

Contents

Preface	<i>page</i> xvii
Installation	xxvi
Notation	xxix
1 Introduction	1
1.1 A Motivating Example	2
1.2 Key Components	4
1.3 Kinds of Machine Learning Problems	7
1.4 Roots	20
1.5 The Road to Deep Learning	22
1.6 Success Stories	25
1.7 The Essence of Deep Learning	27
1.8 Summary	29
1.9 Exercises	29
2 Preliminaries	30
2.1 Data Manipulation	30
2.1.1 Getting Started	30
2.1.2 Indexing and Slicing	33
2.1.3 Operations	34
2.1.4 Broadcasting	35
2.1.5 Saving Memory	36
2.1.6 Conversion to Other Python Objects	37
2.1.7 Summary	37
2.1.8 Exercises	38
2.2 Data Preprocessing	38
2.2.1 Reading the Dataset	38
2.2.2 Data Preparation	39
2.2.3 Conversion to the Tensor Format	40
2.2.4 Discussion	40
2.2.5 Exercises	40
2.3 Linear Algebra	41
2.3.1 Scalars	41

2.3.2	Vectors	42
2.3.3	Matrices	43
2.3.4	Tensors	44
2.3.5	Basic Properties of Tensor Arithmetic	45
2.3.6	Reduction	46
2.3.7	Non-Reduction Sum	47
2.3.8	Dot Products	48
2.3.9	Matrix–Vector Products	48
2.3.10	Matrix–Matrix Multiplication	49
2.3.11	Norms	50
2.3.12	Discussion	52
2.3.13	Exercises	53
2.4	Calculus	54
2.4.1	Derivatives and Differentiation	54
2.4.2	Visualization Utilities	56
2.4.3	Partial Derivatives and Gradients	58
2.4.4	Chain Rule	59
2.4.5	Discussion	59
2.4.6	Exercises	59
2.5	Automatic Differentiation	60
2.5.1	A Simple Function	60
2.5.2	Backward for Non-Scalar Variables	62
2.5.3	Detaching Computation	62
2.5.4	Gradients and Python Control Flow	63
2.5.5	Discussion	64
2.5.6	Exercises	64
2.6	Probability and Statistics	65
2.6.1	A Simple Example: Tossing Coins	66
2.6.2	A More Formal Treatment	69
2.6.3	Random Variables	69
2.6.4	Multiple Random Variables	70
2.6.5	An Example	73
2.6.6	Expectations	74
2.6.7	Discussion	76
2.6.8	Exercises	77
2.7	Documentation	78
2.7.1	Functions and Classes in a Module	79
2.7.2	Specific Functions and Classes	79
3	Linear Neural Networks for Regression	82
3.1	Linear Regression	82
3.1.1	Basics	83
3.1.2	Vectorization for Speed	88
3.1.3	The Normal Distribution and Squared Loss	88
3.1.4	Linear Regression as a Neural Network	90

3.1.5	Summary	92
3.1.6	Exercises	92
3.2	Object-Oriented Design for Implementation	93
3.2.1	Utilities	94
3.2.2	Models	96
3.2.3	Data	97
3.2.4	Training	98
3.2.5	Summary	99
3.2.6	Exercises	99
3.3	Synthetic Regression Data	99
3.3.1	Generating the Dataset	99
3.3.2	Reading the Dataset	100
3.3.3	Concise Implementation of the Data Loader	101
3.3.4	Summary	102
3.3.5	Exercises	102
3.4	Linear Regression Implementation from Scratch	103
3.4.1	Defining the Model	103
3.4.2	Defining the Loss Function	104
3.4.3	Defining the Optimization Algorithm	104
3.4.4	Training	105
3.4.5	Summary	107
3.4.6	Exercises	107
3.5	Concise Implementation of Linear Regression	108
3.5.1	Defining the Model	109
3.5.2	Defining the Loss Function	110
3.5.3	Defining the Optimization Algorithm	110
3.5.4	Training	110
3.5.5	Summary	111
3.5.6	Exercises	112
3.6	Generalization	112
3.6.1	Training Error and Generalization Error	113
3.6.2	Underfitting or Overfitting?	115
3.6.3	Model Selection	117
3.6.4	Summary	118
3.6.5	Exercises	118
3.7	Weight Decay	119
3.7.1	Norms and Weight Decay	119
3.7.2	High-Dimensional Linear Regression	121
3.7.3	Implementation from Scratch	121
3.7.4	Concise Implementation	123
3.7.5	Summary	125
3.7.6	Exercises	125
4	Linear Neural Networks for Classification	126
4.1	Softmax Regression	126

4.1.1	Classification	127
4.1.2	Loss Function	130
4.1.3	Information Theory Basics	131
4.1.4	Summary and Discussion	132
4.1.5	Exercises	133
4.2	The Image Classification Dataset	135
4.2.1	Loading the Dataset	135
4.2.2	Reading a Minibatch	136
4.2.3	Visualization	137
4.2.4	Summary	138
4.2.5	Exercises	138
4.3	The Base Classification Model	139
4.3.1	The Classifier Class	139
4.3.2	Accuracy	139
4.3.3	Summary	140
4.3.4	Exercises	140
4.4	Softmax Regression Implementation from Scratch	141
4.4.1	The Softmax	141
4.4.2	The Model	142
4.4.3	The Cross-Entropy Loss	142
4.4.4	Training	143
4.4.5	Prediction	144
4.4.6	Summary	145
4.4.7	Exercises	145
4.5	Concise Implementation of Softmax Regression	145
4.5.1	Defining the Model	146
4.5.2	Softmax Revisited	146
4.5.3	Training	147
4.5.4	Summary	148
4.5.5	Exercises	148
4.6	Generalization in Classification	148
4.6.1	The Test Set	149
4.6.2	Test Set Reuse	151
4.6.3	Statistical Learning Theory	152
4.6.4	Summary	154
4.6.5	Exercises	155
4.7	Environment and Distribution Shift	155
4.7.1	Types of Distribution Shift	156
4.7.2	Examples of Distribution Shift	158
4.7.3	Correction of Distribution Shift	160
4.7.4	A Taxonomy of Learning Problems	164
4.7.5	Fairness, Accountability, and Transparency in Machine Learning	166
4.7.6	Summary	166
4.7.7	Exercises	167

5	Multilayer Perceptrons	168
5.1	Multilayer Perceptrons	168
5.1.1	Hidden Layers	168
5.1.2	Activation Functions	172
5.1.3	Summary and Discussion	176
5.1.4	Exercises	176
5.2	Implementation of Multilayer Perceptrons	177
5.2.1	Implementation from Scratch	177
5.2.2	Concise Implementation	178
5.2.3	Summary	179
5.2.4	Exercises	180
5.3	Forward Propagation, Backward Propagation, and Computational Graphs	181
5.3.1	Forward Propagation	181
5.3.2	Computational Graph of Forward Propagation	182
5.3.3	Backpropagation	183
5.3.4	Training Neural Networks	184
5.3.5	Summary	184
5.3.6	Exercises	185
5.4	Numerical Stability and Initialization	185
5.4.1	Vanishing and Exploding Gradients	186
5.4.2	Parameter Initialization	188
5.4.3	Summary	190
5.4.4	Exercises	190
5.5	Generalization in Deep Learning	190
5.5.1	Revisiting Overfitting and Regularization	191
5.5.2	Inspiration from Nonparametrics	192
5.5.3	Early Stopping	193
5.5.4	Classical Regularization Methods for Deep Networks	194
5.5.5	Summary	194
5.5.6	Exercises	195
5.6	Dropout	195
5.6.1	Dropout in Practice	196
5.6.2	Implementation from Scratch	197
5.6.3	Concise Implementation	198
5.6.4	Summary	200
5.6.5	Exercises	200
5.7	Predicting House Prices on Kaggle	200
5.7.1	Downloading Data	201
5.7.2	Kaggle	201
5.7.3	Accessing and Reading the Dataset	202
5.7.4	Data Preprocessing	203
5.7.5	Error Measure	204
5.7.6	K -Fold Cross-Validation	205
5.7.7	Model Selection	206
5.7.8	Submitting Predictions on Kaggle	207

5.7.9	Summary and Discussion	207
5.7.10	Exercises	208
6	Builders' Guide	209
6.1	Layers and Modules	209
6.1.1	A Custom Module	211
6.1.2	The Sequential Module	213
6.1.3	Executing Code in the Forward Propagation Method	213
6.1.4	Summary	215
6.1.5	Exercises	215
6.2	Parameter Management	215
6.2.1	Parameter Access	216
6.2.2	Tied Parameters	217
6.2.3	Summary	218
6.2.4	Exercises	218
6.3	Parameter Initialization	218
6.3.1	Built-in Initialization	219
6.3.2	Summary	221
6.3.3	Exercises	221
6.4	Lazy Initialization	221
6.4.1	Summary	222
6.4.2	Exercises	223
6.5	Custom Layers	223
6.5.1	Layers without Parameters	223
6.5.2	Layers with Parameters	224
6.5.3	Summary	225
6.5.4	Exercises	225
6.6	File I/O	225
6.6.1	Loading and Saving Tensors	226
6.6.2	Loading and Saving Model Parameters	227
6.6.3	Summary	228
6.6.4	Exercises	228
6.7	GPUs	228
6.7.1	Computing Devices	229
6.7.2	Tensors and GPUs	230
6.7.3	Neural Networks and GPUs	232
6.7.4	Summary	233
6.7.5	Exercises	234
7	Convolutional Neural Networks	235
7.1	From Fully Connected Layers to Convolutions	236
7.1.1	Invariance	236
7.1.2	Constraining the MLP	237
7.1.3	Convolutions	239
7.1.4	Channels	240

7.1.5	Summary and Discussion	241
7.1.6	Exercises	241
7.2	Convolutions for Images	242
7.2.1	The Cross-Correlation Operation	242
7.2.2	Convolutional Layers	244
7.2.3	Object Edge Detection in Images	244
7.2.4	Learning a Kernel	246
7.2.5	Cross-Correlation and Convolution	247
7.2.6	Feature Map and Receptive Field	247
7.2.7	Summary	248
7.2.8	Exercises	249
7.3	Padding and Stride	249
7.3.1	Padding	250
7.3.2	Stride	252
7.3.3	Summary and Discussion	253
7.3.4	Exercises	254
7.4	Multiple Input and Multiple Output Channels	254
7.4.1	Multiple Input Channels	254
7.4.2	Multiple Output Channels	256
7.4.3	1×1 Convolutional Layer	257
7.4.4	Discussion	258
7.4.5	Exercises	258
7.5	Pooling	259
7.5.1	Maximum Pooling and Average Pooling	260
7.5.2	Padding and Stride	262
7.5.3	Multiple Channels	263
7.5.4	Summary	264
7.5.5	Exercises	264
7.6	Convolutional Neural Networks (LeNet)	264
7.6.1	LeNet	265
7.6.2	Training	268
7.6.3	Summary	268
7.6.4	Exercises	269
8	Modern Convolutional Neural Networks	270
8.1	Deep Convolutional Neural Networks (AlexNet)	271
8.1.1	Representation Learning	272
8.1.2	AlexNet	275
8.1.3	Training	278
8.1.4	Discussion	279
8.1.5	Exercises	280
8.2	Networks Using Blocks (VGG)	280
8.2.1	VGG Blocks	281
8.2.2	VGG Network	282
8.2.3	Training	283

8.2.4	Summary	284
8.2.5	Exercises	284
8.3	Network in Network (NiN)	285
8.3.1	NiN Blocks	286
8.3.2	NiN Model	286
8.3.3	Training	288
8.3.4	Summary	288
8.3.5	Exercises	289
8.4	Multi-Branch Networks (GoogLeNet)	289
8.4.1	Inception Blocks	290
8.4.2	GoogLeNet Model	291
8.4.3	Training	293
8.4.4	Discussion	294
8.4.5	Exercises	294
8.5	Batch Normalization	295
8.5.1	Training Deep Networks	295
8.5.2	Batch Normalization Layers	298
8.5.3	Implementation from Scratch	299
8.5.4	LeNet with Batch Normalization	301
8.5.5	Concise Implementation	302
8.5.6	Discussion	303
8.5.7	Exercises	304
8.6	Residual Networks (ResNet) and ResNeXt	305
8.6.1	Function Classes	305
8.6.2	Residual Blocks	307
8.6.3	ResNet Model	309
8.6.4	Training	311
8.6.5	ResNeXt	311
8.6.6	Summary and Discussion	314
8.6.7	Exercises	315
8.7	Densely Connected Networks (DenseNet)	315
8.7.1	From ResNet to DenseNet	315
8.7.2	Dense Blocks	316
8.7.3	Transition Layers	317
8.7.4	DenseNet Model	318
8.7.5	Training	319
8.7.6	Summary and Discussion	319
8.7.7	Exercises	320
8.8	Designing Convolution Network Architectures	320
8.8.1	The AnyNet Design Space	321
8.8.2	Distributions and Parameters of Design Spaces	323
8.8.3	RegNet	325
8.8.4	Training	326
8.8.5	Discussion	326
8.8.6	Exercises	327

9	Recurrent Neural Networks	328
9.1	Working with Sequences	330
9.1.1	Autoregressive Models	331
9.1.2	Sequence Models	333
9.1.3	Training	335
9.1.4	Prediction	336
9.1.5	Summary	338
9.1.6	Exercises	339
9.2	Converting Raw Text into Sequence Data	339
9.2.1	Reading the Dataset	340
9.2.2	Tokenization	340
9.2.3	Vocabulary	341
9.2.4	Putting It All Together	342
9.2.5	Exploratory Language Statistics	342
9.2.6	Summary	345
9.2.7	Exercises	345
9.3	Language Models	346
9.3.1	Learning Language Models	346
9.3.2	Perplexity	348
9.3.3	Partitioning Sequences	349
9.3.4	Summary and Discussion	351
9.3.5	Exercises	351
9.4	Recurrent Neural Networks	352
9.4.1	Neural Networks without Hidden States	352
9.4.2	Recurrent Neural Networks with Hidden States	353
9.4.3	RNN-Based Character-Level Language Models	355
9.4.4	Summary	356
9.4.5	Exercises	356
9.5	Recurrent Neural Network Implementation from Scratch	356
9.5.1	RNN Model	356
9.5.2	RNN-Based Language Model	358
9.5.3	Gradient Clipping	360
9.5.4	Training	361
9.5.5	Decoding	361
9.5.6	Summary	363
9.5.7	Exercises	363
9.6	Concise Implementation of Recurrent Neural Networks	364
9.6.1	Defining the Model	364
9.6.2	Training and Predicting	365
9.6.3	Summary	365
9.6.4	Exercises	366
9.7	Backpropagation Through Time	366
9.7.1	Analysis of Gradients in RNNs	366
9.7.2	Backpropagation Through Time in Detail	369
9.7.3	Summary	372

9.7.4	Exercises	372
10	Modern Recurrent Neural Networks	373
10.1	Long Short-Term Memory (LSTM)	374
10.1.1	Gated Memory Cell	374
10.1.2	Implementation from Scratch	378
10.1.3	Concise Implementation	379
10.1.4	Summary	380
10.1.5	Exercises	380
10.2	Gated Recurrent Units (GRU)	381
10.2.1	Reset Gate and Update Gate	381
10.2.2	Candidate Hidden State	382
10.2.3	Hidden State	382
10.2.4	Implementation from Scratch	383
10.2.5	Concise Implementation	384
10.2.6	Summary	386
10.2.7	Exercises	386
10.3	Deep Recurrent Neural Networks	386
10.3.1	Implementation from Scratch	388
10.3.2	Concise Implementation	388
10.3.3	Summary	389
10.3.4	Exercises	390
10.4	Bidirectional Recurrent Neural Networks	390
10.4.1	Implementation from Scratch	391
10.4.2	Concise Implementation	392
10.4.3	Summary	392
10.4.4	Exercises	392
10.5	Machine Translation and the Dataset	393
10.5.1	Downloading and Preprocessing the Dataset	393
10.5.2	Tokenization	395
10.5.3	Loading Sequences of Fixed Length	396
10.5.4	Reading the Dataset	397
10.5.5	Summary	398
10.5.6	Exercises	398
10.6	The Encoder–Decoder Architecture	399
10.6.1	Encoder	399
10.6.2	Decoder	400
10.6.3	Putting the Encoder and Decoder Together	400
10.6.4	Summary	400
10.6.5	Exercises	401
10.7	Sequence-to-Sequence Learning for Machine Translation	401
10.7.1	Teacher Forcing	402
10.7.2	Encoder	402
10.7.3	Decoder	404
10.7.4	Encoder–Decoder for Sequence-to-Sequence Learning	406

10.7.5	Loss Function with Masking	406
10.7.6	Training	406
10.7.7	Prediction	407
10.7.8	Evaluation of Predicted Sequences	408
10.7.9	Summary	409
10.7.10	Exercises	409
10.8	Beam Search	410
10.8.1	Greedy Search	410
10.8.2	Exhaustive Search	411
10.8.3	Beam Search	412
10.8.4	Summary	413
10.8.5	Exercises	413
11	Attention Mechanisms and Transformers	414
11.1	Queries, Keys, and Values	416
11.1.1	Visualization	417
11.1.2	Summary	419
11.1.3	Exercises	419
11.2	Attention Pooling by Similarity	420
11.2.1	Kernels and Data	420
11.2.2	Attention Pooling via Nadaraya–Watson Regression	422
11.2.3	Adapting Attention Pooling	423
11.2.4	Summary	424
11.2.5	Exercises	424
11.3	Attention Scoring Functions	425
11.3.1	Dot Product Attention	426
11.3.2	Convenience Functions	426
11.3.3	Scaled Dot Product Attention	428
11.3.4	Additive Attention	429
11.3.5	Summary	431
11.3.6	Exercises	431
11.4	The Bahdanau Attention Mechanism	432
11.4.1	Model	433
11.4.2	Defining the Decoder with Attention	433
11.4.3	Training	435
11.4.4	Summary	436
11.4.5	Exercises	437
11.5	Multi-Head Attention	437
11.5.1	Model	438
11.5.2	Implementation	438
11.5.3	Summary	440
11.5.4	Exercises	440
11.6	Self-Attention and Positional Encoding	440
11.6.1	Self-Attention	441
11.6.2	Comparing CNNs, RNNs, and Self-Attention	441

11.6.3	Positional Encoding	442
11.6.4	Summary	445
11.6.5	Exercises	445
11.7	The Transformer Architecture	446
11.7.1	Model	446
11.7.2	Positionwise Feed-Forward Networks	447
11.7.3	Residual Connection and Layer Normalization	448
11.7.4	Encoder	449
11.7.5	Decoder	451
11.7.6	Training	453
11.7.7	Summary	456
11.7.8	Exercises	456
11.8	Transformers for Vision	457
11.8.1	Model	457
11.8.2	Patch Embedding	459
11.8.3	Vision Transformer Encoder	459
11.8.4	Putting It All Together	460
11.8.5	Training	461
11.8.6	Summary and Discussion	462
11.8.7	Exercises	462
11.9	Large-Scale Pretraining with Transformers	462
11.9.1	Encoder-Only	463
11.9.2	Encoder–Decoder	465
11.9.3	Decoder-Only	467
11.9.4	Scalability	470
11.9.5	Large Language Models	471
11.9.6	Summary and Discussion	472
11.9.7	Exercises	473
	Appendix: Tools for Deep Learning	474
A.1	Using Jupyter Notebooks	474
A.2	Using Amazon SageMaker	479
A.3	Using AWS EC2 Instances	482
A.4	Using Google Colab	490
A.5	Selecting Servers and GPUs	491
A.6	Contributing to This Book	495
A.7	The d2l API Document	500
	References	516
	Index	539