

The Elements of Differentiable Programming¹

Mathieu Blondel²

Google DeepMind

mblondel@google.com

Vincent Roulet³

Google DeepMind

vroulet@google.com

Contents ¹

1	Introduction	4	2
1.1	What is differentiable programming?	4	
1.2	Book goals and scope	6	
1.3	Intended audience	7	
1.4	How to read this book?	7	
1.5	Related work	7	
I	Fundamentals	9	3
2	Differentiation	10	4
2.1	Univariate functions	10	5
2.1.1	Derivatives	10	
2.1.2	Calculus rules	13	
2.1.3	Leibniz's notation	15	
2.2	Multivariate functions	16	
2.2.1	Directional derivatives	16	
2.2.2	Gradients	17	
2.2.3	Jacobians	20	
2.3	Linear differentiation maps	26	
2.3.1	The need for linear maps	26	
2.3.2	Euclidean spaces	27	

2.3.3	Linear maps and their adjoints	28	1
2.3.4	Jacobian-vector products	29	
2.3.5	Vector-Jacobian products	30	
2.3.6	Chain rule	31	
2.3.7	Functions of multiple inputs (fan-in)	32	
2.3.8	Functions of multiple outputs (fan-out)	34	
2.3.9	Extensions to non-Euclidean linear spaces	34	
2.4	Second-order differentiation	36	
2.4.1	Second derivatives	36	
2.4.2	Second directional derivatives	36	
2.4.3	Hessians	37	
2.4.4	Hessian-vector products	39	
2.4.5	Second-order Jacobians	39	
2.5	Higher-order differentiation	40	
2.5.1	Higher-order derivatives	40	
2.5.2	Higher-order directional derivatives	41	
2.5.3	Higher-order Jacobians	41	
2.5.4	Taylor expansions	42	
2.6	Differential geometry	43	
2.6.1	Differentiability on manifolds	43	
2.6.2	Tangent spaces and pushforward operators	44	
2.6.3	Cotangent spaces and pullback operators	45	
2.7	Generalized derivatives	48	
2.7.1	Rademacher's theorem	49	
2.7.2	Clarke derivatives	49	
2.8	Summary	52	

3	Probabilistic learning	54	2
3.1	Probability distributions	54	3
3.1.1	Discrete probability distributions	54	
3.1.2	Continuous probability distributions	55	
3.2	Maximum likelihood estimation	56	
3.2.1	Negative log-likelihood	56	
3.2.2	Consistency w.r.t. the Kullback-Leibler divergence	56	
3.3	Probabilistic supervised learning	57	
3.3.1	Conditional probability distributions	57	

3.3.2	Inference	57	1
3.3.3	Binary classification	58	
3.3.4	Multiclass classification	60	
3.3.5	Regression	61	
3.3.6	Multivariate regression	62	
3.3.7	Integer regression	63	
3.3.8	Loss functions	63	
3.4	Exponential family distributions	65	
3.4.1	Definition	65	
3.4.2	The log-partition function	67	
3.4.3	Maximum entropy principle	68	
3.4.4	Maximum likelihood estimation	69	
3.4.5	Probabilistic learning with exponential families	69	
3.5	Summary	71	

II Differentiable programs 72 2

4	Parameterized programs 73 3	4	
4.1	Representing computer programs	73	
4.1.1	Computation chains	73	
4.1.2	Directed acyclic graphs	74	
4.1.3	Computer programs as DAGs	76	
4.1.4	Arithmetic circuits	78	
4.2	Feedforward networks	79	
4.3	Multilayer perceptrons	79	
4.3.1	Combining affine layers and activations	79	
4.3.2	Link with generalized linear models	80	
4.4	Activation functions	81	
4.4.1	Scalar-to-scalar nonlinearities	81	
4.4.2	Vector-to-scalar nonlinearities	81	
4.4.3	Scalar-to-scalar probability mappings	82	
4.4.4	Vector-to-vector probability mappings	83	
4.5	Residual neural networks	85	
4.6	Recurrent neural networks	86	
4.6.1	Vector to sequence	86	

4.6.2	Sequence to vector	88	1
4.6.3	Sequence to sequence (aligned)	88	
4.6.4	Sequence to sequence (unaligned)	88	
4.7	Summary	89	
5	Control flows	90	2
5.1	Comparison operators	90	
5.2	Soft inequality operators	92	
5.2.1	Heuristic definition	92	
5.2.2	Stochastic process perspective	92	
5.3	Soft equality operators	93	
5.3.1	Heuristic definition	93	
5.3.2	Gaussian process perspective	94	
5.4	Logical operators	95	
5.5	Continuous extensions of logical operators	96	
5.5.1	Probabilistic continuous extension	96	
5.5.2	Triangular norms and co-norms	98	
5.6	If-else statements	98	
5.6.1	Differentiating through branch variables	99	
5.6.2	Differentiating through predicate variables	100	
5.6.3	Continuous relaxations	101	
5.7	Else-if statements	102	
5.7.1	Encoding K branches	103	
5.7.2	Conditionals	104	
5.7.3	Differentiating through branch variables	105	
5.7.4	Differentiating through predicate variables	106	
5.7.5	Continuous relaxations	106	
5.8	For loops	108	
5.9	Scan functions	109	
5.10	While loops	110	
5.10.1	While loops as cyclic graphs	110	
5.10.2	Unrolled while loops	111	
5.10.3	Markov chain perspective	113	
5.11	Summary	116	

6 Finite differences	118	2
6.1 Forward differences	118	3
6.2 Backward differences	119	
6.3 Central differences	120	
6.4 Higher-accuracy finite differences	121	
6.5 Higher-order finite differences	122	
6.6 Complex-step derivatives	123	
6.7 Complexity	124	
6.8 Summary	124	
7 Automatic differentiation	126	4
7.1 Computation chains	126	5
7.1.1 Forward-mode	127	
7.1.2 Reverse-mode	129	
7.1.3 Complexity of entire Jacobians	134	
7.2 Feedforward networks	136	
7.2.1 Computing the adjoint	136	
7.2.2 Computing the gradient	137	
7.3 Computation graphs	139	
7.3.1 Forward-mode	139	
7.3.2 Reverse-mode	140	
7.3.3 Complexity, the Baur-Strassen theorem	140	
7.4 Implementation	141	
7.4.1 Primitive functions	141	
7.4.2 Closure under function composition	142	
7.4.3 Examples of JVPs and VJPs	143	
7.4.4 Automatic linear transposition	144	
7.5 Checkpointing	145	
7.5.1 Recursive halving	146	
7.5.2 Dynamic programming	148	
7.5.3 Online checkpointing	150	
7.6 Reversible layers	151	
7.6.1 General case	151	
7.6.2 Case of orthonormal JVPs	151	

7.7	Randomized forward-mode estimator	152	1
7.8	Summary	152	
8	Second-order automatic differentiation	154	2
8.1	Hessian-vector products	154	3
8.1.1	Four possible methods	154	
8.1.2	Complexity	155	
8.2	Gauss-Newton matrix	159	
8.2.1	An approximation of the Hessian	159	
8.2.2	Gauss-Newton chain rule	160	
8.2.3	Gauss-Newton vector product	160	
8.2.4	Gauss-Newton matrix factorization	161	
8.2.5	Stochastic setting	162	
8.3	Fisher information matrix	162	
8.3.1	Definition using the score function	162	
8.3.2	Link with the Hessian	163	
8.3.3	Equivalence with the Gauss-Newton matrix	163	
8.4	Inverse-Hessian vector product	165	
8.4.1	Definition as a linear map	165	
8.4.2	Implementation with matrix-free linear solvers	165	
8.4.3	Complexity	166	
8.5	Second-order backpropagation	167	
8.5.1	Second-order Jacobian chain rule	167	
8.5.2	Computation chains	169	
8.5.3	Fan-in and fan-out	170	
8.6	Block diagonal approximations	171	
8.6.1	Feedforward networks	171	
8.6.2	Computation graphs	173	
8.7	Diagonal approximations	173	
8.7.1	Computation chains	174	
8.7.2	Computation graphs	175	
8.8	Randomized estimators	176	
8.8.1	Girard-Hutchinson estimator	176	
8.8.2	Bartlett estimator for the factorization	177	
8.8.3	Bartlett estimator for the diagonal	178	
8.9	Summary	179	

9 Inference in graphical models as differentiation	180	1
9.1 Chain rule of probability	180	2
9.2 Conditional independence	181	
9.3 Inference problems	182	
9.3.1 Joint probability distributions	182	
9.3.2 Likelihood	182	
9.3.3 Maximum a-posteriori inference	182	
9.3.4 Marginal inference	183	
9.3.5 Expectation, convex hull, marginal polytope	183	
9.3.6 Complexity of brute force	185	
9.4 Markov chains	185	
9.4.1 The Markov property	186	
9.4.2 Time-homogeneous Markov chains	188	
9.4.3 Higher-order Markov chains	189	
9.5 Bayesian networks	189	
9.5.1 Expressing variable dependencies using DAGs	189	
9.5.2 Parameterizing Bayesian networks	190	
9.5.3 Ancestral sampling	191	
9.6 Markov random fields	191	
9.6.1 Expressing factors using undirected graphs	191	
9.6.2 MRFs as exponential family distributions	192	
9.6.3 Conditional random fields	194	
9.6.4 Sampling	194	
9.7 Inference on chains	194	
9.7.1 The forward-backward algorithm	195	
9.7.2 The Viterbi algorithm	196	
9.8 Inference on trees	198	
9.9 Inference as differentiation	199	
9.9.1 Inference as gradient of the log-partition	199	
9.9.2 Semirings and softmax operators	200	
9.9.3 Inference as backpropagation	202	
9.10 Summary	204	
10 Differentiating through optimization	205	3
10.1 Implicit functions	205	4
10.1.1 Optimization problems	206	

10.1.2	Nonlinear equations	206	1
10.1.3	Application to bilevel optimization	206	
10.2	Envelope theorems	207	
10.2.1	Danskin's theorem	208	
10.2.2	Rockafellar's theorem	209	
10.3	Implicit function theorem	210	
10.3.1	Univariate functions	210	
10.3.2	Multivariate functions	211	
10.3.3	JVP and VJP of implicit functions	213	
10.3.4	Proof of the implicit function theorem	214	
10.4	Adjoint state method	214	
10.4.1	Differentiating nonlinear equations	214	
10.4.2	Relation with envelope theorems	216	
10.4.3	Proof using the method of Lagrange multipliers	216	
10.4.4	Proof using the implicit function theorem	217	
10.4.5	Reverse mode as adjoint method with backsubstitution	217	
10.5	Inverse function theorem	220	
10.5.1	Differentiating inverse functions	220	
10.5.2	Link with the implicit function theorem	220	
10.5.3	Proof of inverse function theorem	221	
10.6	Summary	222	
11	Differentiating through integration	224	2
11.1	Differentiation under the integral sign	224	3
11.2	Differentiating through expectations	225	
11.2.1	The easy case	226	
11.2.2	Exact gradients	226	
11.2.3	Application to expected loss functions	227	
11.2.4	Application to experimental design	228	
11.3	Score function estimators, REINFORCE	229	
11.3.1	Scalar-valued functions	229	
11.3.2	Variance reduction	231	
11.3.3	Vector-valued functions	233	
11.3.4	Second derivatives	234	
11.4	Path gradient estimators, reparametrization trick	235	
11.4.1	Location-scale transforms	235	

11.4.2	Inverse transforms	236	1
11.4.3	Pushforward operators	238	
11.4.4	Change-of-variables theorem	240	2
11.5	Stochastic programs	240	
11.5.1	Stochastic computation graphs	241	
11.5.2	Examples	243	
11.5.3	Unbiased gradient estimators	245	
11.5.4	Local vs. global expectations	247	
11.6	Differential equations	248	
11.6.1	Parameterized differential equations	248	
11.6.2	Continuous adjoint method	251	
11.6.3	Gradients via the continuous adjoint method	252	
11.6.4	Gradients via reverse-mode on discretization	254	
11.6.5	Reversible discretization schemes	255	
11.6.6	Proof of the continuous adjoint method	257	
11.7	Summary	259	

IV Smoothing programs 261 3

12	Smoothing by optimization 262	4	
12.1	Primal approach	262	5
12.1.1	Infimal convolution	262	
12.1.2	Moreau envelope	263	
12.2	Legendre–Fenchel transforms, convex conjugates	265	
12.2.1	Definition	265	
12.2.2	Closed-form examples	266	
12.2.3	Properties	267	
12.2.4	Conjugate calculus	269	
12.2.5	Fast Legendre transform	270	
12.3	Dual approach	270	
12.3.1	Duality between strong convexity and smoothness .	270	
12.3.2	Smoothing by dual regularization	271	
12.3.3	Equivalence between primal and dual regularizations	273	
12.4	Examples	273	
12.4.1	Smoothed ReLU functions	273	

12.4.2 Smoothed max operators	274	1
12.4.3 Relaxed step functions (sigmoids)	276	
12.4.4 Relaxed argmax operators	277	
12.5 Summary	278	
13 Smoothing by integration	279	2
13.1 Convolution	279	3
13.1.1 Convolution operators	279	
13.1.2 Convolution with a kernel	280	
13.1.3 Discrete convolution	281	
13.1.4 Differentiation	283	
13.1.5 Multidimensional convolution	283	
13.1.6 Link between convolution and infimal convolution	283	
13.2 Fourier and Laplace transforms	284	
13.2.1 Convolution theorem	284	
13.2.2 Link between Fourier and Legendre transforms	285	
13.2.3 The soft Legendre-Fenchel transform	285	
13.3 Examples	289	
13.3.1 Smoothed step function	289	
13.3.2 Smoothed ReLU function	290	
13.4 Perturbation of blackbox functions	291	
13.4.1 Expectation in a location-scale family	291	
13.4.2 Gradient estimation by reparametrization	292	
13.4.3 Gradient estimation by SFE, Stein's lemma	293	
13.4.4 Link between reparametrization and SFE	294	
13.4.5 Variance reduction and evolution strategies	295	
13.4.6 Zero-temperature limit	296	
13.5 Gumbel tricks	296	
13.5.1 The Gumbel distribution	296	
13.5.2 Perturbed comparison	297	
13.5.3 Perturbed argmax	298	
13.5.4 Perturbed max	300	
13.5.5 Gumbel trick for sampling	301	
13.5.6 Perturb-and-MAP	301	
13.5.7 Gumbel-softmax	303	
13.6 Summary	304	

V Optimizing differentiable programs

306 1

14 Optimization basics	307	2
14.1 Objective functions	307	3
14.2 Oracles	308	
14.3 Variational perspective of optimization algorithms	309	
14.4 Classes of functions	309	
14.4.1 Lipschitz functions	309	
14.4.2 Smooth functions	310	
14.4.3 Convex functions	312	
14.4.4 Strongly-convex functions	314	
14.4.5 Nonconvex functions	315	
14.5 Performance guarantees	316	
14.6 Summary	319	

15 First-order optimization	320	4
15.1 Gradient descent	320	5
15.1.1 Variational perspective	320	
15.1.2 Convergence for smooth functions	321	
15.1.3 Momentum and accelerated variants	323	
15.2 Stochastic gradient descent	323	
15.2.1 Stochastic gradients	324	
15.2.2 Vanilla SGD	325	
15.2.3 Momentum variants	326	
15.2.4 Adaptive variants	327	
15.3 Projected gradient descent	328	
15.3.1 Variational perspective	328	
15.3.2 Optimality conditions	329	
15.3.3 Commonly-used projections	329	
15.4 Proximal gradient method	330	
15.4.1 Variational perspective	331	
15.4.2 Optimality conditions	331	
15.4.3 Commonly-used proximal operators	332	
15.5 Summary	333	

16 Second-order optimization	1	334	2
16.1 Newton's method		334	
16.1.1 Variational perspective		334	
16.1.2 Regularized Newton method		335	
16.1.3 Approximate direction		336	
16.1.4 Convergence guarantees		336	
16.1.5 Linesearch		336	
16.1.6 Geometric interpretation		337	
16.1.7 Stochastic Newton's method		338	
16.2 Gauss-Newton method		339	
16.2.1 With exact outer function		340	
16.2.2 With approximate outer function		341	
16.2.3 Linesearch		342	
16.2.4 Stochastic Gauss-Newton		342	
16.3 Natural gradient descent		343	
16.3.1 Variational perspective		343	
16.3.2 Stochastic natural gradient descent		344	
16.4 Quasi-Newton methods		345	
16.4.1 BFGS		345	
16.4.2 Limited-memory BFGS		346	
16.5 Approximate Hessian diagonal inverse preconditionners		346	
16.6 Summary		346	
17 Duality	3	348	4
17.1 Dual norms		348	
17.2 Fenchel duality		349	
17.3 Bregman divergences		352	
17.4 Fenchel-Young loss functions		355	
17.5 Summary		356	
References		357	

The Elements of Differentiable Programming¹

Mathieu Blondel¹ and Vincent Roulet^{1,2}

¹Google DeepMind³

ABSTRACT⁴

Artificial intelligence has recently experienced remarkable ⁵ 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 ⁶ 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 ⁷ 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 ¹

Table 1: Naming conventions ²

Notation	Description	³
$\mathcal{X} \subseteq \mathbb{R}^D$	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	
$x \in \mathcal{X}$	Input vector	
$y \in \mathcal{Y}$	Target vector	
$s_k \in \mathcal{S}_k$	State vector k	
$w \in \mathcal{W}$	Network (model) weights	
$\lambda \in \Lambda$	Hyperparameters	
$\theta \in \Theta$	Distribution parameters, logits	
$\pi \in [0, 1]$	Probability value	
$\pi \in \Delta^M$	Probability vector	

Table 2: Naming conventions (continued) 1

Notation	Description	2
f	Network function	
$f(\cdot; \mathbf{x})$	Network function with \mathbf{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}	
μ, σ^2	Mean and variance	
Z	Random noise variable	

1

Introduction¹

1.1 What is differentiable programming?²

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.³

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.⁴

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.⁵

In differentiable programming, a program is also defined as the⁶

composition of elementary operations, forming a **computation graph**.¹ 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?²

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?⁴

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 1

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 3

While autodiff is a key ingredient of differentiable programming, this 4 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 5

The present book aims to provide a comprehensive introduction to 6 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**.¹ 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.²

1.3 Intended audience³

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.⁴

1.4 How to read this book?⁵

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.⁶

1.5 Related work⁷

Differentiable programming builds upon a variety of connected topics.⁸ 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).⁹

A tutorial with a focus on machine learning is provided by Baydin [\(2018\)](#). 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 Equilibrium 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 I¹

Fundamentals²

2

Differentiation¹

In this chapter, we review key differentiation concepts. In particular,² we emphasize on the fundamental role played by linear maps.

2.1 Univariate functions³

2.1.1 Derivatives⁴

Before studying derivatives, we briefly recall the definition of function⁵ continuity.

Definition 2.1 (Continuous function). A function $f : \mathbb{R} \rightarrow \mathbb{R}$ is⁶ continuous at a point $w \in \mathbb{R}$ if

$$\lim_{v \rightarrow w} f(v) = f(w). \quad ^7$$

A function f is said to be continuous if it is continuous at all points⁸ in its domain.

In the following, we use Landau's little o notation. We write⁹

$$g(v) = o(f(v)) \text{ as } v \rightarrow w \quad ^{10}$$

if 1

$$\lim_{v \rightarrow w} \frac{|g(v)|}{|f(v)|} = 0. \quad 2$$

That is, the function f dominates g in the limit $v \rightarrow w$. For example, f 3 is continuous at w if and only if

$$f(w + \delta) = f(w) + o(1) \text{ as } \delta \rightarrow 0. \quad 4$$

We now explain derivatives. Consider a function $f : \mathbb{R} \rightarrow \mathbb{R}$. As 5 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 $f : \mathbb{R} \rightarrow \mathbb{R}$ at $w \in \mathbb{R}$ is defined as 6

$$f'(w) := \lim_{\delta \rightarrow 0} \frac{f(w + \delta) - f(w)}{\delta}, \quad 7$$

provided that the limit exists. If $f'(w)$ is well-defined at a particular 8 w , we say that the function f is **differentiable** at w .

Here, and in the following definitions, if f is differentiable at any 9 $w \in \mathbb{R}$, 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 $f : \mathbb{R} \rightarrow \mathbb{R}$ 10 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 11

$$f(w + \delta) = f(w) + f'(w)\delta + o(\delta) \text{ as } \delta \rightarrow 0. \quad 12$$

Since $f'(w)\delta + o(\delta) = o(1)$ as $\delta \rightarrow 0$, f is continuous at w . 13 \square

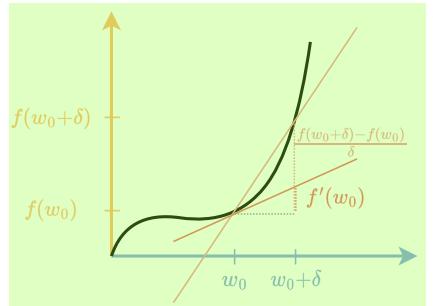


Figure 2.1: A function f can be locally approximated around a point w_0 by a secant, 2 a linear function $w \mapsto aw + b$ with slope a and intercept b , crossing f at w_0 with value $y_0 = f(w_0)$ and crossing at $w_0 + \delta$ with value $u_\delta = f(w_0 + \delta)$. Using $u_0 = aw_0 + b$ and $u_\delta = a(w_0 + \delta) + b$, 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 $\delta \rightarrow 0$. 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 3 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 $\sin w$, 4 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 $f(w) = w^n$ 5

for $w \in \mathbb{R}$, $n \in \mathbb{N} \setminus \{0\}$. For any $\delta \in \mathbb{R}$, we have ¹

$$\begin{aligned}\frac{f(w + \delta) - f(w)}{\delta} &= \frac{(w + \delta)^n - w^n}{\delta} \\ &= \frac{\sum_{k=0}^n \binom{n}{k} \delta^k w^{n-k} - w^n}{\delta} \\ &= \sum_{k=1}^n \binom{n}{k} \delta^{k-1} w^{n-k} \\ &= \binom{n}{1} w^{n-1} + \sum_{k=2}^n \binom{n}{k} \delta^{k-1} w^{n-k},\end{aligned}\tag{2}$$

where, in the second line, we used the binomial theorem. Since ³ $\binom{n}{1} = n$ and $\lim_{\delta \rightarrow 0} \sum_{k=2}^n \binom{n}{k} \delta^{k-1} w^{n-k} = 0$, 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 $f : \mathcal{U} \rightarrow \mathbb{R}$ 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 ⁵

For a given $w \in \mathbb{R}$ and two functions $f : \mathbb{R} \rightarrow \mathbb{R}$ and $g : \mathbb{R} \rightarrow \mathbb{R}$, 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 ¹ or their products exist and lead to the following rules

$$\begin{aligned} \forall a, b \in \mathbb{R}, \quad (af + bg)'(w) &= af'(w) + bg'(w) && \text{(Linearity)} \quad 2 \\ (fg)'(w) &= f'(w)g(w) + f(w)g'(w), && \text{(Product rule)} \end{aligned}$$

where $(fg)(w) = f(w)g(w)$. The linearity can be verified directly from ³ the linearity of the limits. For the product rule, in little o notation, we have, as $\delta \rightarrow 0$,

$$\begin{aligned} (fg)(w + \delta) &= (f(w) + f'(w)\delta + o(\delta))(g(w) + g'(w)\delta + o(\delta)) \quad 4 \\ &= f(w)g(w) + f'(w)g(w)\delta + f(w)g'(w)\delta + o(\delta), \end{aligned}$$

hence the result. ⁵

If the derivatives of g at w and of f at $g(w)$ exist, then the derivative ⁶ of the composition $(f \circ g)(w) := f(g(w))$ at w exist and is given by

$$(f \circ g)'(w) = f'(g(w))g'(w). \quad 7 \quad \text{(Chain rule)}$$

We prove this result more generally in Proposition 2.2. As seen in the ⁸ 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 ⁹ 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 ¹⁰

step by step as follows, denoting $\text{sq}(w) := w^2$, 1

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

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 3 procedure, which is the main idea of automatic differentiation presented in Chapter 7.

2.1.3 Leibniz's notation 4

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 5

$$f' = \frac{du}{dw} \quad \text{with} \quad f'(w) = \left. \frac{du}{dw} \right|_w \quad 6$$

where du and dw denote infinitesimal variations of u and w respectively 7 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 $u = f(v)$

$$\frac{du}{dw} = \frac{du}{dv} \cdot \frac{dv}{dw}. \quad 8$$

This hints that derivatives are multiplied when considering compositions. 9 At evaluation, the chain rule in Leibniz notation recovers the formula presented above as

$$\left. \frac{du}{dw} \right|_w = \left. \frac{du}{dv} \right|_{g(w)} \left. \frac{dv}{dw} \right|_w = f'(g(w))g'(w) = (f \circ g)'(w). \quad 10$$

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

2.2.1 Directional derivatives 3

Let us now consider a function $f : \mathbb{R}^P \rightarrow \mathbb{R}$ of multiple inputs $\mathbf{w} = (w_1, \dots, w_P) \in \mathbb{R}^P$. The most important example in machine learning is a function which, to the parameters $\mathbf{w} \in \mathbb{R}^P$ 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 $f(\mathbf{w} + \delta\mathbf{v}) - f(\mathbf{w})$ of f around $\mathbf{w} \in \mathbb{R}^P$ in the direction $\mathbf{v} \in \mathbb{R}^P$ by an amount $\delta > 0$. This consideration naturally leads to the definition of the directional derivative.

Definition 2.3 (Directional derivative). The **directional derivative** 5 of f at \mathbf{w} in the **direction** \mathbf{v} is given by

$$\partial f(\mathbf{w})[\mathbf{v}] := \lim_{\delta \rightarrow 0} \frac{f(\mathbf{w} + \delta\mathbf{v}) - f(\mathbf{w})}{\delta}, \quad 6$$

provided that the limit exists. 7

One example of directional derivative consists in computing the 8 derivative of a function f at \mathbf{w} in any of the canonical directions

$$\mathbf{e}_i := (0, \dots, 0, \underbrace{1}_{i}, 0, \dots, 0). \quad 9$$

This allows us to define the notion of **partial derivatives**, denoted for $i \in [P]$ 1

$$\partial_i f(\mathbf{w}) := \partial f(\mathbf{w})[\mathbf{e}_i] = \lim_{\delta \rightarrow 0} \frac{f(\mathbf{w} + \delta \mathbf{e}_i) - f(\mathbf{w})}{\delta}. \quad 2$$

This is also denoted in Leibniz's notation as $\partial_i f(\mathbf{w}) = \frac{\partial f(\mathbf{w})}{\partial w_i}$ or $\partial_i f(\mathbf{w}) = \partial_{w_i} f(\mathbf{w})$. By moving along only the i^{th} coordinate of the function, the partial derivative is akin to using the function $\phi(\omega_i) = f(w_1, \dots, \omega_i, \dots, w_P)$ around ω_i , letting all other coordinates fixed at their values \mathbf{w}_i . 3

2.2.2 Gradients 4

We now introduce the gradient vector, which gathers the partial derivatives. We first recall the definitions of linear map and linear form. 5

Definition 2.4 (Linear map, linear form). A function $l : \mathbb{R}^P \rightarrow \mathbb{R}^M$ 6 is a **linear map** if for any $a_1, a_2 \in \mathbb{R}$, $\mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^D$,

$$l[a_1 \mathbf{v}_1 + a_2 \mathbf{v}_2] = a_1 l(\mathbf{v}_1) + a_2 l(\mathbf{v}_2). \quad 7$$

A linear map with values in \mathbb{R} , $l : \mathbb{R}^P \rightarrow \mathbb{R}$, is called a **linear form**. 8

Linearity plays a crucial role in the differentiability of a function. 9

Definition 2.5 (Differentiability, single-output case). A function $f : \mathbb{R}^P \rightarrow \mathbb{R}$ is **differentiable** at $\mathbf{w} \in \mathbb{R}^P$ if its directional derivative is defined along any direction, linear in any direction, and if 10

$$\lim_{\|\mathbf{v}\|_2 \rightarrow 0} \frac{|f(\mathbf{w} + \mathbf{v}) - f(\mathbf{w}) - \partial f(\mathbf{w})[\mathbf{v}]|}{\|\mathbf{v}\|_2} = 0. \quad 11$$

We can now introduce the gradient. 12

Definition 2.6 (Gradient). The **gradient** of a differentiable function $f : \mathbb{R}^P \rightarrow \mathbb{R}$ at a point $\mathbf{w} \in \mathbb{R}^P$ is defined as the vector of partial derivatives 13

$$\nabla f(\mathbf{w}) := \begin{pmatrix} \partial_1 f(\mathbf{w}) \\ \vdots \\ \partial_P f(\mathbf{w}) \end{pmatrix} = \begin{pmatrix} \partial f(\mathbf{w})[\mathbf{e}_1] \\ \vdots \\ \partial f(\mathbf{w})[\mathbf{e}_P] \end{pmatrix}. \quad 14$$

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

$$\partial f(\mathbf{w})[\mathbf{v}] = \sum_{i=1}^P v_i \partial f(\mathbf{w})[\mathbf{e}_i] = \langle \mathbf{v}, \nabla f(\mathbf{w}) \rangle. \quad 2$$

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 $f(\mathbf{w}) = \mathbf{a}^\top \mathbf{w} = \sum_{i=1}^P a_i w_i$ is differentiable as we have $(\mathbf{a}^\top (\mathbf{w} + \mathbf{v}) - \mathbf{a}^\top \mathbf{w} - \mathbf{a}^\top \mathbf{v})/\|\mathbf{v}\|_2 = 0$ for any \mathbf{v} and in particular for $\|\mathbf{v}\| \rightarrow 0$. Moreover, its gradient is naturally given by $\nabla f(\mathbf{w}) = \mathbf{a}$.

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

$$f(\mathbf{w} + \mathbf{v}) = f(\mathbf{w}) + \langle \mathbf{g}, \mathbf{v} \rangle + o(\|\mathbf{v}\|_2), \quad 6$$

then f is differentiable at \mathbf{w} since $\langle \mathbf{g}, \cdot \rangle$ is linear. Moreover, \mathbf{g} is then the gradient of f at \mathbf{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 $f : \mathbb{R}^P \rightarrow \mathbb{R}$ 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. 1

In the remainder of this chapter, all definitions of differentiability are in terms of Fréchet differentiability. 2

Example 2.3 illustrates how to compute the gradient of the logistic loss and validate its differentiability. 3

Example 2.3 (Gradient of logistic loss). Consider the logistic loss 4
 $\ell(\boldsymbol{\theta}, \mathbf{y}) := -\mathbf{y}^\top \boldsymbol{\theta} + \log \sum_{i=1}^M e^{\theta_i}$, that measures the prediction error of the logits $\boldsymbol{\theta} \in \mathbb{R}^M$ w.r.t. the correct label $\mathbf{y} \in \{\mathbf{e}_1, \dots, \mathbf{e}_M\}$. Let us compute the gradient of this loss w.r.t. $\boldsymbol{\theta}$ for fixed \mathbf{y} , i.e., we want to compute the gradient of $f(\boldsymbol{\theta}) := \ell(\boldsymbol{\theta}, \mathbf{y})$. Let us decompose f as $f = l + \text{logsumexp}$ with $l(\boldsymbol{\theta}) := \langle -\mathbf{y}, \boldsymbol{\theta} \rangle$ and

$$\text{logsumexp}(\boldsymbol{\theta}) := \log \sum_{i=1}^M e^{\theta_i}, \quad 5$$

the log-sum-exp function. The function l is linear so differentiable 6 with gradient $\nabla l(\boldsymbol{\theta}) = -\mathbf{y}$. We therefore focus on logsumexp. Denoting $\exp(\boldsymbol{\theta}) = (\exp(\theta_1), \dots, \exp(\theta_M))$, and using that $\exp(1+x) = 1+x+o(x)$, and $\log(1+x) = x+o(x)$, we get

$$\begin{aligned} \text{logsumexp}(\boldsymbol{\theta} + \mathbf{v}) &= \log(\langle \exp(\boldsymbol{\theta} + \mathbf{v}), \mathbf{1} \rangle) \\ &= \log(\langle \exp(\boldsymbol{\theta}), \mathbf{1} \rangle + \langle \exp(\boldsymbol{\theta}), \mathbf{v} \rangle + o(\|\mathbf{v}\|_2)) \\ &= \log(\langle \exp(\boldsymbol{\theta}), \mathbf{1} \rangle) + \left\langle \frac{\exp(\boldsymbol{\theta})}{\langle \exp(\boldsymbol{\theta}), \mathbf{1} \rangle}, \mathbf{v} \right\rangle + o(\|\mathbf{v}\|_2), \end{aligned} \quad 7$$

The above decomposition of $\text{logsumexp}(\boldsymbol{\theta} + \mathbf{v})$ shows that it is 8 differentiable, and that $\nabla \text{logsumexp}(\boldsymbol{\theta}) = \text{softargmax}(\boldsymbol{\theta})$, where

$$\text{softargmax}(\boldsymbol{\theta}) := \left(e^{\theta_1} / \left(\sum_{j=1}^M e^{\theta_j} \right), \dots, e^{\theta_M} / \left(\sum_{j=1}^M e^{\theta_j} \right) \right). \quad 9$$

In total, we then get that $\nabla f(\boldsymbol{\theta}) = -\mathbf{y} + \text{softargmax}(\boldsymbol{\theta})$. 10

Linearity of gradients 1

The notion of differentiability for multi-inputs functions naturally inherits from the linearity of derivatives for single-input functions. For any $u_1, \dots, u_M \in \mathbb{R}$ and any multi-inputs functions f_1, \dots, f_M differentiable at \mathbf{w} , the function $u_1 f_1 + \dots + u_M f_M$ is differentiable at \mathbf{w} and its gradient is 2

$$\nabla(u_1 f_1 + \dots + u_M f_M)(\mathbf{w}) = u_1 \nabla f_1(\mathbf{w}) + \dots + u_M \nabla f_M(\mathbf{w}). \quad 3$$

Why is the gradient useful? 4

The gradient defines the steepest ascent direction of f from \mathbf{w} . To see 5 why, notice that

$$\arg \max_{\mathbf{v} \in \mathbb{R}^P, \|\mathbf{v}\|_2 \leq 1} \partial f(\mathbf{w})[\mathbf{v}] = \arg \max_{\mathbf{v} \in \mathbb{R}^P, \|\mathbf{v}\|_2 \leq 1} \langle \mathbf{v}, \nabla f(\mathbf{w}) \rangle = \nabla f(\mathbf{w}) / \|\nabla f(\mathbf{w})\|_2, \quad 6$$

where we assumed $\nabla f(\mathbf{w}) \neq \mathbf{0}$. The gradient $\nabla f(\mathbf{w})$ is orthogonal to 7 the level set of the function (the set of points \mathbf{w} sharing the same value $f(\mathbf{w})$) and points towards higher values of f as illustrated in Fig. 2.2. Conversely, the negated gradient $-\nabla f(\mathbf{w})$ 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 $\mathbf{w}_{t+1} = \mathbf{w}_t - \gamma \nabla f(\mathbf{w}_t)$, for $\gamma > 0$. It therefore seeks for a minimizer of f by moving along the direction of steepest descent around \mathbf{w}_t given, up to a multiplicative factor, by $-\nabla f(\mathbf{w}_t)$.

2.2.3 Jacobians 8

Let us now consider a multi-output function $f : \mathbb{R}^P \rightarrow \mathbb{R}^M$ defined by 9 $f(\mathbf{w}) := (f_1(\mathbf{w}), \dots, f_M(\mathbf{w}))$, where $f_j : \mathbb{R}^P \rightarrow \mathbb{R}$. 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:

$$\partial f(\mathbf{w})[\mathbf{v}] := \lim_{\delta \rightarrow 0} \frac{f(\mathbf{w} + \delta \mathbf{v}) - f(\mathbf{w})}{\delta} = \lim_{\delta \rightarrow 0} \begin{pmatrix} \frac{f_1(\mathbf{w} + \delta \mathbf{v}) - f_1(\mathbf{w})}{\delta} \\ \vdots \\ \frac{f_M(\mathbf{w} + \delta \mathbf{v}) - f_M(\mathbf{w})}{\delta} \end{pmatrix} \in \mathbb{R}^M, \quad 10$$

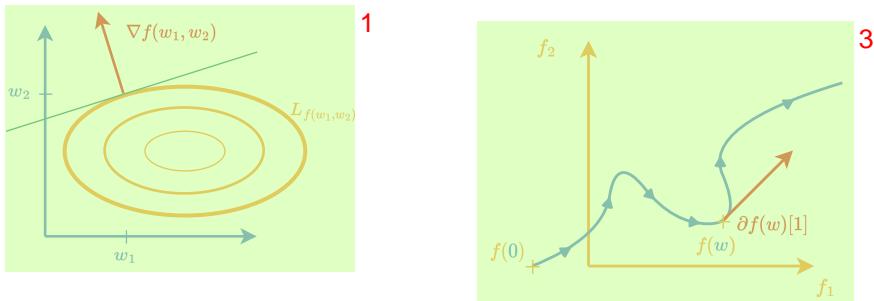


Figure 2.2: The gradient of a function $f : \mathbb{R}^2 \rightarrow \mathbb{R}$ at (w_1, w_2) is the normal vector to the tangent space of the level set $L_{f(w_1, w_2)} = \{(w'_1, w'_2) : f(w'_1, w'_2) = f(w_1, w_2)\}$ and points towards points with higher function values.

Figure 2.3: The directional derivative of a parameterized curve $f : \mathbb{R} \rightarrow \mathbb{R}^2$ 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. 5
The directional derivative of f in the direction $\mathbf{v} \in \mathbb{R}^P$ is therefore the vector that gathers the directional derivative of each f_j , i.e., $\partial f(\mathbf{w})[\mathbf{v}] = (\partial f_j(\mathbf{v})[\mathbf{v}])_{j=1}^M$. In particular, we can define the **partial derivatives** of f at \mathbf{w} as the vectors

$$\partial_i f(\mathbf{w}) := \partial f(\mathbf{w})[e_i] = \begin{pmatrix} \partial_i f_1(\mathbf{w}) \\ \vdots \\ \partial_i f_M(\mathbf{w}) \end{pmatrix} \in \mathbb{R}^M. \quad 6$$

As for the usual definition of the derivative, the directional derivative 7
can provide a linear approximation of a function around a current input
as illustrated in Fig. 2.3 for a parameterized curve $f : \mathbb{R} \rightarrow \mathbb{R}^2$.

Just as in the single-output case, differentiability is defined not only 8
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 $f : \mathbb{R}^P \rightarrow \mathbb{R}^M$ is (Fréchet) **differentiable** at a point $\mathbf{w} \in \mathbb{R}^P$ if its 9
directional derivative is defined along any directions, linear along

any directions, and, 1

$$\lim_{\|\mathbf{v}\|_2 \rightarrow 0} \frac{\|f(\mathbf{w} + \mathbf{v}) - f(\mathbf{w}) - \partial f(\mathbf{w})[\mathbf{v}]\|_2}{\|\mathbf{v}\|_2} = 0. \quad 2$$

The partial derivatives of all function coordinates are gathered in 3
the **Jacobian matrix**.

Definition 2.8 (Jacobian). The **Jacobian** of a differentiable function $f : \mathbb{R}^P \rightarrow \mathbb{R}^M$ at \mathbf{w} is defined as the matrix of all partial derivatives of all coordinate functions provided they exist, 4

$$\partial f(\mathbf{w}) := \begin{pmatrix} \partial_1 f_1(\mathbf{w}) & \dots & \partial_P f_1(\mathbf{w}) \\ \vdots & \ddots & \vdots \\ \partial_1 f_M(\mathbf{w}) & \dots & \partial_P f_M(\mathbf{w}) \end{pmatrix} \in \mathbb{R}^{M \times P}. \quad 5$$

The Jacobian can be represented by stacking columns of partial 6
derivatives or rows of gradients,

$$\partial f(\mathbf{w}) = (\partial_1 f(\mathbf{w}), \dots, \partial_P f(\mathbf{w})) = \begin{pmatrix} \nabla f_1(\mathbf{w})^\top \\ \vdots \\ \nabla f_M(\mathbf{w})^\top \end{pmatrix}. \quad 7$$

By linearity, the directional derivative of f at \mathbf{w} along any input 8
direction $\mathbf{v} = \sum_{i=1}^P v_i \mathbf{e}_i \in \mathbb{R}^P$ is then given by

$$\partial f(\mathbf{w})[\mathbf{v}] = \sum_{i=1}^P v_i \partial_i f(\mathbf{w}) = \partial f(\mathbf{w})\mathbf{v} \in \mathbb{R}^M. \quad 9$$

Notice that we use bold ∂ to indicate the Jacobian matrix. The 10
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 $f(\mathbf{w} + \mathbf{v})$
around $\mathbf{v} = \mathbf{0}$. If we find a linear map l such that

$$f(\mathbf{w} + \mathbf{v}) = f(\mathbf{w}) + l[\mathbf{v}] + o(\|\mathbf{v}\|_2), \quad 11$$

then f is differentiable at \mathbf{w} . Moreover, if l is represented by matrix \mathbf{J} 12
such that $l[\mathbf{v}] = \mathbf{J}\mathbf{v}$ then $\mathbf{J} = \partial f(\mathbf{w})$.

As a simple example, any linear function $f(\mathbf{w}) = \mathbf{A}\mathbf{w}$ for $\mathbf{A} \in \mathbb{R}^{M \times P}$ ¹ is differentiable, since all its coordinate-wise components are single-output linear functions, and the Jacobian of f at any \mathbf{w} is given by $\partial f(\mathbf{w}) = \mathbf{A}$.

Remark 2.3 (Special cases of the Jacobian). For single-output functions $f : \mathbb{R}^P \rightarrow \mathbb{R}$, i.e., $M = 1$, the Jacobian matrix reduces to a row vector identified as the transpose of the gradient, i.e.,²

$$\partial f(\mathbf{w}) = \nabla f(\mathbf{w})^\top \in \mathbb{R}^{1 \times P}. \quad 3$$

For a single-input function $f : \mathbb{R} \rightarrow \mathbb{R}^M$, the Jacobian reduces to a single column vector of directional derivatives, denoted⁴

$$\partial f(w) = f'(w) := \begin{pmatrix} f'_1(w) \\ \vdots \\ f'_M(w) \end{pmatrix} \in \mathbb{R}^{M \times 1}. \quad 5$$

For a single-input single-output function $f : \mathbb{R} \rightarrow \mathbb{R}$, the Jacobian⁶ reduces to the derivative of f , i.e.,

$$\partial f(w) = f'(w) \in \mathbb{R}. \quad 7$$

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 2.3.⁸

Example 2.4 (Jacobian matrix of the softplus activation). Consider⁹ the element-wise application of the softplus defined for $\mathbf{w} \in \mathbb{R}^P$ by

$$f(\mathbf{w}) := \begin{pmatrix} \sigma(w_1) \\ \vdots \\ \sigma(w_P) \end{pmatrix} \in \mathbb{R}^P \quad \text{where} \quad \sigma(w) := \log(1 + e^w). \quad 10$$

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

$$\boldsymbol{\partial}f(\mathbf{w}) = \text{diag}(\sigma'(w_1), \dots, \sigma'(w_P)) := \begin{pmatrix} \sigma'(w_1) & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \sigma'(w_P) \end{pmatrix}. \quad 2$$

Variations along outputs 3

Rather than considering variations of f along an **input** direction $\mathbf{v} \in \mathbb{R}^P$, 4 we may also consider the variations of f along an **output** direction $\mathbf{u} \in \mathbb{R}^M$, namely, computing the gradients $\nabla(\mathbf{u}^\top f)(\mathbf{w})$ of single-output functions, where we defined

$$(\mathbf{u}^\top f)(\mathbf{w}) := \mathbf{u}^\top f(\mathbf{w}) \in \mathbb{R}. \quad 5$$

In particular, we may consider computing the gradients $\nabla f_j(\mathbf{w})$ of each 6 function coordinate $f_j = \mathbf{e}_j^\top f$ at \mathbf{w} , where \mathbf{e}_j is the j^{th} canonical vector in \mathbb{R}^M . The infinitesimal variations of f at \mathbf{w} along any output direction $\mathbf{u} = \sum_{j=1}^M u_j \mathbf{e}_j \in \mathbb{R}^M$ are given by

$$\nabla(\mathbf{u}^\top f)(\mathbf{w}) = \sum_{j=1}^M u_j \nabla f_j(\mathbf{w}) = \boldsymbol{\partial}f(\mathbf{w})^\top \mathbf{u} \in \mathbb{R}, \quad 7$$

where $\boldsymbol{\partial}f(\mathbf{w})^\top$ is the Jacobian's transpose. Using the definition of 8 derivative as a limit, we obtain for $i \in [P]$

$$\nabla_i(\mathbf{u}^\top f)(\mathbf{w}) = [\boldsymbol{\partial}f(\mathbf{w})^\top \mathbf{u}]_i = \lim_{\delta \rightarrow 0} \frac{\mathbf{u}^\top (f(\mathbf{w} + \delta \mathbf{e}_i) - f(\mathbf{w}))}{\delta}. \quad 9$$

Chain rule 10

Equipped with a generic definition of differentiability and the associated 11 objects, gradients and Jacobians, we can now generalize the chain rule,

previously introduced for single-input single-output functions. 1

Proposition 2.2 (Chain rule). Consider $f : \mathbb{R}^P \rightarrow \mathbb{R}^M$ and $g : \mathbb{R}^M \rightarrow \mathbb{R}^R$. If f is differentiable at $\mathbf{w} \in \mathbb{R}^P$ and g is differentiable at $f(\mathbf{w}) \in \mathbb{R}^M$, then the composition $g \circ f$ is differentiable at $\mathbf{w} \in \mathbb{R}^P$ and its Jacobian is given by 2

$$\partial(g \circ f)(\mathbf{w}) = \partial g(f(\mathbf{w})) \partial f(\mathbf{w}). 3$$

Proof. We progressively approximate $g \circ f(\mathbf{w} + \mathbf{v})$ using the differentiability of f at \mathbf{w} and g at $f(\mathbf{w})$, 4

$$\begin{aligned} g(f(\mathbf{w} + \mathbf{v})) &= g(f(\mathbf{w}) + \partial f(\mathbf{w})\mathbf{v} + o(\|\mathbf{v}\|)) \\ &= g(f(\mathbf{w})) + \partial g(f(\mathbf{w})) \partial f(\mathbf{w})\mathbf{v} + o(\|\mathbf{v}\|). \end{aligned} 5$$

Hence, $g \circ f$ is differentiable at \mathbf{w} with Jacobian $\partial g(f(\mathbf{w})) \partial f(\mathbf{w})$. □ 6

Proposition 2.2 can be seen as the cornerstone of any derivative 7 computations. For example, it can be used to rederive the linearity or the product rule associated to the derivatives of single-input single-output functions.

When g is scalar-valued, combined with Remark 2.3, we obtain a 8 simple expression for $\nabla(g \circ f)$.

Proposition 2.3 (Chain rule, scalar-valued case). Consider $f : \mathbb{R}^P \rightarrow \mathbb{R}^M$ and $g : \mathbb{R}^M \rightarrow \mathbb{R}$. The gradient of the composition is given by 9

$$\nabla(g \circ f)(\mathbf{w}) = \partial f(\mathbf{w})^\top \nabla g(f(\mathbf{w})). 10$$

This is illustrated with linear regression in Example 2.5. 11

Example 2.5 (Linear regression). Consider the squared residuals of 12 a linear regression of N inputs $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^D$ onto N targets $y_1, \dots, y_N \in \mathbb{R}$ with a vector $\mathbf{w} \in \mathbb{R}^D$, that is, $f(\mathbf{w}) = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 = \sum_{i=1}^N (\mathbf{x}_i^\top \mathbf{w} - y_i)^2$ for $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N)^\top \in \mathbb{R}^{N \times D}$ and $\mathbf{y} = (y_1, \dots, y_N)^\top \in \mathbb{R}^N$.

The function f can be decomposed into a linear mapping 13 $f_1(\mathbf{w}) = \mathbf{X}\mathbf{w}$ and a squared error $f_2(\mathbf{p}) = \|\mathbf{p} - \mathbf{y}\|_2^2$, so that $f = f_2 \circ f_1$. We can then apply the chain rule in Proposition 2.3 to

get 1

$$\nabla f(\mathbf{w}) = \partial f_1(\mathbf{w})^\top \nabla f_2(f_1(\mathbf{w})) \quad 2$$

provided that f_1, f_2 are differentiable at \mathbf{w} and $f_1(\mathbf{w})$, respectively. 3

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

$$\nabla f(\mathbf{w}) = 2\mathbf{X}^\top(f_1(\mathbf{w}) - \mathbf{y}) = 2\mathbf{X}^\top(\mathbf{X}\mathbf{w} - \mathbf{y}). \quad 4$$

2.3 Linear differentiation maps 5

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. 6

2.3.1 The need for linear maps 7

So far, we have focused on functions $f: \mathbb{R}^P \rightarrow \mathbb{R}^M$, 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 $f(\mathbf{W}) = \mathbf{W}\mathbf{x}$, where $\mathbf{x} \in \mathbb{R}^D$ and $\mathbf{W} \in \mathbb{R}^{M \times D}$. This function takes a matrix as input, not a vector. Of course, a matrix $\mathbf{W} \in \mathbb{R}^{M \times D}$ can always be “flattened” into a vector $\mathbf{w} \in \mathbb{R}^{MD}$, by stacking the columns of \mathbf{W} . We denote this operation by $\mathbf{w} = \text{vec}(\mathbf{W})$ and its inverse by $\mathbf{W} = \text{vec}^{-1}(\mathbf{w})$. We can then equivalently write $f(\mathbf{W})$ as $\tilde{f}(\mathbf{w}) = f(\text{vec}^{-1}(\mathbf{w})) = \text{vec}^{-1}(\mathbf{w})\mathbf{x}$, so that the previous framework applies. However, we will now see that this would be inefficient. 8

Indeed, the resulting Jacobian of \tilde{f} at any \mathbf{w} consists in a matrix 1 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 $\mathbf{W} \in \mathbb{R}^{M \times D}$ in a direction $\mathbf{V} \in \mathbb{R}^{M \times D}$ would consist in (i) vectorizing \mathbf{V} into $\mathbf{v} = \text{vec}(\mathbf{V})$, (ii) computing the matrix-vector product $\partial\tilde{f}(\mathbf{w})\mathbf{v}$ at a cost of M^3D^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 2 infer that the directional derivative of f at any $\mathbf{W} \in \mathbb{R}^{M \times D}$ in any direction $\mathbf{V} \in \mathbb{R}^{M \times D}$ is simply given by the function itself applied on \mathbf{V} . Namely, we have $\partial f(\mathbf{W})[\mathbf{V}] = f(\mathbf{V}) = \mathbf{V}\mathbf{x}$, 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 $\partial\tilde{f}(\mathbf{w})$. 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 3

Linear spaces, a.k.a. **vector spaces**, are spaces equipped (and closed 4 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 $\mathbf{u}, \mathbf{v} \in \mathcal{E}$, and $a \in \mathbb{R}$, we have $\mathbf{u} + \mathbf{v} \in \mathcal{E}$ and $a \cdot \mathbf{u} \in \mathcal{E}$. **Euclidean spaces** are linear spaces equipped with a basis $\mathbf{e}_1, \dots, \mathbf{e}_P \in \mathcal{E}$. Any element $\mathbf{v} \in \mathcal{E}$ can be decomposed as $\mathbf{v} = \sum_{i=1}^P v_i \mathbf{e}_i$ for some unique scalars $v_1, \dots, v_P \in \mathbb{R}$. 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 $\mathbf{E}_{ij} \in \{0, 1\}^{P_1 \times P_2}$ 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, $\mathbf{W} \in \mathbb{R}^{P_1 \times P_2}$ can be written $\mathbf{W} = \sum_{i,j=1}^{P_1, P_2} W_{ij} \mathbf{E}_{ij}$.

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 $\langle \cdot, \cdot \rangle : \mathcal{E} \times \mathcal{E} \rightarrow \mathbb{R}$ that is

- bilinear, that is, $\mathbf{x} \mapsto \langle \mathbf{x}, \mathbf{w} \rangle$ and $\mathbf{y} \mapsto \langle \mathbf{v}, \mathbf{y} \rangle$ are linear for any $\mathbf{w}, \mathbf{v} \in \mathcal{E}$
- symmetric, that is, $\langle \mathbf{w}, \mathbf{v} \rangle = \langle \mathbf{w}, \mathbf{v} \rangle$ for any $\mathbf{w}, \mathbf{v} \in \mathcal{E}$
- positive definite, that is, $\langle \mathbf{w}, \mathbf{w} \rangle \geq 0$ for any $\mathbf{w} \in \mathcal{E}$, and $\langle \mathbf{w}, \mathbf{w} \rangle = 0$ if and only if $\mathbf{w} = 0$.

An inner product defines a norm $\|\mathbf{w}\| := \sqrt{\langle \mathbf{w}, \mathbf{w} \rangle}$.³

The norm induced by an inner product defines a distance $\|\mathbf{w} - \mathbf{v}\|$ ⁴ between $\mathbf{w}, \mathbf{v} \in \mathcal{E}$, and therefore a notion of convergence.

For vectors, where $\mathcal{E} = \mathbb{R}^P$, the inner product is the usual one⁵ $\langle \mathbf{w}, \mathbf{v} \rangle = \sum_{i=1}^P w_i v_i$. 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 $\mathbf{W}, \mathbf{V} \in \mathbb{R}^{P_1 \times P_2}$ by

$$\langle \mathbf{W}, \mathbf{V} \rangle := \langle \text{vec}(\mathbf{W}), \text{vec}(\mathbf{V}) \rangle = \sum_{i,j=1}^{P_1, P_2} W_{ij} V_{ij} = \text{tr}(\mathbf{W}^\top \mathbf{V}), \quad 6$$

where $\text{tr}(\mathbf{Z}) := \sum_{i=1}^P Z_{ii}$ is the trace operator defined for square matrices⁷ $\mathbf{Z} \in \mathbb{R}^{P \times P}$. For tensors of order R , which generalize matrices to $\mathcal{E} = \mathbb{R}^{P_1 \times \dots \times P_R}$, the inner product is defined similarly for $\mathbf{W}, \mathbf{V} \in \mathbb{R}^{P_1 \times \dots \times P_R}$ by

$$\langle \mathbf{W}, \mathbf{V} \rangle := \langle \text{vec}(\mathbf{W}), \text{vec}(\mathbf{V}) \rangle = \sum_{i_1, \dots, i_R=1}^{P_1, \dots, P_R} \mathbf{W}_{i_1 \dots i_R} \mathbf{V}_{i_1 \dots i_R}, \quad 8$$

where $\mathbf{W}_{i_1 \dots i_R}$ is the $(i_1, \dots, i_R)^{\text{th}}$ entry of \mathbf{W} .⁹

2.3.3 Linear maps and their adjoints¹⁰

The notion of linear map defined in Definition 2.4 naturally extends¹¹ to Euclidean spaces. Namely, a function $l : \mathcal{E} \rightarrow \mathcal{F}$ from a Euclidean

space \mathcal{E} onto a Euclidean space \mathcal{F} is a **linear map** if for any $\mathbf{w}, \mathbf{v} \in \mathcal{E}$ ¹ and $a, b \in \mathbb{R}$, we have $l[a\mathbf{w} + b\mathbf{v}] = a \cdot l[\mathbf{w}] + b \cdot l[\mathbf{v}]$. When $\mathcal{E} = \mathbb{R}^P$ and $\mathcal{F} = \mathbb{R}^M$, there always exists a matrix $\mathbf{A} \in \mathbb{R}^{M \times P}$ such that $l[\mathbf{x}] = \mathbf{Ax}$. Therefore, we can think of \mathbf{A} as the “materialization” of l .

We can define the adjoint operator of a linear map.²

Definition 2.10 (Adjoint operator). Given two Euclidean spaces \mathcal{E} ³ 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 $l : \mathcal{E} \rightarrow \mathcal{F}$ is the unique linear map $l^* : \mathcal{F} \rightarrow \mathcal{E}$ such that for any $\mathbf{v} \in \mathcal{E}$ and $\mathbf{u} \in \mathcal{F}$,

$$\langle l[\mathbf{v}], \mathbf{u} \rangle_{\mathcal{F}} = \langle \mathbf{v}, l^*[\mathbf{u}] \rangle_{\mathcal{E}}. \quad 4$$

The adjoint can be thought as the counterpart of the matrix transpose for linear maps. When $l[\mathbf{v}] = \mathbf{Av}$, we have $l^*[\mathbf{u}] = \mathbf{A}^\top \mathbf{u}$ since⁵

$$\langle l[\mathbf{v}], \mathbf{u} \rangle_{\mathcal{F}} = \langle \mathbf{Av}, \mathbf{u} \rangle_{\mathcal{F}} = \langle \mathbf{v}, \mathbf{A}^\top \mathbf{u} \rangle_{\mathcal{E}} = \langle \mathbf{v}, l^*[\mathbf{u}] \rangle_{\mathcal{E}}. \quad 6$$

2.3.4 Jacobian-vector products⁷

We now define the directional derivative using linear maps, leading⁸ 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 $f : \mathcal{E} \rightarrow \mathcal{F}$ is **differentiable** at a point $\mathbf{w} \in \mathcal{E}$ if the **directional derivative** along $\mathbf{v} \in \mathcal{E}$ ⁹

$$\partial f(\mathbf{w})[\mathbf{v}] := \lim_{\delta \rightarrow 0} \frac{f(\mathbf{w} + \delta\mathbf{v}) - f(\mathbf{w})}{\delta} = l[\mathbf{v}], \quad 10$$

is well-defined for any $\mathbf{v} \in \mathcal{E}$, linear in \mathbf{v} and if¹¹

$$\lim_{\|\mathbf{v}\|_2 \rightarrow 0} \frac{\|f(\mathbf{w} + \mathbf{v}) - f(\mathbf{w}) - l[\mathbf{v}]\|_2}{\|\mathbf{v}\|_2} = 0. \quad 12$$

We can now formally define the Jacobian-vector product.¹³

Definition 2.12 (Jacobian-vector product). For a differentiable function $f : \mathcal{E} \rightarrow \mathcal{F}$, the linear map $\partial f(\mathbf{w}) : \mathcal{E} \rightarrow \mathcal{F}$, mapping \mathbf{v} to $\partial f(\mathbf{w})[\mathbf{v}]$ is called the **Jacobian-vector product** (JVP) by analogy with Definition 2.8. Note that $\partial f : \mathcal{E} \rightarrow (\mathcal{E} \rightarrow \mathcal{F})$. 1

Strictly speaking, \mathbf{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. 2

Recovering the gradient 3

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. 4

Proposition 2.4 (Gradient). If a function $f : \mathcal{E} \rightarrow \mathbb{R}$ is differentiable at $\mathbf{w} \in \mathcal{E}$, then there exists $\nabla f(\mathbf{w}) \in \mathcal{E}$, called the **gradient** of f at \mathbf{w} such that the directional derivative of f at \mathbf{w} along any input direction $\mathbf{v} \in \mathcal{E}$ is given by 5

$$\partial f(\mathbf{w})[\mathbf{v}] = \langle \nabla f(\mathbf{w}), \mathbf{v} \rangle_{\mathcal{E}}. \quad 6$$

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. 7

2.3.5 Vector-Jacobian products 8

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. 9

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

$$\nabla \langle \mathbf{u}, f \rangle_{\mathcal{F}}(\mathbf{w}) = \partial f(\mathbf{w})^*[\mathbf{u}] \quad 2$$

where we denoted $\langle \mathbf{u}, f \rangle_{\mathcal{F}}(\mathbf{w}) := \langle \mathbf{u}, f(\mathbf{w}) \rangle_{\mathcal{F}}$. Note that $\partial f(\cdot)^* : \mathcal{E} \rightarrow \mathcal{F}$ ($\mathcal{F} \rightarrow \mathcal{E}$).

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

$$\begin{aligned} \partial(\langle \mathbf{u}, f \rangle_{\mathcal{F}})(\mathbf{w})[\mathbf{v}] &= \langle \mathbf{u}, \partial f(\mathbf{w})[\mathbf{v}] \rangle_{\mathcal{F}} \quad 5 \\ &= \langle \partial f(\mathbf{w})^*[\mathbf{u}], \mathbf{v} \rangle_{\mathcal{F}}. \end{aligned}$$

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

2.3.6 Chain rule ⁷

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 $f : \mathcal{E} \rightarrow \mathcal{F}$ and $g : \mathcal{F} \rightarrow \mathcal{G}$ for $\mathcal{E}, \mathcal{F}, \mathcal{G}$ some Euclidean spaces. If f is differentiable at $\mathbf{w} \in \mathcal{E}$ and g is differentiable at $f(\mathbf{w}) \in \mathcal{F}$, then the composition $g \circ f$ is differentiable at $\mathbf{w} \in \mathcal{E}$. Its JVP is given by

$$\partial(g \circ f)(\mathbf{w})[\mathbf{v}] = \partial g(f(\mathbf{w}))[\partial f(\mathbf{w})[\mathbf{v}]] \quad 10$$

and its VJP is given by 1

$$\partial(g \circ f)(\mathbf{w})^*[\mathbf{u}] = \partial f(\mathbf{w})^*[\partial g(f(\mathbf{w}))^*[\mathbf{u}]]. \quad 2$$

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 $f : \mathcal{E} \rightarrow \mathcal{F}$ and $g : \mathcal{F} \rightarrow \mathbb{R}$, the gradient of the composition is given by 4

$$\nabla(g \circ f)(\mathbf{w}) = \partial f(\mathbf{w})^*[\nabla g(f(\mathbf{w}))]. \quad 5$$

2.3.7 Functions of multiple inputs (fan-in) 6

Oftentimes, the inputs of a function do not belong to only one Euclidean space but to a product of them. An example is $f(\mathbf{x}, \mathbf{W}) = \mathbf{W}\mathbf{x}$, 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 $f(\mathbf{w}_1, \dots, \mathbf{w}_S)$ defined on $\mathcal{E} = \mathcal{E}_1 \times \dots \times \mathcal{E}_S$, 7 where $\mathbf{w}_i \in \mathcal{E}_i$. We denote the partial derivative with respect to the i^{th} input \mathbf{w}_i along $\mathbf{v}_i \in \mathcal{E}_i$ as $\partial_i f(\mathbf{w}_1, \dots, \mathbf{w}_S)[\mathbf{v}_i]$. 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 $f(\mathbf{w}) = f(\mathbf{w}_1, \dots, \mathbf{w}_S)$ with signature $f : \mathcal{E} \rightarrow \mathcal{F}$, where $\mathbf{w} := (\mathbf{w}_1, \dots, \mathbf{w}_S) \in \mathcal{E}$ and $\mathcal{E} := \mathcal{E}_1 \times \dots \times \mathcal{E}_S$. Then the JVP with the input direction $\mathbf{v} = (\mathbf{v}_1, \dots, \mathbf{v}_S) \in \mathcal{E}$ is given by 9

$$\begin{aligned} \partial f(\mathbf{w})[\mathbf{v}] &= \partial f(\mathbf{w}_1, \dots, \mathbf{w}_S)[\mathbf{v}_1, \dots, \mathbf{v}_S] \in \mathcal{F} \quad 10 \\ &= \sum_{i=1}^S \partial_i f(\mathbf{w}_1, \dots, \mathbf{w}_S)[\mathbf{v}_i]. \end{aligned}$$

The VJP with the output direction $\mathbf{u} \in \mathcal{F}$ is given by 1

$$\begin{aligned}\partial f(\mathbf{w})^*[\mathbf{u}] &= \partial f(\mathbf{w}_1, \dots, \mathbf{w}_S)^*[\mathbf{u}] \in \mathcal{E} \\ &= (\partial_1 f(\mathbf{w}_1, \dots, \mathbf{w}_S)^*[\mathbf{u}], \dots, \partial_S f(\mathbf{w}_1, \dots, \mathbf{w}_S)^*[\mathbf{u}]).\end{aligned}\quad 2$$

Example 2.6 (Matrix-vector product). Consider $f(\mathbf{x}, \mathbf{W}) = \mathbf{Wx}$, 3 where $\mathbf{W} \in \mathbb{R}^{M \times D}$ and $\mathbf{x} \in \mathbb{R}^D$. 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 $\mathbf{v} \in \mathbb{R}^D$ and $\mathbf{V} \in \mathbb{R}^{M \times D}$, we obtain

$$\partial f(\mathbf{x}, \mathbf{W})[\mathbf{v}, \mathbf{V}] = \mathbf{Wv} + \mathbf{Vx} \in \mathcal{F}. \quad 4$$

We can also access the individual JVPs as 5

$$\begin{aligned}\partial_1 f(\mathbf{x}, \mathbf{W})[\mathbf{v}] &= \mathbf{Wv} \in \mathcal{F}, \quad 6 \\ \partial_2 f(\mathbf{x}, \mathbf{W})[\mathbf{V}] &= \mathbf{Vx} \in \mathcal{F}.\end{aligned}$$

For the VJP, letting $\mathbf{u} \in \mathbb{R}^M$, we obtain 7

$$\partial f(\mathbf{x}, \mathbf{W})^*[\mathbf{u}] = (\mathbf{W}^\top \mathbf{u}, \mathbf{ux}^\top) \in \mathcal{E}. \quad 8$$

We can access the individual VJPs by 9

$$\begin{aligned}\partial_1 f(\mathbf{x}, \mathbf{W})^*[\mathbf{u}] &= \mathbf{W}^\top \mathbf{u} \in \mathcal{E}_1, \quad 10 \\ \partial_2 f(\mathbf{x}, \mathbf{W})^*[\mathbf{u}] &= \mathbf{ux}^\top \in \mathcal{E}_2.\end{aligned}$$

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 $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2)$, where \mathbf{x}_1 is a text part and \mathbf{x}_2 is an image part, and the network parameters are naturally grouped into three layers $\mathbf{w} = (\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3)$, we can write $f(\mathbf{x}, \mathbf{w}) = f((\mathbf{x}_1, \mathbf{x}_2), (\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3))$. 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. 11

Remark 2.5 (Hiding away inputs). It will often be convenient to 12 ignore inputs when differentiating. We use the semicolon for this

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

2.3.8 Functions of multiple outputs (fan-out) 2

Similarly, it is often convenient to deal with functions of multiple 3 outputs.

Proposition 2.9 (Multiple outputs). Consider a differentiable function of the form $f(\mathbf{w}) = (f_1(\mathbf{w}), \dots, f_T(\mathbf{w}))$, with signatures $f: \mathcal{E} \rightarrow \mathcal{F}$ and $f_i: \mathcal{E} \rightarrow \mathcal{F}_i$, where $\mathcal{F} := \mathcal{F}_1 \times \dots \times \mathcal{F}_T$. Then the JVP with the input direction $\mathbf{v} \in \mathcal{E}$ is given by 4

$$\partial f(\mathbf{w})[\mathbf{v}] = (\partial f_1(\mathbf{w})[\mathbf{v}], \dots, \partial f_T(\mathbf{w})[\mathbf{v}]) \in \mathcal{F}. \quad 5$$

The VJP with the output direction $\mathbf{u} = (\mathbf{u}_1, \dots, \mathbf{u}_T) \in \mathcal{F}$ is 6

$$\begin{aligned} \partial f(\mathbf{w})^*[\mathbf{u}] &= \partial f(\mathbf{w})^*[\mathbf{u}_1, \dots, \mathbf{u}_T] \in \mathcal{E}^7 \\ &= \sum_{i=1}^T \partial f_i(\mathbf{w})^*[\mathbf{u}_i]. \end{aligned}$$

Combined with the chain rule, we obtain that the Jacobian of 8

$$\mathbf{h}(\mathbf{w}) := g(f(\mathbf{w})) = g(f_1(\mathbf{w}), \dots, f_T(\mathbf{w})) \quad 9$$

is $\partial \mathbf{h}(\mathbf{w}) = \sum_{i=1}^T \partial_i f(g(\mathbf{w})) \circ \partial g_i(\mathbf{w})$ and therefore the JVP is 10

$$\partial \mathbf{h}(\mathbf{w})[\mathbf{v}] = \sum_{i=1}^T \partial_i f(g(\mathbf{w}))[\partial g_i(\mathbf{w})[\mathbf{v}]]. \quad 11$$

2.3.9 Extensions to non-Euclidean linear spaces 12

We focused on Euclidean spaces, i.e., linear spaces with a finite basis. 13 However, the notions introduced earlier can be defined in more generic

spaces.¹

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 $f : \mathcal{E} \rightarrow \mathcal{F}$ 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 $l[\mathbf{v}] \leq C\|\mathbf{v}\|$, 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 $f : \mathcal{E} \rightarrow \mathbb{R}$, the JVP $\partial f(\mathbf{w}) : \mathcal{E} \rightarrow \mathbb{R}$ is a linear form, Riesz's representation theorem ensures the existence of the gradient as the element $g \in \mathcal{E}$ such that $\partial f(\mathbf{w})\mathbf{v} = \langle g, \mathbf{v} \rangle$ for any $\mathbf{v} \in \mathcal{E}$. 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 ¹ 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

2.4.1 Second derivatives ³

For a single-input, single-output differentiable function $f : \mathbb{R} \rightarrow \mathbb{R}$, ⁴ its derivative at any point is itself a function $f' : \mathbb{R} \rightarrow \mathbb{R}$. We may then consider the derivative of the derivative at any point: the **second derivative**.

Definition 2.13 (Second derivative). The **second derivative** $f^{(2)}(w)$ ⁵ of a differentiable function $f : \mathbb{R} \rightarrow \mathbb{R}$ at $w \in \mathbb{R}$ is defined as the derivative of f' at w , that is,

$$f^{(2)}(w) := \lim_{\delta \rightarrow 0} \frac{f'(w + \delta) - f'(w)}{\delta}, \quad \text{⁶}$$

provided that the limit is well-defined. If the second derivative ⁷ 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 ⁸ 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 ⁹

For a multi-input function $f : \mathbb{R}^P \rightarrow \mathbb{R}$, 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 \mathbf{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 $f : \mathbb{R}^P \rightarrow \mathbb{R}$ at $\mathbf{w} \in \mathbb{R}^P$ along $\mathbf{v}, \mathbf{v}' \in \mathbb{R}^P$ ¹⁰ ¹¹

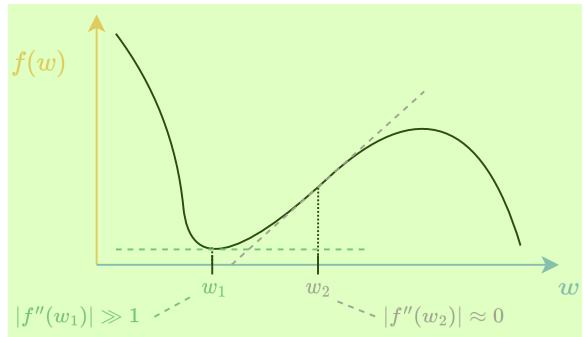


Figure 2.4: Points at which the second derivative is small are points along which the function is well approximated by its tangent line. On the other hand, point with large second derivative tend to be badly approximated by the tangent line.

is defined as the directional derivative of $\mathbf{w} \mapsto \partial f(\mathbf{w})[\mathbf{v}]$ along \mathbf{v}' ,³ that is,

$$\partial^2 f(\mathbf{w})[\mathbf{v}, \mathbf{v}'] := \lim_{\delta \rightarrow 0} \frac{\partial f(\mathbf{w} + \delta \mathbf{v}')[\mathbf{v}] - \partial f(\mathbf{w})[\mathbf{v}]}{\delta},$$
⁴

provided that $\partial f(\mathbf{w})[\mathbf{v}]$ is well-defined around \mathbf{w} and that the limit⁵ exists.

Of particular interest are the variations of a function around the⁶ canonical directions: the **second partial derivatives**, defined as

$$\partial_{ij}^2 f(\mathbf{w}) := \partial^2 f(\mathbf{w})[\mathbf{e}_i, \mathbf{e}_j]$$
⁷

for $\mathbf{e}_i, \mathbf{e}_j$ the i^{th} and j^{th} canonical directions in \mathbb{R}^P , respectively. In⁸ Leibniz notation, the second partial derivatives are denoted

$$\partial_{ij}^2 f(\mathbf{w}) = \frac{\partial^2 f(\mathbf{w})}{\partial w_i \partial w_j}.$$
⁹

2.4.3 Hessians¹⁰

For a multi-input function, twice differentiability is simply defined as¹¹ the differentiability of any directional derivative $\partial f(\mathbf{w})[\mathbf{v}]$ w.r.t. \mathbf{w} .