlier the momentum method can be modified to handle non-quadratic smooth strongly convex functions. This leads to Nesterov's accelerated method in the deterministic setting. This has

been adapted to the stochastic with a so-called **Nesterov momentum** (Sutskever *et al.*, 2013)

$$\boldsymbol{v}^{t+1} := \nu\boldsymbol{v}^t + \boldsymbol{g}(\boldsymbol{w}^t + \nu\boldsymbol{v}^t; S^t)$$
$$\boldsymbol{w}^{t+1} := \boldsymbol{w}^t - \gamma\boldsymbol{v}^{t+1}.$$

15.2.4 Adaptive variants

In any gradient descent-like algorithm, selecting the stepsize is key for good performance. While a constant stepsize may be used if the function is smooth, we may not know in advance the smoothness constant of the objective, which means that additional procedures may be required to select appropriately the stepsize. In the deterministic case, line-searches such as the Armijo or Wolfe's rules (Wright and Nocedal, 1999) can be used to check whether the selected stepsize decreases sufficiently the objective at each iteration. Such rules have be adapted in the stochastic setting (Vaswani *et al.*, 2019).

Another way to decrease the sensitivity of the algorithm with respect to the stepsize has been to estimate first and second-order moments of the gradients and use the latter as a form of preconditioning to smooth the trajectory of the iterates. This led to the popular **Adam** optimizer (Kingma and Ba, 2014). It takes the form,

$$\boldsymbol{m}^{t+1} := \nu_1\boldsymbol{m}^t + (1 - \nu_1)\boldsymbol{g}^t$$
$$\boldsymbol{v}^{t+1} := \nu_2\boldsymbol{v}^t + (1 - \nu_2)(\boldsymbol{g}^t)^2$$
$$\hat{\boldsymbol{m}}^{t+1} := \boldsymbol{m}^{t+1}/(1 - \nu_1^t)$$
$$\hat{\boldsymbol{v}}^{t+1} := \boldsymbol{v}^{t+1}/(1 - \nu_2^t)$$
$$\boldsymbol{w}^{t+1} := \boldsymbol{w}^t - \gamma\,\hat{\boldsymbol{m}}^{t+1}/\left(\sqrt{\hat{\boldsymbol{v}}^{t+1}} + \varepsilon\right),$$

where $\boldsymbol{g}^t := \boldsymbol{g}(\boldsymbol{w}^t; S^t)$, $(\boldsymbol{g}^t)^2$ denotes the element-wise square of $\boldsymbol{g}^t$ and $\nu_1, \nu_2, \gamma, \varepsilon$ are hyper-parameters of the algorithm. Numerous variants exist, such as varying the stepsize γ above along the iterations.

15.3   Projected gradient descent

Oftentimes, we seek to find the solution of a minimization problem subject to **constraints** on the variables, of the form

$$\min_{\boldsymbol{w}\in\mathcal{C}} L(\boldsymbol{w}), \tag{15.3}$$

where $\mathcal{C} \subseteq \mathcal{W} = \mathbb{R}^P$ is a set of constraints. We say that an approximate solution $\widehat{\boldsymbol{w}}$ to Eq. (15.3) is **feasible** if $\widehat{\boldsymbol{w}} \in \mathcal{C}$. Naturally, the design of algorithms for the constrained setting now depends, not only on information about L, but also on information about $\mathcal{C}$.

Similarly to L, different **oracles** can be considered about $\mathcal{C}$. One of the most commonly used oracle is the **Euclidean projection**

> **Definition 15.2** (Euclidean projection). The Euclidean projection onto the set $\mathcal{C}$ is defined by
>
> $$\text{proj}_{\mathcal{C}}(\boldsymbol{w}) \coloneqq \arg\min_{\boldsymbol{v}\in\mathcal{C}} \|\boldsymbol{w} - \boldsymbol{v}\|_2^2.$$

This projection, which is well-defined when $\mathcal{C}$ is a convex set, can be used in projected gradient descent, that we briefly review below. Other possible oracles are **linear maximization oracles** (LMO) used in Frank-Wolfe algorithms and **Bregman projection oracles**, used in mirror descent algorithms. The algorithm choice can be dictated by what oracle about $\mathcal{C}$ is available.

15.3.1   Variational perspective

Projected gradient descent is a natural generalization of gradient descent, based on the Euclidean projection oracle. Its iterates read

$$\boldsymbol{w}^{t+1} \coloneqq \text{proj}_{\mathcal{C}}(\boldsymbol{w}^t - \gamma \nabla L(\boldsymbol{w}^t)).$$

At each iteration, we attempt to decrease the objective by moving along the negative gradient direction, while ensuring that the next iterate remains feasible, thanks to the projection step.

Similarly to the variational perspective of gradient descent in Eq. (15.2), the projected gradient descent update is equivalent to

$$\boldsymbol{w}^{t+1} = \arg\min_{\boldsymbol{w} \in \mathcal{C}} L(\boldsymbol{w}^t) + \langle \nabla L(\boldsymbol{w}^t), \boldsymbol{w} - \boldsymbol{w}^t \rangle + \frac{1}{2\gamma}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2.$$

This shows that projected gradient descent minimizes a trade-off between staying close to $\boldsymbol{w}^t$ and minimizing the linearization of L around $\boldsymbol{w}^t$, while staying in $\mathcal{C}$.

In terms of convergence rates, they remain the same as gradient descent (Nesterov, 2018). For example, projected gradient descent on a smooth convex function still converges at a rate $R(T) = O(1/T)$.

There are numerous extensions of vanilla projected gradient descent. Similarly to gradient descent, the stepsize can be automatically adjusted using linesearch techniques and there exists accelerated variants. If we replace $\nabla L(\boldsymbol{w})$ with a stochastic gradient $\nabla L(\boldsymbol{w}; S)$, we obtain a stochastic projected gradient descent.

15.3.2 Optimality conditions

In the unconstrained case, a minimum necessarily has a zero gradient. In the constrained setting, there may not be any feasible parameters with zero gradient. Instead, the optimality of a point is characterized by the fact that no better solution can be found by moving along the gradient at that point, while staying in the constraints. Formally, it means that for any $\gamma > 0$, a minimizer $\boldsymbol{w}^\star$ of L on $\mathcal{C}$ satisfies

$$\boldsymbol{w}^\star = \text{proj}_{\mathcal{C}}(\boldsymbol{w}^\star - \gamma \nabla L(\boldsymbol{w}^\star)).$$

It can be shown that this condition is equivalent (Nesterov, 2018) to

$$\langle \nabla L(\boldsymbol{w}^\star), \boldsymbol{w} - \boldsymbol{w}^\star \rangle \geq 0 \quad \forall \boldsymbol{w} \in \mathcal{C}.$$

15.3.3 Commonly-used projections

We now briefly review a few useful Euclidean projections.

- If $\mathcal{C} = \mathbb{R}^P$, we obviously have

$$\text{proj}_{\mathcal{C}}(\boldsymbol{w}) = \boldsymbol{w}.$$

Therefore, in the unconstrained setting, projected gradient descent indeed recovers gradient descent.

- If $\mathcal{C} = [a, b]^P$ (box constraints), we have

$$\mathrm{proj}_{\mathcal{C}}(\boldsymbol{w}) = \mathrm{clip}(\boldsymbol{w}, a, b) := \min\{\max\{\boldsymbol{w}, a\}, b\}.$$

where the min and max are applied coordinate-wise.

- As a special case of the above, if $\mathcal{C} = \mathbb{R}_+^P$ (non-negative orthant),

$$\mathrm{proj}_{\mathcal{C}}(\boldsymbol{w}) = \max\{\boldsymbol{w}, 0\},$$

also known as non-negative part or ReLu.

- If $\mathcal{C} = \triangle^P$ (unit probability simplex),

$$\mathrm{proj}_{\mathcal{C}}(\boldsymbol{w}) = \max\{\boldsymbol{w} - \tau\,\mathbf{1}, 0\},$$

where $\tau \in \mathbb{R}$ is a constant ensuring that $\mathrm{proj}_{\mathcal{C}}(\boldsymbol{w})$ normalizes to 1. It is known that τ can be found in $O(P \log P)$ using a sort. This can be improved to $O(P)$ using a median-finding like algorithm.

15.4   Proximal gradient method

The constrained setting (with $\mathcal{C}$ a convex set) can be recast as unconstrained optimization, by extending our analysis to functions taking infinite values. Let us denote the indicator function of the set $\mathcal{C}$ by

$$\iota_{\mathcal{C}}(\boldsymbol{w}) := \begin{cases} 0 & \text{if } \boldsymbol{w} \in \mathcal{C} \\ +\infty & \text{otherwise} \end{cases}.$$

Clearly, the constrained problem in Eq. (15.3) can then be rewritten as

$$\min_{\boldsymbol{w} \in \mathcal{W}} L(\boldsymbol{w}) + \iota_{\mathcal{C}}(\boldsymbol{w}).$$

This suggests that constrained optimization is a special case of **composite objectives** of the form

$$\min_{\boldsymbol{w} \in \mathcal{W}} L(\boldsymbol{w}) + \Omega(\boldsymbol{w}),$$

where Ω is a convex but potentially non-differentiable function. We assume that we have access to an oracle associated with Ω called the **proximal operator**.

Definition 15.3 (Proximal operator). The proximal operator associated with $\Omega \colon \mathcal{W} \to \mathbb{R}$ is

$$\mathrm{prox}_\Omega(\boldsymbol{w}) := \arg\min_{\boldsymbol{v} \in \mathcal{W}} \frac{1}{2}\|\boldsymbol{w} - \boldsymbol{v}\|_2^2 + \Omega(\boldsymbol{v}).$$

This leads to the proximal gradient method, reviewed below.

15.4.1 Variational perspective

With this method, the update reads

$$\boldsymbol{w}^{t+1} = \mathrm{prox}_{\gamma\Omega}(\boldsymbol{w}^t - \gamma\nabla L(\boldsymbol{w}^t)).$$

This update again enjoys an intuitive variational perspective, namely,

$$\boldsymbol{w}^{t+1} = \arg\min_{\boldsymbol{w} \in \mathcal{W}} L(\boldsymbol{w}^t) + \langle \nabla L(\boldsymbol{w}^t), \boldsymbol{w} - \boldsymbol{w}^t \rangle + \frac{1}{2\gamma}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2 + \Omega(\boldsymbol{w}).$$

That is, we linearize L around $\boldsymbol{w}^t$, but keep Ω as is.

The proximal gradient method is popularly used when the objective function contains a sparsity-inducing regularizer Ω. For example, for the LASSO (Tibshirani, 1996), which aims at predicting targets $\boldsymbol{y} = (y_1, \ldots, y_n)^\top \in \mathbb{R}^N$ from observations $\boldsymbol{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)^\top \in \mathbb{R}^{N \times P}$, we set $L(\boldsymbol{w}) = \frac{1}{2}\|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|_2^2$ and $\Omega(\boldsymbol{w}) = \lambda\|\boldsymbol{w}\|_1$, where $\lambda > 0$ controls the regularization strength. In this case, prox_Ω is the so-called soft-thresholding operator (see below).

Convergence guarantees of the proximal gradient method remain the same as for gradient descent, such as a $O(1/T)$ rate for smooth convex functions.

15.4.2 Optimality conditions

An optimal solution of the problem is characterized by the **fixed point** equation

$$\boldsymbol{w}^\star = \mathrm{prox}_{\gamma\Omega}(\boldsymbol{w}^\star - \gamma\nabla L(\boldsymbol{w}^\star)),$$

for all $\gamma > 0$ (Nesterov, 2018). In other words, the proximal gradient method (which includes gradient descent and projected gradient descent as special cases), can be seen as fixed point iteration schemes. Such

a viewpoint suggests using acceleration methods from the fixed point literature such as Anderson acceleration (Pollock and Rebholz, 2021). It is also useful when designing implicit differentiation schemes as presented in Chapter 7.

15.4.3   Commonly-used proximal operators

We now briefly review a few useful proximal operators.

- If $\Omega(\boldsymbol{w}) = 0$, we have

$$\text{prox}_{\gamma\Omega}(\boldsymbol{w}) = \boldsymbol{w}.$$

  Therefore, with this proximal operator, the proximal gradient method recovers gradient descent.

- If $\Omega(\boldsymbol{w}) = \iota_C(\boldsymbol{w})$, we have

$$\text{prox}_{\gamma\Omega}(\boldsymbol{w}) = \text{proj}_C(\boldsymbol{w}).$$

  Therefore, with this proximal operator, the proximal gradient method recovers projected gradient descent.

- If $\Omega(\boldsymbol{w}) = \lambda\|\boldsymbol{w}\|_1$, we have

$$\text{prox}_{\gamma\Omega}(\boldsymbol{w}) = (\text{sign}(\boldsymbol{w}) \cdot \max(|\boldsymbol{w}| - \gamma\lambda, 0)),$$

  where the operations are applied coordinate-wise. This is the so-called soft-thresholding operator.

- $\Omega(\boldsymbol{w}) = \lambda \sum_{g \in G} \|\boldsymbol{w}_g\|_2$ where G is a partition of $[P]$ and $\boldsymbol{w}_g$ denotes the subvector restricted to g, then we have

$$\left[\text{prox}_{\gamma\Omega}(\boldsymbol{w})\right]_g = \max(1 - \lambda \cdot \gamma/\|\boldsymbol{w}_g\|_2, 0)\boldsymbol{w}_g,$$

  which is used in the group lasso (Yuan and Lin, 2006) and can be used to encourage group sparsity.

For a review of more proximal operators, see for instance (Bach *et al.*, 2012; Parikh, Boyd, *et al.*, 2014).

15.5 Summary

From a variational perspective, gradient descent is the algorithm obtained when linearizing the objective function and using a quadratic regularization term. Projected gradient descent is the algorithm obtained when there is an additional constraint (the Euclidean projection naturally appearing, due to the quadratic regularization term). When the objective is the sum of a differentiable function and a non-differentiable function, proximal gradient is the algorithm obtained when the differentiable function is linearized but the non-differentiable function is kept as is. We also reviewed various stochastic gradient based algorithms, including vanilla SGD, SGD with momentum and Adam.

16

Second-order optimization

We review in this chapter methods whose iterations take the form

$$\boldsymbol{w}^{t+1} := \boldsymbol{w}^t - \gamma^t B^t \nabla L(\boldsymbol{w}^t),$$

where γ^t is a stepsize and B^t is a pre-conditioning matrix involving second-order derivatives.

16.1 Newton's method

16.1.1 Variational perspective

We saw in Eq. (15.2) that gradient descent can be motivated from a variational perspective, in which we use a linear approximation of the objective around the current iterate, obtained from the current gradient. Similarly, if we have access not only to the gradient but also to the Hessian of the objective, we can use a quadratic approximation of the objective around the current iterate. More precisely, given a function $L(\boldsymbol{w})$, we may consider minimizing the second-order Taylor approximation of $L(\boldsymbol{w})$ around the current iterate $\boldsymbol{w}^t$,

$$L(\boldsymbol{w}) \approx L(\boldsymbol{w}^t) + \langle \nabla L(\boldsymbol{w}^t), \boldsymbol{w} - \boldsymbol{w}^t \rangle + \frac{1}{2} \langle \boldsymbol{w} - \boldsymbol{w}^t, \nabla^2 L(\boldsymbol{w}^t)(\boldsymbol{w} - \boldsymbol{w}^t) \rangle.$$

Newton's method simply iteratively minimizes this quadratic approximation around the current iteration $\boldsymbol{w}^t$, namely,

$$\boldsymbol{w}^{t+1} = \underset{\boldsymbol{w}\in\mathcal{W}}{\arg\min}\, L(\boldsymbol{w}^t) + \langle\nabla L(\boldsymbol{w}^t), \boldsymbol{w}-\boldsymbol{w}^t\rangle + \frac{1}{2}\langle\boldsymbol{w}-\boldsymbol{w}^t, \nabla^2 L(\boldsymbol{w}^t)(\boldsymbol{w}-\boldsymbol{w}^t)\rangle.$$

$$(16.1)$$

If the Hessian is positive definite at $\boldsymbol{w}^t$, which we denote by $\nabla^2 L(\boldsymbol{w}^t) \succ 0$, then the minimum is well-defined and unique (this is for example the case if L is strictly convex). The iterates can then be written analytically as

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \nabla^2 L(\boldsymbol{w}^t)^{-1}\nabla L(\boldsymbol{w}^t).$$

If the Hessian is not positive definite, the minimum may not be defined. Ignoring this issue and taking the analytical formulation could be dangerous, as it could amount to computing the maximum of the quadratic instead if, for example, the quadratic was strictly concave (i.e., $\nabla^2 L(\boldsymbol{w}) \prec 0$).

16.1.2   Regularized Newton method

A simple technique to circumvent this issue consists in adding a regularization term to the Hessian. Namely, from a variational viewpoint, we can add a proximity term $\frac{1}{2}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2$, encouraging to stay close to the current $\boldsymbol{w}^t$. The iterates of this regularized Newton method then take the form

$$\boldsymbol{w}^{t+1} = \underset{\boldsymbol{w}\in\mathcal{W}}{\arg\min}\ L(\boldsymbol{w}^t) + \langle\nabla L(\boldsymbol{w}^t), \boldsymbol{w}-\boldsymbol{w}^t\rangle\frac{1}{2}\langle\boldsymbol{w}-\boldsymbol{w}^t, \nabla^2 L(\boldsymbol{w}^t)(\boldsymbol{w}-\boldsymbol{w}^t)\rangle$$

$$+ \frac{\eta^t}{2}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2,$$

where η^t controls the regularization strength. Assuming $\eta^t > 0$ is strong enough to make $\nabla^2 L(\boldsymbol{w}^t) + \eta^t\,\mathrm{I}$ positive-definite, we have

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \boldsymbol{d}^t,$$

where we defined the direction

$$\boldsymbol{d}^t := (\nabla^2 L(\boldsymbol{w}^t) + \eta^t\,\mathrm{I})^{-1}\nabla L(\boldsymbol{w}^t). \qquad (16.2)$$

Other techniques to circumvent this issue include using cubic regularization and modifying the spectral decomposition of the Hessian, by thresholding the eigenvalues or taking their absolute values. We refer the interested reader to, e.g., (Nesterov, 2018; Wright and Nocedal, 1999) for more details.

16.1.3   Approximate direction

We observe a main impediment for implementing such a second-order optimization algorithm: even if we had access to the Hessian of the objective for free and this Hessian was positive definite, computing the exact direction $\boldsymbol{d}^t$ in Eq. (16.2) requires computing an inverse-Hessian vector product (IHVP) with the gradient $\nabla L(\boldsymbol{w}^t)$. Doing so exactly requires solving a linear system

$$(\nabla^2 L(\boldsymbol{w}^t) + \eta^t \, \mathrm{I})\boldsymbol{d}^t = \nabla L(\boldsymbol{w}^t),$$

which a priori takes $O(P^3)$ time. In practice, however, we can compute IHVPs approximately, as explained in Section 8.4.

16.1.4   Convergence guarantees

While implementing Newton's method comes at a higher computational cost, it can also benefit from faster convergence rates. Briefly, if Newton's method is initialized at a point $\boldsymbol{w}^0 \in \mathcal{W}$ close enough from the minimizer $\boldsymbol{w}^\star$ of a μ-strongly convex function with M-Lipschitz continuous Hessian (namely $\|\boldsymbol{w}^0 - \boldsymbol{w}^*\|_2 \le \frac{2\mu}{3M}$), then Newton's method converges at a quadratic rate (Nesterov, 2018), that is, $R(t) \le O(\exp(\exp(-t)))$ (see Section 14.5 for a brief introduction to performance guarantees). This is far superior to gradient descent. Such an efficiency motivated the development of interior point methods, that have been a breakthrough in constrained optimization, thanks to the use of log-barrier penalties (Nesterov, 2018).

16.1.5   Linesearch

In practice, we may not have access to an initial point close enough from the minimizer. In that case, even for strictly convex functions for

which Newton's steps are well-defined, taking $\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \boldsymbol{d}^t$ may not ensure a decrease of the objective values. Nevertheless, the direction $\boldsymbol{d}^t$ may define a descent direction as defined below.

> **Definition 16.1** (Descent direction). A point $\boldsymbol{d} \in \mathcal{W}$ defines a **descent direction** $-\boldsymbol{d}$ for an objective L at $\boldsymbol{w}$, if there exists a positive stepsize $\gamma > 0$ such that
>
> $$L(\boldsymbol{w} - \gamma \boldsymbol{d}) \leq L(\boldsymbol{w}).$$
>
> If L is differentiable, $-\boldsymbol{d}$ is a descent direction if $\langle -\boldsymbol{d}, \nabla L(\boldsymbol{w}) \rangle < 0$.

For Newton's method without regularization, $\boldsymbol{d}^t = \nabla^2 L(\boldsymbol{w}^t)^{-1} \nabla L(\boldsymbol{w}^t)$ is then a descent direction at $\boldsymbol{w}^t$, as long as $\nabla L(\boldsymbol{w}^t) \neq 0$ and $\nabla^2 L(\boldsymbol{w}^t) \succ 0$. If $\nabla^2 L(\boldsymbol{w}^t) \not\succ 0$, choosing $\eta^t > 0$ such that $\nabla^2 L(\boldsymbol{w}^t) + \eta^t \, \mathrm{I} \succ 0$, also ensures that $\boldsymbol{d}^t = -(\nabla^2 L(\boldsymbol{w}^t) + \eta^t \, \mathrm{I})^{-1} \nabla L(\boldsymbol{w}^t)$ is a descent direction (as long as $\nabla L(\boldsymbol{w}^t) \neq 0$). Newton's method is then generally equipped with a linesearch method that attempts to take steps of the form x

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \gamma^t \boldsymbol{d}^t$$

with γ^t chosen as the largest stepsize among $\{\rho^\tau, \tau \in \mathbb{N}\}$ for $\rho \in (0, 1)$ until a sufficient decrease of the objective is satisfied such as, for $c \in (0, 1)$,

$$L(\boldsymbol{w}^t - \gamma^t \boldsymbol{d}^t) \leq L(\boldsymbol{w}^t) - c\gamma^t \langle \nabla L(\boldsymbol{w}^t), \nabla^2 L(\boldsymbol{w}^t)^{-1} \nabla L(\boldsymbol{w}^t) \rangle.$$

For strongly convex functions, such an implementation exhibits two phases: a first phase during which Newton's steps are "damped" by using a stepsize $\gamma^t < 1$ and a second phase of super-fast convergence during which stepsizes $\gamma^t = 1$ are taken, and the objective decreases very fast. Even far from the optimum, Newton directions can advantageously adapt to the local geometry of the objective to speed-up convergence compared to a regular gradient descent as explained below.

16.1.6 Geometric interpretation

To understand the efficiency of Newton's method compared to gradient descent, consider the minimization of a simple quadratic

$$L(\boldsymbol{w}) = \frac{1}{2} a w_1^2 + \frac{1}{2} b w_2^2$$

for $a \gg b \geq 0$, as illustrated in Fig. 16.1. A gradient descent moves along the directions $\nabla L(\boldsymbol{w}) = (aw_1, bw_2)^\top$ and its stepsize is limited by the variations in the first coordinate leading to some oscillations. If we were simply rescaling the gradient by (a, b), i.e., taking steps of the form

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \gamma \, \mathbf{diag}(a^{-1}, b^{-1})L(\boldsymbol{w}^t),$$

the variations in both coordinates would be normalized to one and the stepsize could simply be chosen to $\gamma = 1$ to directly get $\boldsymbol{w}^\star$. In other words, by adapting the geometry of the directions with the geometry induced by the objective, we can circumvent the oscillations.

That's exactly what Newton's method does by modifying the gradient direction using the inverse of the Hessian. Formally, at iteration t, consider the modified objective

$$\tilde{L}(\boldsymbol{v}) = L(A\boldsymbol{v}) \text{ for } A = \nabla^2 L(\boldsymbol{w}^t)^{-1/2},$$

with L strictly convex and A the inverse matrix square root of the Hessian. One easily verifies that a Newton step is equivalent to a gradient step on $\tilde{L}$, that is,

$$\boldsymbol{v}^{t+1} = \boldsymbol{v}^t - \nabla \tilde{L}(\boldsymbol{v}^t) \iff \boldsymbol{w}^{t+1} = \boldsymbol{w}^t - (\nabla^2 L(\boldsymbol{w}^t))^{-1}\nabla L(\boldsymbol{w}^t)$$

where

$$\boldsymbol{w}^t = A\boldsymbol{v}^t = \nabla^2 L(\boldsymbol{w}^t)^{-1/2}\boldsymbol{v}^t.$$

In the geometry induced by A, the objective is generally better conditioned as illustrated in Fig. 16.1. This explains the efficiency of Newton's method. In particular for any strongly convex quadratic, a Newton step reaches the optimum in one iteration, while a gradient step can take many more iterations.

16.1.7   Stochastic Newton's method

Consider now an expected loss

$$\min_{\boldsymbol{w} \in \mathcal{W}} \ L(\boldsymbol{w}) \coloneqq \mathbb{E}_{S \sim \rho}\left[L(\boldsymbol{w}; S)\right].$$

In that case, an estimate of the Hessian can be constructed just like for the gradient using that

$$\mathbb{E}_{S \sim \rho}\left[\nabla^2 L(\boldsymbol{w}; S)\right] = \nabla^2 L(\boldsymbol{w}).$$
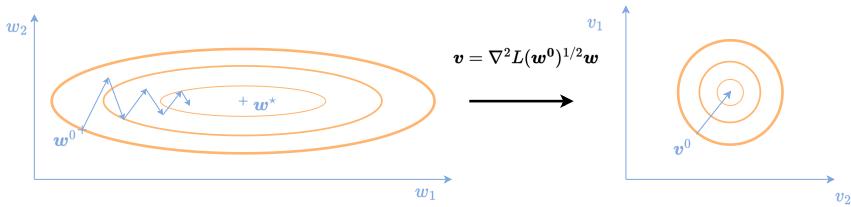
Figure 16.1: Left: Minimization of a quadratic $L(\boldsymbol{w}) = \frac{1}{2}aw_1^2 + \frac{1}{2}bw_2^2$ by gradient descent. For $a \gg b \geq 0$, a gradient descent typically oscillates. Right: minimization by Newton's method amounts to change the geometry of the problem to avoid oscillations.

Denote then

$$g(\boldsymbol{w}; S) \approx \nabla L(\boldsymbol{w}), \quad H(\boldsymbol{w}; S') \approx \nabla^2 L(\boldsymbol{w})$$

some stochastic estimates of respectively of the gradient and the Hessian with S, S' independently drawn from p or from mini-batch approaximations with varying mini-batch sizes. One implementation of a **stochastic Newton method** can then be

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \gamma^t (H(\boldsymbol{w}^t; S') + \eta^t \,\mathrm{I})^{-1} \boldsymbol{g}(\boldsymbol{w}^t; S),$$

for $\eta^t \geq 0$ such that $(H(\boldsymbol{w}^t; S') + \eta^t)^{-1} \succ 0$ and γ^t fixed or chosen to satisfy some sufficient decrease condition. We refer the interested reader to, e.g., (Xu *et al.*, 2020), for more details and variants.

16.2 Gauss-Newton method

Newton's method (16.1) is usually not properly defined for non-convex objective functions, since the Hessian may not be positive definite at the current iterate. We saw in Section 8.2 that the Gauss-Newton matrix can be used to define a positive-semidefinite approximation of the Hessian. Here, we revisit the Gauss-Newton method from a variational and **partial linearization** perspective. While the original Gauss-Newton method originates from nonlinear least-squares, we will first describe an extension to arbitrary convex loss functions, since it is both more general and easier to explain.

16.2.1   With exact outer function

Consider a composite objective of the form

$$L(\boldsymbol{w}) := \ell(f(\boldsymbol{w})),$$

where $\ell : \mathcal{M} \to \mathbb{R}$ is a **convex** function, such as a convex loss function applied on a given sample, and $f : \mathcal{W} \to \mathcal{M}$ is a **nonlinear** function, such as a neural network with parameters $\boldsymbol{w} \in \mathcal{W}$, evaluated on the same sample. We saw that gradient descent and Newton's method amount to using **linear** and **quadratic** approximations of $L(\boldsymbol{w})$ around the current iterate $\boldsymbol{w}^t$, respectively. As a middle ground between the two, the Gauss-Newton method uses the linearization of f around $\boldsymbol{w}^t$

$$f(\boldsymbol{w}) \approx f(\boldsymbol{w}^t) + \partial f(\boldsymbol{w}^t)(\boldsymbol{w} - \boldsymbol{w}^t)$$

but keeps ℓ as is to obtain the objective

$$
\begin{aligned}
\boldsymbol{w}^{t+1} &:= \underset{\boldsymbol{w} \in \mathcal{W}}{\arg\min}\, \ell(f(\boldsymbol{w}^t) + \partial f(\boldsymbol{w}^t)(\boldsymbol{w} - \boldsymbol{w}^t)) \\
&= \underset{\boldsymbol{w} \in \mathcal{W}}{\arg\min}\, \ell(\partial f(\boldsymbol{w}^t)\boldsymbol{w} + f(\boldsymbol{w}^t) - \partial f(\boldsymbol{w}^t)\boldsymbol{w}^t) \\
&= \underset{\boldsymbol{w} \in \mathcal{W}}{\arg\min}\, \ell(J^t\boldsymbol{w} + \boldsymbol{\delta}^t),
\end{aligned}
$$

where we defined the shorthands $J^t := \partial f(\boldsymbol{w}^t)$ and $\boldsymbol{\delta}^t := f(\boldsymbol{w}^t) - \partial f(\boldsymbol{w}^t)\boldsymbol{w}^t$. We call $\ell(J^t\boldsymbol{w} + \boldsymbol{\delta}^t)$ the **partial linearization** of $L = \ell \circ f$ at $\boldsymbol{w}^t$, as opposed to the full linearization of L used in gradient descent.

Since the composition of a convex function and of linear function is convex, this objective is **convex** even if $L(\boldsymbol{w})$ is nonconvex. In practice, we often add a proximity term as regularization to define

$$\boldsymbol{w}^{t+1} := \underset{\boldsymbol{w} \in \mathcal{W}}{\arg\min}\, \ell(J^t\boldsymbol{w} + \boldsymbol{\delta}^t) + \frac{\eta^t}{2}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2. \qquad (16.3)$$

We can see this update as an approximation of the **proximal point** update

$$\underset{\boldsymbol{w} \in \mathcal{W}}{\arg\min}\, L(\boldsymbol{w}) + \frac{\eta^t}{2}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2,$$

where $L(\boldsymbol{w})$ has been replaced by its partial linearization. Solving Eq. (16.3) using gradient-based solvers requires to compute the gradient

of $\boldsymbol{w} \mapsto \ell(J^t \boldsymbol{w} + \delta^t)$, which is $\boldsymbol{w} \mapsto (J^t)^* \nabla \ell(J^t \boldsymbol{w} + \delta^t)$. Computing this gradient by autodiff therefore requires to perform a forward pass to compute the JVP $J^t \boldsymbol{w}$ and a backward pass to compute the VJP $(J^t)^* \nabla \ell(\boldsymbol{z})$. See Section 2.3 for an introduction to these operators and Chapter 7 for an introduction to autodiff.

The Gauss-Newton method with arbitrary convex outer loss is often called modified Gauss-Newton (Nesterov, 2007) or prox-linear (Drusvyatskiy and Paquette, 2019). The classical Gauss-Newton and Levenberg-Marquardt (Levenberg, 1944; Marquardt, 1963) methods originate from nonlinear least-squares and are recovered when $\ell(\boldsymbol{z})$ is quadratic (Kelley, 1995), such as $\ell(\boldsymbol{z}) := \frac{1}{2}\|\boldsymbol{z} - \boldsymbol{y}\|_2^2$, for $\boldsymbol{y}$ some reference target. The Gauss-Newton method corresponds classically to not using regularization (i.e., $\eta^t = 0$) and the Levenberg-Marquardt method uses regularization (usually called damping, potentially changing η^t across iterations). See e.g., (Messerer *et al.*, 2021), for a survey of different variants.

16.2.2   With approximate outer function

Another variant of the Gauss-Newton method consists in replacing the convex loss ℓ with its quadratic approximation around $\boldsymbol{z}^t := f(\boldsymbol{w}^t)$,

$$q^t(\boldsymbol{z}) := \ell(\boldsymbol{z}^t) + \langle \nabla \ell(\boldsymbol{z}^t), \boldsymbol{z} - \boldsymbol{z}^t \rangle + \frac{1}{2}\langle \boldsymbol{z} - \boldsymbol{z}^t, \nabla^2 \ell(\boldsymbol{z}^t)(\boldsymbol{z} - \boldsymbol{z}^t) \rangle \approx \ell(\boldsymbol{z})$$

to define the update

$$\boldsymbol{w}^{t+1} := \operatorname*{arg\,min}_{\boldsymbol{w} \in \mathcal{W}} q^t(J^t \boldsymbol{w} + \delta^t) + \frac{\eta^t}{2}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2.$$

Notice that ℓ has been replaced by its quadratic approximation q^t. This objective is always a **convex quadratic**, unlike the objective of the Newton method in Eq. (16.1), which is a priori a **nonconvex quadratic**, if f is nonlinear. Simple calculations show that

$$\boldsymbol{w}^{t+1} = \operatorname*{arg\,min}_{\boldsymbol{w} \in \mathcal{W}} \; L(\boldsymbol{w}^t) + \langle \boldsymbol{q}^t, J^t(\boldsymbol{w} - \boldsymbol{w}^t) \rangle$$

$$+ \frac{1}{2}\langle \boldsymbol{w} - \boldsymbol{w}^t, (J^t)^* Q^t J^t(\boldsymbol{w} - \boldsymbol{w}^t) \rangle + \frac{\eta^t}{2}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2$$

where $\boldsymbol{q}^t := \nabla\ell(f(\boldsymbol{w}^t)) \in \mathcal{M} = \mathbb{R}^Z, Q^t := \nabla^2\ell(f(\boldsymbol{w}^t)) \in \mathbb{R}^{Z\times Z}$. The closed form solution is

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - ((J^t)^*Q^tJ^t + \eta^t\,\mathrm{I})^{-1}(J^t)^*\boldsymbol{q}^t$$
$$= \boldsymbol{w}^t - (\nabla^2_{\mathrm{GN}}(\ell \circ f)(\boldsymbol{w}^t) + \eta^t\,\mathrm{I})^{-1}\nabla L(\boldsymbol{w}^t),$$

where we used the (generalized) **Gauss-Newton matrix** of $L = \ell \circ f$, defined in Section 8.2.

16.2.3   Linesearch

Similarly to Newton's method, the iterates of a Gauss-Newton method may diverge when used alone. However, the direction $-(\nabla^2_{\mathrm{GN}}(\ell\circ f)(\boldsymbol{w}^t)+\eta^t\,\mathrm{I})^{-1}\nabla L(\boldsymbol{w}^t)$ defines a descent direction for any $\eta^t > 0$ and can be combined with a stepsize γ^t (typically chosen using a linesearch) to obtain iterates of the form

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \gamma^t(\nabla^2_{\mathrm{GN}}(\ell \circ f)(\boldsymbol{w}^t) + \eta^t\,\mathrm{I})^{-1}\nabla L(\boldsymbol{w}^t).$$

16.2.4   Stochastic Gauss-Newton

In deep learning, the objective generally consists in an expectation over samples of the composition between a loss function and a network function:

$$L(\boldsymbol{w}) = \mathbb{E}_{S\sim\rho}[L(\boldsymbol{w}; S)] = \mathbb{E}_{(X,Y)\sim\rho}[\ell(f(\boldsymbol{w}; X); Y)]$$

where $S = (X, Y)$ denotes a sample pair of input X with associated label Y. In that case, as already studied in Section 8.2, the Gauss-Newton matrix $\nabla^2_{\mathrm{GN}}L$ is the expectation of the individual Gauss-Newton matrices

$$\nabla^2_{\mathrm{GN}}L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y}) := \partial f(\boldsymbol{w}; \boldsymbol{x})^\top \nabla^2\ell(f(\boldsymbol{w}; \boldsymbol{x}))\partial f(\boldsymbol{w}; \boldsymbol{x}),$$
$$\nabla^2_{\mathrm{GN}}L(\boldsymbol{w}) := \mathbb{E}_{(X,Y)\sim\rho}[\nabla^2_{\mathrm{GN}}L(\boldsymbol{w}; \boldsymbol{x}, \boldsymbol{y})].$$

We can estimate the gradient and the Gauss-Newton matrix by, respectively, $\boldsymbol{g}(\boldsymbol{w}; S) \approx \nabla L(\boldsymbol{w})$, and $G(\boldsymbol{w}; S') \approx \nabla^2_{\mathrm{GN}}L(\boldsymbol{w})$ for $S, S' \sim \rho$ or using mini-batch approximations. A **stochastic** Gauss-Newton method therefore performs iterates

$$\boldsymbol{w}^{t+1} := \boldsymbol{w}^t - \gamma^t(G(\boldsymbol{w}; S') + \eta^t\,\mathrm{I})^{-1}\boldsymbol{g}(\boldsymbol{w}, S),$$

for $\eta^t \geq 0$ and γ^t fixed or selected to satisfy some criterion.

16.3 Natural gradient descent

Natural gradient descent (Amari, 1998) follows a similar principle as gradient descent: linearize the objective around the current iterate and minimize this approximation together with a proximity term. It differs from gradient descent in the choice of the proximity term: rather than using a squared Euclidean distance between the **parameters**, it uses a Kullback-Leibler divergence between the **probability distributions** these parameters define.

Negative log-likelihood

We consider objectives of the form

$$\min_{\boldsymbol{w} \in \mathcal{W}} L(\boldsymbol{w}) = \mathbb{E}_{S \sim \rho} \left[L(\boldsymbol{w}; S) \right] = \mathbb{E}_{S \sim \rho} \left[- \log q_{\boldsymbol{w}}(S) \right],$$

where ρ is an unknown data distribution (but from which we can sample) and where $q_{\boldsymbol{w}}$ is a probability distribution parameterized by $\boldsymbol{w}$. As reviewed in Chapter 3, the negative log-likelihood can be used as a loss function (many loss functions can be seen from this perspective, including the squared and logistic loss functions). In the unsupervised setting, where $S = Y$, we simply use $q_{\boldsymbol{w}}(Y)$ as is. In the supervised setting, where $S = (X, Y)$, we use the product rule $\mathbb{P}(X, Y) = \mathbb{P}(X)\mathbb{P}(Y|X)$ to parameterize $q_{\boldsymbol{w}}(S)$ as

$$q_{\boldsymbol{w}}(\boldsymbol{x}, \boldsymbol{y}) := \rho_X(\boldsymbol{x}) p_{\boldsymbol{\theta}}(\boldsymbol{y}),$$

where ρ_X is the marginal distribution for X, $p_{\boldsymbol{\theta}}(\boldsymbol{y})$ is the PMF/PDF of a probability distribution and $\boldsymbol{\theta} = f(\boldsymbol{w}; \boldsymbol{x})$ is for instance a neural network with parameters $\boldsymbol{w} \in \mathcal{W}$ and input $\boldsymbol{x} \in \mathcal{X}$.

16.3.1 Variational perspective

Natural gradient descent is motivated by updates of the form

$$\boldsymbol{w}^{t+1} = \arg \min_{\boldsymbol{w} \in \mathcal{W}} L(\boldsymbol{w}^t) + \langle \nabla L(\boldsymbol{w}^t), \boldsymbol{w} - \boldsymbol{w}^t \rangle + \mathrm{KL}(q_{\boldsymbol{w}^t}, q_{\boldsymbol{w}}),$$

where $\mathrm{KL}(p, q) := \int p(\boldsymbol{z}) \log \frac{p(\boldsymbol{z})}{q(\boldsymbol{z})} d\boldsymbol{z}$ is the Kullback-Leibler (KL) divergence. Unlike gradient descent, the proximity term is therefore between

the current distribution $q_{\boldsymbol{w}^t}$ and a candidate probability distribution $q_{\boldsymbol{w}}$. The above problem is intractable in general, as the KL may not have a closed form. Nevertheless, its quadratic approximation can be shown (Amari, 1998) to admit a simple form,

$$\mathrm{KL}(q_{\boldsymbol{w}^t}, q_{\boldsymbol{w}}) \approx \frac{1}{2}\langle \boldsymbol{w} - \boldsymbol{w}^t, \nabla_{\mathrm{F}}^2 L(\boldsymbol{w}^t)(\boldsymbol{w} - \boldsymbol{w}^t)\rangle$$

where we used the Fisher information matrix $\nabla_{\mathrm{F}}^2 L(\boldsymbol{w})$, studied in Section 8.3. Equipped with this quadratic approximation of the KL divergence, natural gradient descent amounts to compute iterates as

$$\boldsymbol{w}^{t+1} := \underset{\boldsymbol{w} \in \mathcal{W}}{\arg\min} \ L(\boldsymbol{w}^t) + \langle \nabla L(\boldsymbol{w}^t), \boldsymbol{w} - \boldsymbol{w}^t\rangle$$

$$+ \frac{1}{2}\langle \boldsymbol{w} - \boldsymbol{w}^t, \nabla_{\mathrm{F}}^2 L(\boldsymbol{w}^t)(\boldsymbol{w} - \boldsymbol{w}^t)\rangle + \frac{\eta^t}{2}\|\boldsymbol{w} - \boldsymbol{w}^t\|_2^2,$$

where a quadratic proximity-term was added to ensure a unique solution. This is a srictly convex problem as $\nabla_{\mathrm{F}}^2 L(\boldsymbol{w}^t)$ is positive semi-definite. The closed-form solution is

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - (\nabla_{\mathrm{F}}^2 L(\boldsymbol{w}^t) + \eta^t \, \mathrm{I})^{-1}\nabla L(\boldsymbol{w}^t).$$

Because the Gauss-Newton and Fisher information matrices are equivalent when $p_{\boldsymbol{\theta}}$ is an exponential family distribution (Proposition 8.6), the Gauss-Newton and natural gradient methods coincide in this case.

16.3.2 Stochastic natural gradient descent

In practice, we may not have access to $\nabla L(\boldsymbol{w}^t)$ in closed form as it is an expectation over ρ. Moreover, $\nabla_{\mathrm{F}}^2 L(\boldsymbol{w}^t)$ may not be computable in closed form either. To estimate the Fisher information matrix, we can use that (see Section 8.3) using the shorthand $\boldsymbol{\theta} := f(\boldsymbol{w}, X)$,

$$\nabla_{\mathrm{F}}^2 L(\boldsymbol{w}) = \mathbb{E}_{X \sim \rho_X}\mathbb{E}_{Y \sim p_{\boldsymbol{\theta}}}[\nabla L(\boldsymbol{w}; X, Y) \otimes \nabla L(\boldsymbol{w}; X, Y)].$$

We can then build estimates $\boldsymbol{g}(\boldsymbol{w}^t; S) \approx \nabla L(\boldsymbol{w}^t, S)$ and $F(\boldsymbol{w}^t; S') \approx \nabla_{\mathrm{F}}^2 L(\boldsymbol{w}^t)$ for S sampled from ρ and S' sampled from $q_{\boldsymbol{w}^t}(\boldsymbol{x}, \boldsymbol{y}) = p_{\mathcal{X}}(\boldsymbol{x})\rho_{\boldsymbol{\theta}}(\boldsymbol{y})$. A stochastic natural gradient descent can then be implemented as

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \gamma^t(F(\boldsymbol{w}^t; S') + \eta^t \, \mathrm{I})^{-1}\boldsymbol{g}(\boldsymbol{w}^t; S),$$

where γ^t is a stepsize, possibly chosen by linesearch.

In deep learning, the product with the inverse Fisher or Gauss-Newton matrices can remain costly to compute. Several approximations have been proposed, such as KFAC (Martens and Grosse, 2015; Botev *et al.*, 2017), which uses a computationally efficient structural approximation to these matrices.

16.4 Quasi-Newton methods

16.4.1 BFGS

A celebrated example of **quasi-Newton** method is the BFGS method (Broyden, 1970; Fletcher, 1970; Goldfarb, 1970; Shanno, 1970), whose acronym follows from its author names. The rationale of the BFGS update stems once again from a variational viewpoint. We wish to build a simple quadratic model of the objective $h^t(\boldsymbol{w}) = L(\boldsymbol{w}^t) + \langle \nabla L(\boldsymbol{w}^t), \boldsymbol{w} - \boldsymbol{w}^t \rangle + \frac{1}{2}\langle \boldsymbol{w} - \boldsymbol{w}^t, Q^t(\boldsymbol{w} - \boldsymbol{w}^t) \rangle$ for some Q^t built along the iterations rather than taken as $\nabla^2 L(\boldsymbol{w}^t)$. One desirable property of such quadratic model would be that its gradients at consecutive iterates match the gradients of the original function, i.e., $\nabla h^t(\boldsymbol{w}^t) = \nabla L(\boldsymbol{w}^t)$ and $\nabla h^t(\boldsymbol{w}^{t-1}) = \nabla L(\boldsymbol{w}^{t-1})$. A simpler condition, called the **secant condition** consists in considering the differences of these vectors, that is, ensuring that

$$\nabla h^t(\boldsymbol{w}^t) - \nabla h^t(\boldsymbol{w}^{t-1}) = \nabla L(\boldsymbol{w}^t) - \nabla L(\boldsymbol{w}^{t-1})$$
$$\iff Q^t(\boldsymbol{w}^t - \boldsymbol{w}^{t-1}) = \nabla L(\boldsymbol{w}^t) - \nabla L(\boldsymbol{w}^{t-1})$$
$$\iff \boldsymbol{w}^t - \boldsymbol{w}^{t-1} = B^t(\nabla L(\boldsymbol{w}^t) - \nabla L(\boldsymbol{w}^{t-1})),$$

for $B^t = (Q^t)^{-1}$. Building B^t, a surrogate of the inverse of the Hessian satisfying the secant equation, can then be done as

$$B^{t+1} := \left(\mathrm{I} - \rho^t \boldsymbol{s}^t (\boldsymbol{y}^t)^\top \right) B^t \left(\mathrm{I} - \rho^t \boldsymbol{s}^t (\boldsymbol{y}^t)^\top \right) + \rho^t \boldsymbol{s}^t (\boldsymbol{s}^t)^\top$$

where

$$\boldsymbol{s}^t := \boldsymbol{w}^{t+1} - \boldsymbol{w}^t$$
$$\boldsymbol{y}^t := \nabla L(\boldsymbol{w}^{t+1}) - \nabla L(\boldsymbol{w}^t)$$
$$\rho^t := \frac{1}{\langle \boldsymbol{s}^t, \boldsymbol{y}^t \rangle}.$$

A typical implementation of BFGS stores $B_t \in \mathbb{R}^{P \times P}$ in memory, which is prohibitive when P is large.

16.4.2 Limited-memory BFGS

In practice, the limited-memory counterpart of BFGS, called LBFGS (Liu and Nocedal, 1989), is often preferred. The key observation of LBFGS is that we do not need to materialize B_t in memory: we only need to multiply it with the gradient $\nabla L(\boldsymbol{w}^t)$. That is, we can see B_t as a linear map. Fortunately, the product between B^t and any vector $\boldsymbol{v}$ can be computed efficiently if we store $(\boldsymbol{s}^1, \boldsymbol{y}^1, \rho^1), \ldots, (\boldsymbol{s}^t, \boldsymbol{y}^t, \rho^t)$ in memory. In practice, a small history of past values is used to reduce memory and computational cost. Because LBFGS has the benefits of second-order-like methods with much reduced cost, it has become a de-facto algorithm, outperforming most other algorithms for medium-scale problems without particular structure (Liu and Nocedal, 1989).

16.5 Approximate Hessian diagonal inverse preconditionners

One application of the approximations of the Hessian diagonal developed in Section 8.7 is to obtain cheap approximations of the Hessian diagonal inverse,

$$B^t := \mathbf{diag}(|H_{11}^t|^{-1}, \ldots, |H_{PP}^t|^{-1}).$$

Such a scaling would for instance be sufficient to make the quadratic example presented in Fig. 16.1 work. Many optimization algorithms, including the popular ADAM, can be viewed as using a preconditioner that approximates the inverse of the Hessian's diagonal.

16.6 Summary

In this chapter, we reviewed Newton's method, the Gauss-Newton method, natural gradient descent, quasi-Newton methods and precon-ditioning methods. We adopted a variational viewpoint, where the method's next iterate is computed as the solution of a trade-off between minimizing an approximation of the function (linear, partially linear,

quadratic) and a proximity term (squared Euclidean, KL). All methods were shown to use iterates of the form

$$\boldsymbol{w}^{t+1} := \boldsymbol{w}^t - \gamma^t B^t \nabla L(\boldsymbol{w}^t)$$

but have different trade-offs between the cost it takes to evaluate $B^t \nabla L(\boldsymbol{w}^t)$ and the richness of the information used about L.

17

Duality

In this chapter, we review duality principles in optimization.

17.1 Dual norms

We introduce in this section dual norms, since they are useful in this book.

> **Definition 17.1** (Dual norms). Given a norm $\|\boldsymbol{u}\|$, its dual is
>
> $$\|\boldsymbol{v}\|_* := \max_{\|\boldsymbol{u}\| \leq 1} \langle \boldsymbol{u}, \boldsymbol{v} \rangle.$$

Therefore, the dual norm of $\| \cdot \|$ is the **support function** of the unit ball induced by the norm $\| \cdot \|$,

$$B_{\|\cdot\|} := \{\boldsymbol{u} \in \mathbb{R}^D : \|\boldsymbol{u}\| \leq 1\}.$$

We give examples of pairs of dual norms below.

Example 17.1 (Dual norm of p-norms). The p-norm is defined by

$$\|\boldsymbol{u}\|_p := \left(\sum_{j=1}^{D} |u_j|^p\right)^{1/p}.$$

Its dual is $\|\boldsymbol{v}\|_q$ where q is such that $\frac{1}{p} + \frac{1}{q} = 1$. For instance, the dual norm of the 2-norm is itself, since $\frac{1}{2} + \frac{1}{2} = 1$. The 1-norm and the ∞-norm are dual of each other, since $\frac{1}{1} + \frac{1}{\infty} = 1$.

The definition of dual norm implies a generalization of **Cauchy–Schwarz's inequality**: for all $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^D$

$$|\langle \boldsymbol{u}, \boldsymbol{v} \rangle| \leq \|\boldsymbol{u}\|_* \|\boldsymbol{v}\|.$$

See, e.g., Beck (2017, Lemma 1.4).

Proposition 17.1 (Conjugate of norms and squared norms). We know that the conjugate of the support function is the indicator function. Therefore, if $f(\boldsymbol{u}) = \|\boldsymbol{u}\|$, then

$$f^*(\boldsymbol{v}) = \iota_{B_{\|\cdot\|}}(\boldsymbol{v}) = \begin{cases} 0 & \text{if } \|\boldsymbol{v}\|_* \leq 1 \\ \infty & \text{otherwise} \end{cases}.$$

On the other hand, if $f(\boldsymbol{u}) = \frac{1}{2}\|\boldsymbol{u}\|^2$, then

$$f^*(\boldsymbol{v}) = \frac{1}{2}\|\boldsymbol{v}\|_*^2.$$

17.2 Fenchel duality

We consider in this section standard objectives of the form

$$\min_{\boldsymbol{w} \in \mathcal{W}} L(\boldsymbol{w}) := \min_{\boldsymbol{w} \in \mathcal{W}} \ell(f(\boldsymbol{w})) + R(\boldsymbol{w}),$$

where $f \colon \mathcal{W} \to \mathcal{M}$, $\ell \colon \mathcal{M} \to \mathbb{R}$ and $R \colon \mathcal{W} \to \mathbb{R}$. We first show that the minimization of this objective, called the **primal**, can be lower bounded by a **concave** maximization objective, called the **dual**, even if the primal is nonconvex.

Proposition 17.2 (Weak duality). Let $f: \mathcal{W} \to \mathcal{M}$ (potentially non-linear), $\ell: \mathcal{M} \to \mathbb{R}$ (potentially nonconvex) and $R: \mathcal{W} \to \mathbb{R}$ (potentially nonconvex). Then

$$\min_{\boldsymbol{w} \in \mathcal{W}} \ell(f(\boldsymbol{w})) + R(\boldsymbol{w}) \geq \max_{\boldsymbol{\alpha} \in \mathcal{M}} -R^f(\boldsymbol{\alpha}) - \ell^*(-\boldsymbol{\alpha}),$$

where we used the conjugate

$$\ell^*(-\boldsymbol{\alpha}) := \max_{\boldsymbol{\theta} \in \mathcal{M}} \langle -\boldsymbol{\alpha}, \boldsymbol{\theta} \rangle - \ell(\boldsymbol{\theta})$$

and the "generalized conjugate"

$$R^f(\boldsymbol{\alpha}) := \max_{\boldsymbol{w} \in \mathcal{W}} \langle \boldsymbol{\alpha}, f(\boldsymbol{w}) \rangle - R(\boldsymbol{w}).$$

Moreover, ℓ^* and R^f are both convex functions.

We emphasize that the result in Proposition 17.2 is fully general, in the sense that it does not assume the linearity of f or the convexity of ℓ and R. The caveat, of course, is that R^f and ℓ^* are difficult to compute in general, if f is nonlinear, and if ℓ and R are nonconvex.

Proof.

$$\min_{\boldsymbol{w} \in \mathcal{W}} \ell(f(\boldsymbol{w})) + R(\boldsymbol{w})$$

$$= \min_{\substack{\boldsymbol{w} \in \mathcal{W} \\ \boldsymbol{\theta} \in \mathcal{M}}} \ell(\boldsymbol{\theta}) + R(\boldsymbol{w}) \quad \text{s.t.} \quad \boldsymbol{\theta} = f(\boldsymbol{w})$$

$$= \min_{\substack{\boldsymbol{w} \in \mathcal{W} \\ \boldsymbol{\theta} \in \mathcal{M}}} \max_{\boldsymbol{\alpha} \in \mathcal{M}} \ell(\boldsymbol{\theta}) + R(\boldsymbol{w}) + \langle \boldsymbol{\alpha}, \boldsymbol{\theta} - f(\boldsymbol{w}) \rangle$$

$$\geq \max_{\boldsymbol{\alpha} \in \mathcal{M}} \min_{\substack{\boldsymbol{w} \in \mathcal{W} \\ \boldsymbol{\theta} \in \mathcal{M}}} \ell(\boldsymbol{\theta}) + R(\boldsymbol{w}) + \langle \boldsymbol{\alpha}, \boldsymbol{\theta} - f(\boldsymbol{w}) \rangle$$

$$= \max_{\boldsymbol{\alpha} \in \mathcal{M}} \min_{\boldsymbol{w} \in \mathcal{W}} \langle \boldsymbol{\alpha}, -f(\boldsymbol{w}) \rangle + R(\boldsymbol{w}) + \min_{\boldsymbol{\theta} \in \mathcal{M}} \ell(\boldsymbol{\theta}) + \langle \boldsymbol{\alpha}, \boldsymbol{\theta} \rangle$$

$$= \max_{\boldsymbol{\alpha} \in \mathcal{M}} -\max_{\boldsymbol{w} \in \mathcal{W}} \langle \boldsymbol{\alpha}, f(\boldsymbol{w}) \rangle - R(\boldsymbol{w}) - \max_{\boldsymbol{\theta} \in \mathcal{M}} \langle -\boldsymbol{\alpha}, \boldsymbol{\theta} \rangle - \ell(\boldsymbol{\theta})$$

$$= \max_{\boldsymbol{\alpha} \in \mathcal{M}} -R^f(\boldsymbol{\alpha}) - \ell^*(-\boldsymbol{\alpha}).$$

$\square$

In the case when $f(\boldsymbol{w}) = A\boldsymbol{w}$, where A is a linear map, and when both ℓ and R are convex, we can state a much stronger result.

Proposition 17.3 (Strong duality). Let A be a linear map from $\mathcal{W}$ to $\mathcal{M}$. Let $\ell \colon \mathcal{M} \to \mathbb{R}$ and $R \colon \mathcal{W} \to \mathbb{R}$ be convex functions. Let A^* denote the adjoint of A (Section 2.3). Then,

$$\min_{\boldsymbol{w} \in \mathcal{W}} \ell(A\boldsymbol{w}) + R(\boldsymbol{w}) = \max_{\boldsymbol{\alpha} \in \mathcal{M}} -R^*(A^*\boldsymbol{\alpha}) - \ell^*(-\boldsymbol{\alpha}).$$

Furthermore, the primal solution satisfies

$$\boldsymbol{w}^\star \in \arg\max_{\boldsymbol{w} \in \mathcal{W}} \langle A\boldsymbol{\alpha}^\star, \boldsymbol{w} \rangle - R(\boldsymbol{w}).$$

When R is strictly convex, the primal solution is uniquely determined by

$$\boldsymbol{w}^\star = \nabla R^*(A^*\boldsymbol{\alpha}^\star).$$

Proof. Since $f(\boldsymbol{w}) = A\boldsymbol{w}$, we have

$$
\begin{aligned}
R^f(\boldsymbol{\alpha}) &:= \max_{\boldsymbol{w} \in \mathcal{W}} \langle \boldsymbol{\alpha}, f(\boldsymbol{w}) \rangle - R(\boldsymbol{w}) \\
&= \max_{\boldsymbol{w} \in \mathcal{W}} \langle \boldsymbol{\alpha}, A\boldsymbol{w} \rangle - R(\boldsymbol{w}) \\
&= \max_{\boldsymbol{w} \in \mathcal{W}} \langle A^*\boldsymbol{\alpha}, \boldsymbol{w} \rangle - R(\boldsymbol{w}) \\
&= R^*(A^*\boldsymbol{\alpha}).
\end{aligned}
$$

Furthermore, the inequality in the proof of Proposition 17.2 is an equality, since the min max is that of a convex-concave function. $\square$

The maximization problem in Proposition 17.3 is called the **Fenchel dual**. By strong duality, the value of the maximum and the value of the minimum are equal. We can therefore choose to equivalently solve the dual instead of the primal. This can be advantageous when the space $\mathcal{M}$ is smaller than $\mathcal{W}$.

We now apply the Fenchel dual to obtain the dual of regularized multiclass linear classification.

Table 17.1: Examples of loss conjugates. For regression losses (squared, absolute), where $\boldsymbol{y}_i \in \mathbb{R}^M$, we define $\boldsymbol{t}_i = \phi(\boldsymbol{y}_i) = \boldsymbol{y}_i$. For classification losses (logistic, perceptron, hinge), where $y_i \in [M]$, we define $\boldsymbol{t}_i = \phi(y_i) = \boldsymbol{e}_{y_i}$. To simplify some expressions, we defined the change of variable $\boldsymbol{\mu}_i \coloneqq \boldsymbol{y}_i - \boldsymbol{\alpha}_i$.

	$\ell_i(\boldsymbol{\theta}_i)$	$\ell_i^*(-\boldsymbol{\alpha}_i)$
Squared	$\frac{1}{2}\|\boldsymbol{\theta}_i - \boldsymbol{t}_i\|_2^2$	$\frac{1}{2}\|\boldsymbol{\alpha}_i\|_2^2 - \langle \boldsymbol{t}_i, \boldsymbol{\alpha}_i \rangle$
Absolute	$\|\boldsymbol{\theta}_i - \boldsymbol{t}_i\|_1$	$\iota_{[-1,1]^M}(\boldsymbol{\alpha}_i) - \langle \boldsymbol{t}_i, \boldsymbol{\alpha}_i \rangle$
Logistic	$\mathrm{LSE}(\boldsymbol{\theta}_i) - \langle \boldsymbol{\theta}, \boldsymbol{t}_i \rangle$	$\langle \boldsymbol{\mu}_i, \log \boldsymbol{\mu}_i \rangle + \iota_{\triangle^M}(\boldsymbol{\mu}_i)$
Perceptron	$\max_{i \in [M]} \theta_i - \theta_y$	$\iota_{\triangle^M}(\boldsymbol{\mu}_i)$
Hinge	$\max_{i \in [M]}[i \neq y] + \theta_i - \theta_y$	$\iota_{\triangle^M}(\boldsymbol{\mu}_i) - \langle \boldsymbol{1} - \boldsymbol{t}_i, \boldsymbol{\mu}_i \rangle$

Example 17.2 (Sum of separable loss functions). When the loss is $\ell(\boldsymbol{\theta}) \coloneqq \sum_{i=1}^N \ell_i(\boldsymbol{\theta}_i)$, where $\boldsymbol{\theta} = A\boldsymbol{w} = (A_1\boldsymbol{w}, \ldots, A_N\boldsymbol{w}) \in \mathcal{M}^N$ and A_i is a linear map from $\mathcal{W}$ to $\mathcal{M}$, we obtain

$$\min_{\boldsymbol{w} \in \mathcal{W}} \sum_{i=1}^N \ell_i(A_i\boldsymbol{w}) + R(\boldsymbol{w}) = \max_{\boldsymbol{\alpha} \in \mathcal{M}^N} -R(A^*\boldsymbol{\alpha}) - \sum_{i=1}^N \ell_i^*(-\boldsymbol{\alpha}_i),$$

where $A^*\boldsymbol{\alpha} = (A_1^*\boldsymbol{\alpha}_1, \ldots, A_N^*\boldsymbol{\alpha}_N)$. Typically, we define

$$A_i\boldsymbol{w} \coloneqq \boldsymbol{W}\boldsymbol{x}_i,$$

where $\boldsymbol{W} \in \mathbb{R}^{M \times D}$ is a reshaped version of $\boldsymbol{w} \in \mathcal{W}$, $\boldsymbol{x}_i \in \mathbb{R}^D$ is a training sample, and M is the number of classes. In this case, we then have

$$A_i^*\boldsymbol{\alpha}_i = \boldsymbol{\alpha}_i\boldsymbol{x}_i^\top.$$

Examples of loss function conjugates are given in Table 17.1.

17.3 Bregman divergences

Bregman divergences are a measure of difference between two points.

Definition 17.2 (Bregman divergence). The Bregman divergence gen-

erated by a differentiable convex function $f \colon \mathbb{R}^D \to \mathbb{R}$ is

$$B_f(\boldsymbol{u}, \boldsymbol{v}) := f(\boldsymbol{u}) - f(\boldsymbol{v}) - \langle \nabla f(\boldsymbol{v}), \boldsymbol{u} - \boldsymbol{v} \rangle$$
$$= \langle \nabla f(\boldsymbol{v}), \boldsymbol{v} \rangle - f(\boldsymbol{v}) - [\langle \nabla f(\boldsymbol{v}), \boldsymbol{u} \rangle - f(\boldsymbol{u})] \,,$$

where $\boldsymbol{u}, \boldsymbol{v} \in \mathrm{dom}(f)$.

Intuitively, the Bregman divergence is the difference between $f(\boldsymbol{u})$ and its linearization $\boldsymbol{u} \mapsto f(\boldsymbol{v}) + \langle \nabla f(\boldsymbol{v}), \boldsymbol{u} - \boldsymbol{v} \rangle$ around $\boldsymbol{v}$. This is illustrated in Fig. 17.1.

Example 17.3 (Examples of Bregman divergences). If $f(\boldsymbol{u}) = \frac{1}{2}\|\boldsymbol{u}\|_2^2$, where $\mathrm{dom}(f) = \mathbb{R}^D$, then

$$B_f(\boldsymbol{u}, \boldsymbol{v}) = \frac{1}{2}\|\boldsymbol{u} - \boldsymbol{v}\|_2^2,$$

the **squared Euclidean distance**. If $f(\boldsymbol{u}) = \langle \boldsymbol{u}, \log \boldsymbol{u} \rangle$, where $\mathrm{dom}(f) = \mathbb{R}_+^D$, then

$$B_f(\boldsymbol{u}, \boldsymbol{v}) = \sum_{j=1}^{D} u_j \log \frac{u_j}{v_j} - \sum_{j=1}^{D} u_j + \sum_{j=1}^{D} v_j,$$

the (generalized) **Kullback-Leibler divergence**.

Properties

Bregman divergences enjoy several useful properties.

Proposition 17.4 (Properties of Bregman divergences). Let $f \colon \mathbb{R}^D \to \mathbb{R}$ be a differentiable convex function.

1. **Non-negativity:** $B_f(\boldsymbol{u}, \boldsymbol{v}) \geq 0$ for all $\boldsymbol{u}, \boldsymbol{v} \in \mathrm{dom}(f)$.

2. **Positivity:** $B_f(\boldsymbol{u}, \boldsymbol{v}) = 0$ if and only if $\boldsymbol{u} = \boldsymbol{v}$ (when f is strictly convex).

3. **Convexity:** $B_f(\boldsymbol{u}, \boldsymbol{v})$ is convex in $\boldsymbol{u}$.

4. **Dual-space form:** $B_f(\boldsymbol{u}, \boldsymbol{v}) = B_{f^*}(\boldsymbol{b}, \boldsymbol{a})$, where $\boldsymbol{b} = \nabla f(\boldsymbol{v}) \in$
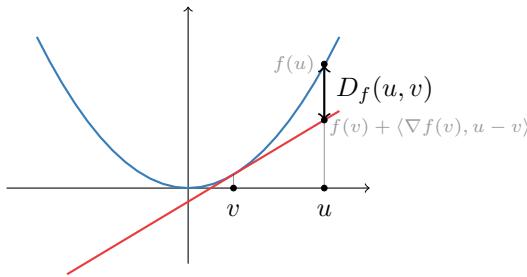
Figure 17.1: The Bregman divergence generated by f is the difference between $f(\boldsymbol{u})$ and its linearization around $\boldsymbol{v}$.

$\mathrm{dom}(f^*)$ and $\boldsymbol{a} = \nabla f(\boldsymbol{u}) \in \mathrm{dom}(f^*)$.

Proof. The properties follow immediately from the convexity of $f(\boldsymbol{u})$.

1. From Definition 14.6.

2. From the unicity of minimizers.

3. From the fact that $\boldsymbol{u} \mapsto B_f(\boldsymbol{u}, \boldsymbol{v})$ is the sum of $f(\boldsymbol{u})$ and a linear function of $\boldsymbol{u}$.

$\square$

The Bregman divergence can be used to define natural generalizations of the Euclidean projection and proximal operators, reviewed in Section 15.3 and Section 15.4.

Definition 17.3 (Bregman proximal and projection operators). Let $\boldsymbol{v} \in \mathrm{dom}(f)$. The Bregman proximal operator is

$$\mathrm{bprox}_{f,g}(\boldsymbol{v}) := \underset{\boldsymbol{u} \in \mathrm{dom}(f) \cap \mathrm{dom}(g)}{\arg\min} B_f(\boldsymbol{u}, \boldsymbol{v}) + g(\boldsymbol{u}).$$

In particular, the Bregman projection onto $\mathcal{C} \subseteq \mathrm{dom}(f)$ is

$$\mathrm{bproj}_{f,\mathcal{C}}(\boldsymbol{v}) := \underset{\boldsymbol{u} \in \mathcal{C}}{\arg\min}\, B_f(\boldsymbol{u}, \boldsymbol{v}).$$

It turns out that these operators are intimately connected to the gradient mapping of the convex conjugate.

Proposition 17.5 (Link with conjugate's gradient). If $\Omega = f + g$, then for all $\boldsymbol{\theta} \in \text{dom}(f^*)$

$$\nabla\Omega^*(\boldsymbol{\theta}) = \text{bprox}_{f,g}(\nabla f^*(\boldsymbol{\theta})).$$

In particular, if $\Omega = f + \iota_C$, then for all $\boldsymbol{\theta} \in \text{dom}(f^*)$

$$\nabla\Omega^*(\boldsymbol{\theta}) = \text{bproj}_{f,C}(\nabla f^*(\boldsymbol{\theta})).$$

We give two examples below.

Example 17.4 (Bregman projections on the simplex). If $f(\boldsymbol{u}) = \frac{1}{2}\|\boldsymbol{u}\|_2^2$, then

$$\text{bproj}_{f,\triangle^D}(\boldsymbol{v}) = \arg\min_{\boldsymbol{u}\in\triangle^D} \frac{1}{2}\|\boldsymbol{u} - \boldsymbol{v}\|_2^2.$$

If $f(\boldsymbol{u}) = \langle\boldsymbol{u}, \log\boldsymbol{u} - \mathbf{1}\rangle$, then

$$\text{bproj}_{f,\triangle^D}(\boldsymbol{v}) = \arg\min_{\boldsymbol{u}\in\mathbb{R}_+^D} \text{KL}(\boldsymbol{u}, \boldsymbol{v}) = \text{softmax}(\boldsymbol{\theta}),$$

where $\boldsymbol{v} = \nabla f^*(\boldsymbol{\theta}) = \exp(\boldsymbol{\theta})$.

Therefore, the softmax can be seen as a projection onto the probability simplex in the Kullback-Leilbler divergence sense!

17.4 Fenchel-Young loss functions

We end this chapter with a brief review of the Fenchel-Young family of loss functions (Blondel *et al.*, 2020), which includes all loss functions in Table 17.1.

Definition 17.4 (Fenchel-Young loss). The Fenchel-Young loss function generated by Ω is

$$\ell_\Omega(\boldsymbol{\theta}, \boldsymbol{t}) := \Omega^*(\boldsymbol{\theta}) + \Omega(\boldsymbol{t}) - \langle\boldsymbol{\theta}, \boldsymbol{t}\rangle$$

where $\boldsymbol{\theta} \in \text{dom}(\Omega^*)$ and $\boldsymbol{t} \in \text{dom}(\Omega)$.

Typically, we set $\boldsymbol{\theta} = f(\boldsymbol{x}, \boldsymbol{w})$, where f is a model prediction function with parameters $\boldsymbol{w}$ and $\boldsymbol{t} = \phi(\boldsymbol{y})$, where $\phi\colon \mathcal{Y} \to \text{dom}(\Omega)$. For instance,

suppose we work with categorical outputs $y \in [M]$. Then, we can set $\phi(y) = \boldsymbol{e}_y$, where $\boldsymbol{e}_y$ is the one-hot encoding of y.

The important point to notice is that the Fenchel-Young loss is defined over arguments in **mixed spaces**: $\boldsymbol{\theta}$ belongs to the dual space, while $\boldsymbol{t}$ belongs to the primal space. In fact, the Fenchel-Young loss is intimately connected to the Bregman divergence, since $B_\Omega(\boldsymbol{t}, \boldsymbol{v}) = \Omega^*(\boldsymbol{\theta}) + \Omega(\boldsymbol{t}) - \langle \boldsymbol{\theta}, \boldsymbol{t} \rangle$, if we set $\boldsymbol{\theta} = \nabla\Omega(\boldsymbol{v})$. The key properties of Fenchel-Young loss functions are summarized below.

Proposition 17.6 (Properties of Fenchel-Young loss functions).

1. **Non-negativity:** $\ell_\Omega(\boldsymbol{\theta}, \boldsymbol{t}) \geq 0$ for all $\boldsymbol{\theta} \in \mathrm{dom}(\Omega^*)$ and $\boldsymbol{t} \in \mathrm{dom}(\Omega)$.

2. **Positivity:** $\ell_\Omega(\boldsymbol{\theta}, \boldsymbol{t}) = 0$ if and only if $\nabla\Omega^*(\boldsymbol{\theta}) = \boldsymbol{t}$, assuming Ω is strictly convex.

3. **Convexity:** $\ell_\Omega(\boldsymbol{\theta}, \boldsymbol{t})$ is convex in $\boldsymbol{\theta}$ (regardless of Ω) and in $\boldsymbol{t}$ (if Ω is convex)

4. **Relation with composite Bregman divergence:**

$$0 \leq \underbrace{B_\Omega(\boldsymbol{t}, \nabla\Omega^*(\boldsymbol{\theta}))}_{\text{possibly nonconvex in } \boldsymbol{\theta}} \leq \underbrace{\ell_\Omega(\boldsymbol{\theta}, \boldsymbol{t})}_{\text{convex in } \boldsymbol{\theta}}.$$

See Blondel *et al.* (2020) for an in-depth study of more properties.

17.5   Summary

The convex conjugate serves as a powerful abstraction in **Fenchal duality**, decoupling the dual expression and function-specific terms. The convex conjugate is also tightly connected to **Bregman divergences** and can be used to derive the family of **Fenchel-Young loss** functions, which can be seen as mixed-space Bregman divergences.

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