

**Computers connected to subscribing institutions download at:  
<https://rd.springer.com/book/10.1007/978-3-319-94463-0>**

Neural Networks and Deep Learning

**Computers connected to subscribing institutions download at:  
<https://rd.springer.com/book/10.1007/978-3-319-94463-0>**

**Computers connected to subscribing institutions download at:  
<https://rd.springer.com/book/10.1007/978-3-319-94463-0>**

Charu C. Aggarwal

# Neural Networks and Deep Learning

A Textbook

**Computers connected to subscribing institutions download at:  
<https://rd.springer.com/book/10.1007/978-3-319-94463-0>**

Charu C. Aggarwal  
IBM T. J. Watson Research Center  
International Business Machines  
Yorktown Heights, NY, USA

ISBN 978-3-319-94462-3      ISBN 978-3-319-94463-0 (eBook)  
<https://doi.org/10.1007/978-3-319-94463-0>

Library of Congress Control Number: 2018947636

© Springer International Publishing AG, part of Springer Nature 2018

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, express or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG  
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

**Computers connected to subscribing institutions download at:  
<https://rd.springer.com/book/10.1007/978-3-319-94463-0>**

To my wife Lata, my daughter Sayani,  
and my late parents Dr. Prem Sarup and Mrs. Pushplata Aggarwal.

**Computers connected to subscribing institutions download at:  
<https://rd.springer.com/book/10.1007/978-3-319-94463-0>**

## Preface

---

---

“Any A.I. smart enough to pass a Turing test is smart enough to know to fail it.”—Ian McDonald

Neural networks were developed to simulate the human nervous system for machine learning tasks by treating the computational units in a learning model in a manner similar to human neurons. The grand vision of neural networks is to create artificial intelligence by building machines whose architecture simulates the computations in the human nervous system. This is obviously not a simple task because the computational power of the fastest computer today is a minuscule fraction of the computational power of a human brain. Neural networks were developed soon after the advent of computers in the fifties and sixties. Rosenblatt’s perceptron algorithm was seen as a fundamental cornerstone of neural networks, which caused an initial excitement about the prospects of artificial intelligence. However, after the initial euphoria, there was a period of disappointment in which the data hungry and computationally intensive nature of neural networks was seen as an impediment to their usability. Eventually, at the turn of the century, greater data availability and increasing computational power lead to increased successes of neural networks, and this area was reborn under the new label of “deep learning.” Although we are still far from the day that artificial intelligence (AI) is close to human performance, there are specific domains like image recognition, self-driving cars, and game playing, where AI has matched or exceeded human performance. It is also hard to predict what AI might be able to do in the future. For example, few computer vision experts would have thought two decades ago that any automated system could ever perform an intuitive task like categorizing an image more accurately than a human.

Neural networks are *theoretically* capable of learning any mathematical function with sufficient training data, and some variants like recurrent neural networks are known to be *Turing complete*. Turing completeness refers to the fact that a neural network can simulate any learning algorithm, *given sufficient training data*. The sticking point is that the amount of data required to learn even simple tasks is often extraordinarily large, which causes a corresponding increase in training time (if we assume that enough training data is available in the first place). For example, the training time for image recognition, which is a simple task for a human, can be on the order of weeks even on high-performance systems. Furthermore, there are practical issues associated with the stability of neural network training, which are being resolved even today. Nevertheless, given that the speed of computers is

expected to increase rapidly over time, and fundamentally more powerful paradigms like quantum computing are on the horizon, the computational issue might not eventually turn out to be quite as critical as imagined.

Although the biological analogy of neural networks is an exciting one and evokes comparisons with science fiction, the mathematical understanding of neural networks is a more mundane one. The neural network abstraction can be viewed as a modular approach of enabling learning algorithms that are based on continuous optimization on a computational graph of dependencies between the input and output. To be fair, this is not very different from traditional work in control theory; indeed, some of the methods used for optimization in control theory are strikingly similar to (and historically preceded) the most fundamental algorithms in neural networks. However, the large amounts of data available in recent years together with increased computational power have enabled experimentation with deeper architectures of these computational graphs than was previously possible. The resulting success has changed the broader perception of the potential of deep learning.

The chapters of the book are organized as follows:

1. *The basics of neural networks*: Chapter 1 discusses the basics of neural network design. Many traditional machine learning models can be understood as special cases of neural learning. Understanding the relationship between traditional machine learning and neural networks is the first step to understanding the latter. The simulation of various machine learning models with neural networks is provided in Chapter 2. This will give the analyst a feel of how neural networks push the envelope of traditional machine learning algorithms.
2. *Fundamentals of neural networks*: Although Chapters 1 and 2 provide an overview of the training methods for neural networks, a more detailed understanding of the training challenges is provided in Chapters 3 and 4. Chapters 5 and 6 present radial-basis function (RBF) networks and restricted Boltzmann machines.
3. *Advanced topics in neural networks*: A lot of the recent success of deep learning is a result of the specialized architectures for various domains, such as recurrent neural networks and convolutional neural networks. Chapters 7 and 8 discuss recurrent and convolutional neural networks. Several advanced topics like deep reinforcement learning, neural Turing mechanisms, and generative adversarial networks are discussed in Chapters 9 and 10.

We have taken care to include some of the “forgotten” architectures like RBF networks and Kohonen self-organizing maps because of their potential in many applications. The book is written for graduate students, researchers, and practitioners. Numerous exercises are available along with a solution manual to aid in classroom teaching. Where possible, an application-centric view is highlighted in order to give the reader a feel for the technology.

Throughout this book, a vector or a multidimensional data point is annotated with a bar, such as  $\bar{X}$  or  $\bar{y}$ . A vector or multidimensional point may be denoted by either small letters or capital letters, as long as it has a bar. Vector dot products are denoted by centered dots, such as  $\bar{X} \cdot \bar{Y}$ . A matrix is denoted in capital letters without a bar, such as  $R$ . Throughout the book, the  $n \times d$  matrix corresponding to the entire training data set is denoted by  $D$ , with  $n$  documents and  $d$  dimensions. The individual data points in  $D$  are therefore  $d$ -dimensional row vectors. On the other hand, vectors with one component for each data



**Computers connected to subscribing institutions download at:**

*PREFACE* <https://rd.springer.com/book/10.1007/978-3-319-94463-0> **IX**

point are usually  $n$ -dimensional column vectors. An example is the  $n$ -dimensional column vector  $\bar{y}$  of class variables of  $n$  data points. An observed value  $y_i$  is distinguished from a predicted value  $\hat{y}_i$  by a circumflex at the top of the variable.

Yorktown Heights, NY, USA

Charu C. Aggarwal

**Computers connected to subscribing institutions download at:  
<https://rd.springer.com/book/10.1007/978-3-319-94463-0>**

---

---

## Acknowledgments

---

---

I would like to thank my family for their love and support during the busy time spent in writing this book. I would also like to thank my manager Nagui Halim for his support during the writing of this book.

Several figures in this book have been provided by the courtesy of various individuals and institutions. The Smithsonian Institution made the image of the Mark I perceptron (cf. Figure 1.5) available at no cost. Saket Sathe provided the outputs in Chapter 7 for the tiny Shakespeare data set, based on code available/described in [233, 580]. Andrew Zisserman provided Figures 8.12 and 8.16 in the section on convolutional visualizations. Another visualization of the feature maps in the convolution network (cf. Figure 8.15) was provided by Matthew Zeiler. NVIDIA provided Figure 9.10 on the convolutional neural network for self-driving cars in Chapter 9, and Sergey Levine provided the image on self-learning robots (cf. Figure 9.9) in the same chapter. Alec Radford provided Figure 10.8, which appears in Chapter 10. Alex Krizhevsky provided Figure 8.9(b) containing *AlexNet*.

This book has benefitted from significant feedback and several collaborations that I have had with numerous colleagues over the years. I would like to thank Quoc Le, Saket Sathe, Karthik Subbian, Jiliang Tang, and Suhang Wang for their feedback on various portions of this book. Shuai Zheng provided feedback on the section on regularized autoencoders in Chapter 4. I received feedback on the sections on autoencoders from Lei Cai and Hao Yuan. Feedback on the chapter on convolutional neural networks was provided by Hongyang Gao, Shuiwang Ji, and Zhengyang Wang. Shuiwang Ji, Lei Cai, Zhengyang Wang and Hao Yuan also reviewed the Chapters 3 and 7, and suggested several edits. They also suggested the ideas of using Figures 8.6 and 8.7 for elucidating the convolution/deconvolution operations.

For their collaborations, I would like to thank Tarek F. Abdelzaher, Jinghui Chen, Jing Gao, Quanquan Gu, Manish Gupta, Jiawei Han, Alexander Hinneburg, Thomas Huang, Nan Li, Huan Liu, Ruoming Jin, Daniel Keim, Arijit Khan, Latifur Khan, Mohammad M. Masud, Jian Pei, Magda Procopiuc, Guojun Qi, Chandan Reddy, Saket Sathe, Jaideep Srivastava, Karthik Subbian, Yizhou Sun, Jiliang Tang, Min-Hsuan Tsai, Haixun Wang, Jianyong Wang, Min Wang, Suhang Wang, Joel Wolf, Xifeng Yan, Mohammed Zaki, ChengXiang Zhai, and Peixiang Zhao. I would also like to thank my advisor James B. Orlin for his guidance during my early years as a researcher.

**Computers connected to subscribing institutions download at:**

XII

ACKNOWLEDGMENTS

**<https://rd.springer.com/book/10.1007/978-3-319-94463-0>**

I would like to thank Lata Aggarwal for helping me with some of the figures created using PowerPoint graphics in this book. My daughter, Sayani, was helpful in incorporating special effects (e.g., image color, contrast, and blurring) in several JPEG images used at various places in this book.

---

---

# Contents

---

---

<b>1</b>	<b>An Introduction to Neural Networks</b>	<b>1</b>
1.1	Introduction . . . . .	1
1.1.1	Humans Versus Computers: Stretching the Limits of Artificial Intelligence . . . . .	3
1.2	The Basic Architecture of Neural Networks . . . . .	4
1.2.1	Single Computational Layer: The Perceptron . . . . .	5
1.2.1.1	What Objective Function Is the Perceptron Optimizing? . . . . .	8
1.2.1.2	Relationship with Support Vector Machines . . . . .	10
1.2.1.3	Choice of Activation and Loss Functions . . . . .	11
1.2.1.4	Choice and Number of Output Nodes . . . . .	14
1.2.1.5	Choice of Loss Function . . . . .	14
1.2.1.6	Some Useful Derivatives of Activation Functions . . . . .	16
1.2.2	Multilayer Neural Networks . . . . .	17
1.2.3	The Multilayer Network as a Computational Graph . . . . .	20
1.3	Training a Neural Network with Backpropagation . . . . .	21
1.4	Practical Issues in Neural Network Training . . . . .	24
1.4.1	The Problem of Overfitting . . . . .	25
1.4.1.1	Regularization . . . . .	26
1.4.1.2	Neural Architecture and Parameter Sharing . . . . .	27
1.4.1.3	Early Stopping . . . . .	27
1.4.1.4	Trading Off Breadth for Depth . . . . .	27
1.4.1.5	Ensemble Methods . . . . .	28
1.4.2	The Vanishing and Exploding Gradient Problems . . . . .	28
1.4.3	Difficulties in Convergence . . . . .	29
1.4.4	Local and Spurious Optima . . . . .	29
1.4.5	Computational Challenges . . . . .	29
1.5	The Secrets to the Power of Function Composition . . . . .	30
1.5.1	The Importance of Nonlinear Activation . . . . .	32
1.5.2	Reducing Parameter Requirements with Depth . . . . .	34
1.5.3	Unconventional Neural Architectures . . . . .	35
1.5.3.1	Blurring the Distinctions Between Input, Hidden, and Output Layers . . . . .	35
1.5.3.2	Unconventional Operations and Sum-Product Networks . . . . .	36

- 1.6 Common Neural Architectures . . . . . 37
  - 1.6.1 Simulating Basic Machine Learning with Shallow Models . . . . . 37
  - 1.6.2 Radial Basis Function Networks . . . . . 37
  - 1.6.3 Restricted Boltzmann Machines . . . . . 38
  - 1.6.4 Recurrent Neural Networks . . . . . 38
  - 1.6.5 Convolutional Neural Networks . . . . . 40
  - 1.6.6 Hierarchical Feature Engineering and Pretrained Models . . . . . 42
- 1.7 Advanced Topics . . . . . 44
  - 1.7.1 Reinforcement Learning . . . . . 44
  - 1.7.2 Separating Data Storage and Computations . . . . . 45
  - 1.7.3 Generative Adversarial Networks . . . . . 45
- 1.8 Two Notable Benchmarks . . . . . 46
  - 1.8.1 The MNIST Database of Handwritten Digits . . . . . 46
  - 1.8.2 The ImageNet Database . . . . . 47
- 1.9 Summary . . . . . 48
- 1.10 Bibliographic Notes . . . . . 48
  - 1.10.1 Video Lectures . . . . . 50
  - 1.10.2 Software Resources . . . . . 50
- 1.11 Exercises . . . . . 51
- 2 Machine Learning with Shallow Neural Networks . . . . . 53**
  - 2.1 Introduction . . . . . 53
  - 2.2 Neural Architectures for Binary Classification Models . . . . . 55
    - 2.2.1 Revisiting the Perceptron . . . . . 56
    - 2.2.2 Least-Squares Regression . . . . . 58
      - 2.2.2.1 Widrow-Hoff Learning . . . . . 59
      - 2.2.2.2 Closed Form Solutions . . . . . 61
    - 2.2.3 Logistic Regression . . . . . 61
      - 2.2.3.1 Alternative Choices of Activation and Loss . . . . . 63
    - 2.2.4 Support Vector Machines . . . . . 63
  - 2.3 Neural Architectures for Multiclass Models . . . . . 65
    - 2.3.1 Multiclass Perceptron . . . . . 65
    - 2.3.2 Weston-Watkins SVM . . . . . 67
    - 2.3.3 Multinomial Logistic Regression (Softmax Classifier) . . . . . 68
    - 2.3.4 Hierarchical Softmax for Many Classes . . . . . 69
  - 2.4 Backpropagated Saliency for Feature Selection . . . . . 70
  - 2.5 Matrix Factorization with Autoencoders . . . . . 70
    - 2.5.1 Autoencoder: Basic Principles . . . . . 71
      - 2.5.1.1 Autoencoder with a Single Hidden Layer . . . . . 72
      - 2.5.1.2 Connections with Singular Value Decomposition . . . . . 74
      - 2.5.1.3 Sharing Weights in Encoder and Decoder . . . . . 74
      - 2.5.1.4 Other Matrix Factorization Methods . . . . . 76
    - 2.5.2 Nonlinear Activations . . . . . 76
    - 2.5.3 Deep Autoencoders . . . . . 78
    - 2.5.4 Application to Outlier Detection . . . . . 80
    - 2.5.5 When the Hidden Layer Is Broader than the Input Layer . . . . . 81
      - 2.5.5.1 Sparse Feature Learning . . . . . 81
    - 2.5.6 Other Applications . . . . . 82

- 2.5.7 Recommender Systems: Row Index to Row Value Prediction . . . . . 83
- 2.5.8 Discussion . . . . . 86
- 2.6 Word2vec: An Application of Simple Neural Architectures . . . . . 87
  - 2.6.1 Neural Embedding with Continuous Bag of Words . . . . . 87
  - 2.6.2 Neural Embedding with Skip-Gram Model . . . . . 90
  - 2.6.3 Word2vec (SGNS) Is Logistic Matrix Factorization . . . . . 95
  - 2.6.4 Vanilla Skip-Gram Is Multinomial Matrix Factorization . . . . . 98
- 2.7 Simple Neural Architectures for Graph Embeddings . . . . . 98
  - 2.7.1 Handling Arbitrary Edge Counts . . . . . 100
  - 2.7.2 Multinomial Model . . . . . 100
  - 2.7.3 Connections with DeepWalk and Node2vec . . . . . 100
- 2.8 Summary . . . . . 101
- 2.9 Bibliographic Notes . . . . . 101
  - 2.9.1 Software Resources . . . . . 102
- 2.10 Exercises . . . . . 103

**3 Training Deep Neural Networks 105**

- 3.1 Introduction . . . . . 105
- 3.2 Backpropagation: The Gory Details . . . . . 107
  - 3.2.1 Backpropagation with the Computational Graph Abstraction . . . . . 107
  - 3.2.2 Dynamic Programming to the Rescue . . . . . 111
  - 3.2.3 Backpropagation with Post-Activation Variables . . . . . 113
  - 3.2.4 Backpropagation with Pre-activation Variables . . . . . 115
  - 3.2.5 Examples of Updates for Various Activations . . . . . 117
    - 3.2.5.1 The Special Case of Softmax . . . . . 117
  - 3.2.6 A Decoupled View of Vector-Centric Backpropagation . . . . . 118
  - 3.2.7 Loss Functions on Multiple Output Nodes and Hidden Nodes . . . . . 121
  - 3.2.8 Mini-Batch Stochastic Gradient Descent . . . . . 121
  - 3.2.9 Backpropagation Tricks for Handling Shared Weights . . . . . 123
  - 3.2.10 Checking the Correctness of Gradient Computation . . . . . 124
- 3.3 Setup and Initialization Issues . . . . . 125
  - 3.3.1 Tuning Hyperparameters . . . . . 125
  - 3.3.2 Feature Preprocessing . . . . . 126
  - 3.3.3 Initialization . . . . . 128
- 3.4 The Vanishing and Exploding Gradient Problems . . . . . 129
  - 3.4.1 Geometric Understanding of the Effect of Gradient Ratios . . . . . 130
  - 3.4.2 A Partial Fix with Activation Function Choice . . . . . 133
  - 3.4.3 Dying Neurons and “Brain Damage” . . . . . 133
    - 3.4.3.1 Leaky ReLU . . . . . 133
    - 3.4.3.2 Maxout . . . . . 134
- 3.5 Gradient-Descent Strategies . . . . . 134
  - 3.5.1 Learning Rate Decay . . . . . 135
  - 3.5.2 Momentum-Based Learning . . . . . 136
    - 3.5.2.1 Nesterov Momentum . . . . . 137
  - 3.5.3 Parameter-Specific Learning Rates . . . . . 137
    - 3.5.3.1 AdaGrad . . . . . 138
    - 3.5.3.2 RMSProp . . . . . 138
    - 3.5.3.3 RMSProp with Nesterov Momentum . . . . . 139

3.5.3.4	AdaDelta . . . . .	139
3.5.3.5	Adam . . . . .	140
3.5.4	Cliffs and Higher-Order Instability . . . . .	141
3.5.5	Gradient Clipping . . . . .	142
3.5.6	Second-Order Derivatives . . . . .	143
3.5.6.1	Conjugate Gradients and Hessian-Free Optimization . . . . .	145
3.5.6.2	Quasi-Newton Methods and BFGS . . . . .	148
3.5.6.3	Problems with Second-Order Methods: Saddle Points . . . . .	149
3.5.7	Polyak Averaging . . . . .	151
3.5.8	Local and Spurious Minima . . . . .	151
3.6	Batch Normalization . . . . .	152
3.7	Practical Tricks for Acceleration and Compression . . . . .	156
3.7.1	GPU Acceleration . . . . .	157
3.7.2	Parallel and Distributed Implementations . . . . .	158
3.7.3	Algorithmic Tricks for Model Compression . . . . .	160
3.8	Summary . . . . .	163
3.9	Bibliographic Notes . . . . .	163
3.9.1	Software Resources . . . . .	165
3.10	Exercises . . . . .	165
<b>4</b>	<b>Teaching Deep Learners to Generalize</b>	<b>169</b>
4.1	Introduction . . . . .	169
4.2	The Bias-Variance Trade-Off . . . . .	174
4.2.1	Formal View . . . . .	175
4.3	Generalization Issues in Model Tuning and Evaluation . . . . .	178
4.3.1	Evaluating with Hold-Out and Cross-Validation . . . . .	179
4.3.2	Issues with Training at Scale . . . . .	180
4.3.3	How to Detect Need to Collect More Data . . . . .	181
4.4	Penalty-Based Regularization . . . . .	181
4.4.1	Connections with Noise Injection . . . . .	182
4.4.2	$L_1$ -Regularization . . . . .	183
4.4.3	$L_1$ - or $L_2$ -Regularization? . . . . .	184
4.4.4	Penalizing Hidden Units: Learning Sparse Representations . . . . .	185
4.5	Ensemble Methods . . . . .	186
4.5.1	Bagging and Subsampling . . . . .	186
4.5.2	Parametric Model Selection and Averaging . . . . .	187
4.5.3	Randomized Connection Dropping . . . . .	188
4.5.4	Dropout . . . . .	188
4.5.5	Data Perturbation Ensembles . . . . .	191
4.6	Early Stopping . . . . .	192
4.6.1	Understanding Early Stopping from the Variance Perspective . . . . .	192
4.7	Unsupervised Pretraining . . . . .	193
4.7.1	Variations of Unsupervised Pretraining . . . . .	197
4.7.2	What About Supervised Pretraining? . . . . .	197
4.8	Continuation and Curriculum Learning . . . . .	199
4.8.1	Continuation Learning . . . . .	199
4.8.2	Curriculum Learning . . . . .	200
4.9	Parameter Sharing . . . . .	200



4.10	Regularization in Unsupervised Applications . . . . .	201
4.10.1	Value-Based Penalization: Sparse Autoencoders . . . . .	202
4.10.2	Noise Injection: De-noising Autoencoders . . . . .	202
4.10.3	Gradient-Based Penalization: Contractive Autoencoders . . . . .	204
4.10.4	Hidden Probabilistic Structure: Variational Autoencoders . . . . .	207
4.10.4.1	Reconstruction and Generative Sampling . . . . .	210
4.10.4.2	Conditional Variational Autoencoders . . . . .	212
4.10.4.3	Relationship with Generative Adversarial Networks . . . . .	213
4.11	Summary . . . . .	213
4.12	Bibliographic Notes . . . . .	214
4.12.1	Software Resources . . . . .	215
4.13	Exercises . . . . .	215
<b>5</b>	<b>Radial Basis Function Networks</b>	<b>217</b>
5.1	Introduction . . . . .	217
5.2	Training an RBF Network . . . . .	220
5.2.1	Training the Hidden Layer . . . . .	221
5.2.2	Training the Output Layer . . . . .	222
5.2.2.1	Expression with Pseudo-Inverse . . . . .	224
5.2.3	Orthogonal Least-Squares Algorithm . . . . .	224
5.2.4	Fully Supervised Learning . . . . .	225
5.3	Variations and Special Cases of RBF Networks . . . . .	226
5.3.1	Classification with Perceptron Criterion . . . . .	226
5.3.2	Classification with Hinge Loss . . . . .	227
5.3.3	Example of Linear Separability Promoted by RBF . . . . .	227
5.3.4	Application to Interpolation . . . . .	228
5.4	Relationship with Kernel Methods . . . . .	229
5.4.1	Kernel Regression as a Special Case of RBF Networks . . . . .	229
5.4.2	Kernel SVM as a Special Case of RBF Networks . . . . .	230
5.4.3	Observations . . . . .	231
5.5	Summary . . . . .	231
5.6	Bibliographic Notes . . . . .	232
5.7	Exercises . . . . .	232
<b>6</b>	<b>Restricted Boltzmann Machines</b>	<b>235</b>
6.1	Introduction . . . . .	235
6.1.1	Historical Perspective . . . . .	236
6.2	Hopfield Networks . . . . .	237
6.2.1	Optimal State Configurations of a Trained Network . . . . .	238
6.2.2	Training a Hopfield Network . . . . .	240
6.2.3	Building a Toy Recommender and Its Limitations . . . . .	241
6.2.4	Increasing the Expressive Power of the Hopfield Network . . . . .	242
6.3	The Boltzmann Machine . . . . .	243
6.3.1	How a Boltzmann Machine Generates Data . . . . .	244
6.3.2	Learning the Weights of a Boltzmann Machine . . . . .	245
6.4	Restricted Boltzmann Machines . . . . .	247
6.4.1	Training the RBM . . . . .	249
6.4.2	Contrastive Divergence Algorithm . . . . .	250
6.4.3	Practical Issues and Improvisations . . . . .	251

6.5	Applications of Restricted Boltzmann Machines . . . . .	251
6.5.1	Dimensionality Reduction and Data Reconstruction . . . . .	252
6.5.2	RBMs for Collaborative Filtering . . . . .	254
6.5.3	Using RBMs for Classification . . . . .	257
6.5.4	Topic Models with RBMs . . . . .	260
6.5.5	RBMs for Machine Learning with Multimodal Data . . . . .	262
6.6	Using RBMs Beyond Binary Data Types . . . . .	263
6.7	Stacking Restricted Boltzmann Machines . . . . .	264
6.7.1	Unsupervised Learning . . . . .	266
6.7.2	Supervised Learning . . . . .	267
6.7.3	Deep Boltzmann Machines and Deep Belief Networks . . . . .	267
6.8	Summary . . . . .	268
6.9	Bibliographic Notes . . . . .	268
6.10	Exercises . . . . .	270
<b>7</b>	<b>Recurrent Neural Networks</b> . . . . .	<b>271</b>
7.1	Introduction . . . . .	271
7.1.1	Expressiveness of Recurrent Networks . . . . .	274
7.2	The Architecture of Recurrent Neural Networks . . . . .	274
7.2.1	Language Modeling Example of RNN . . . . .	277
7.2.1.1	Generating a Language Sample . . . . .	278
7.2.2	Backpropagation Through Time . . . . .	280
7.2.3	Bidirectional Recurrent Networks . . . . .	283
7.2.4	Multilayer Recurrent Networks . . . . .	284
7.3	The Challenges of Training Recurrent Networks . . . . .	286
7.3.1	Layer Normalization . . . . .	289
7.4	Echo-State Networks . . . . .	290
7.5	Long Short-Term Memory (LSTM) . . . . .	292
7.6	Gated Recurrent Units (GRUs) . . . . .	295
7.7	Applications of Recurrent Neural Networks . . . . .	297
7.7.1	Application to Automatic Image Captioning . . . . .	298
7.7.2	Sequence-to-Sequence Learning and Machine Translation . . . . .	299
7.7.2.1	Question-Answering Systems . . . . .	301
7.7.3	Application to Sentence-Level Classification . . . . .	303
7.7.4	Token-Level Classification with Linguistic Features . . . . .	304
7.7.5	Time-Series Forecasting and Prediction . . . . .	305
7.7.6	Temporal Recommender Systems . . . . .	307
7.7.7	Secondary Protein Structure Prediction . . . . .	309
7.7.8	End-to-End Speech Recognition . . . . .	309
7.7.9	Handwriting Recognition . . . . .	309
7.8	Summary . . . . .	310
7.9	Bibliographic Notes . . . . .	310
7.9.1	Software Resources . . . . .	311
7.10	Exercises . . . . .	312

<b>8</b>	<b>Convolutional Neural Networks</b>	<b>315</b>
8.1	Introduction . . . . .	315
8.1.1	Historical Perspective and Biological Inspiration . . . . .	316
8.1.2	Broader Observations About Convolutional Neural Networks . . . . .	317
8.2	The Basic Structure of a Convolutional Network . . . . .	318
8.2.1	Padding . . . . .	322
8.2.2	Strides . . . . .	324
8.2.3	Typical Settings . . . . .	324
8.2.4	The ReLU Layer . . . . .	325
8.2.5	Pooling . . . . .	326
8.2.6	Fully Connected Layers . . . . .	327
8.2.7	The Interleaving Between Layers . . . . .	328
8.2.8	Local Response Normalization . . . . .	330
8.2.9	Hierarchical Feature Engineering . . . . .	331
8.3	Training a Convolutional Network . . . . .	332
8.3.1	Backpropagating Through Convolutions . . . . .	333
8.3.2	Backpropagation as Convolution with Inverted/Transposed Filter . . . . .	334
8.3.3	Convolution/Backpropagation as Matrix Multiplications . . . . .	335
8.3.4	Data Augmentation . . . . .	337
8.4	Case Studies of Convolutional Architectures . . . . .	338
8.4.1	AlexNet . . . . .	339
8.4.2	ZFNet . . . . .	341
8.4.3	VGG . . . . .	342
8.4.4	GoogLeNet . . . . .	345
8.4.5	ResNet . . . . .	347
8.4.6	The Effects of Depth . . . . .	350
8.4.7	Pretrained Models . . . . .	351
8.5	Visualization and Unsupervised Learning . . . . .	352
8.5.1	Visualizing the Features of a Trained Network . . . . .	353
8.5.2	Convolutional Autoencoders . . . . .	357
8.6	Applications of Convolutional Networks . . . . .	363
8.6.1	Content-Based Image Retrieval . . . . .	363
8.6.2	Object Localization . . . . .	364
8.6.3	Object Detection . . . . .	365
8.6.4	Natural Language and Sequence Learning . . . . .	366
8.6.5	Video Classification . . . . .	367
8.7	Summary . . . . .	368
8.8	Bibliographic Notes . . . . .	368
8.8.1	Software Resources and Data Sets . . . . .	370
8.9	Exercises . . . . .	371
<b>9</b>	<b>Deep Reinforcement Learning</b>	<b>373</b>
9.1	Introduction . . . . .	373
9.2	Stateless Algorithms: Multi-Armed Bandits . . . . .	375
9.2.1	Naïve Algorithm . . . . .	376
9.2.2	$\epsilon$ -Greedy Algorithm . . . . .	376
9.2.3	Upper Bounding Methods . . . . .	376
9.3	The Basic Framework of Reinforcement Learning . . . . .	377
9.3.1	Challenges of Reinforcement Learning . . . . .	379

9.3.2	Simple Reinforcement Learning for Tic-Tac-Toe . . . . .	380
9.3.3	Role of Deep Learning and a Straw-Man Algorithm . . . . .	380
9.4	Bootstrapping for Value Function Learning . . . . .	383
9.4.1	Deep Learning Models as Function Approximators . . . . .	384
9.4.2	Example: Neural Network for Atari Setting . . . . .	386
9.4.3	On-Policy Versus Off-Policy Methods: SARSA . . . . .	387
9.4.4	Modeling States Versus State-Action Pairs . . . . .	389
9.5	Policy Gradient Methods . . . . .	391
9.5.1	Finite Difference Methods . . . . .	392
9.5.2	Likelihood Ratio Methods . . . . .	393
9.5.3	Combining Supervised Learning with Policy Gradients . . . . .	395
9.5.4	Actor-Critic Methods . . . . .	395
9.5.5	Continuous Action Spaces . . . . .	397
9.5.6	Advantages and Disadvantages of Policy Gradients . . . . .	397
9.6	Monte Carlo Tree Search . . . . .	398
9.7	Case Studies . . . . .	399
9.7.1	AlphaGo: Championship Level Play at Go . . . . .	399
9.7.1.1	Alpha Zero: Enhancements to Zero Human Knowledge . . . . .	402
9.7.2	Self-Learning Robots . . . . .	404
9.7.2.1	Deep Learning of Locomotion Skills . . . . .	404
9.7.2.2	Deep Learning of Visuomotor Skills . . . . .	406
9.7.3	Building Conversational Systems: Deep Learning for Chatbots . . . . .	407
9.7.4	Self-Driving Cars . . . . .	410
9.7.5	Inferring Neural Architectures with Reinforcement Learning . . . . .	412
9.8	Practical Challenges Associated with Safety . . . . .	413
9.9	Summary . . . . .	414
9.10	Bibliographic Notes . . . . .	414
9.10.1	Software Resources and Testbeds . . . . .	416
9.11	Exercises . . . . .	416
<b>10</b>	<b>Advanced Topics in Deep Learning</b> . . . . .	<b>419</b>
10.1	Introduction . . . . .	419
10.2	Attention Mechanisms . . . . .	421
10.2.1	Recurrent Models of Visual Attention . . . . .	422
10.2.1.1	Application to Image Captioning . . . . .	424
10.2.2	Attention Mechanisms for Machine Translation . . . . .	425
10.3	Neural Networks with External Memory . . . . .	429
10.3.1	A Fantasy Video Game: Sorting by Example . . . . .	430
10.3.1.1	Implementing Swaps with Memory Operations . . . . .	431
10.3.2	Neural Turing Machines . . . . .	432
10.3.3	Differentiable Neural Computer: A Brief Overview . . . . .	437
10.4	Generative Adversarial Networks (GANs) . . . . .	438
10.4.1	Training a Generative Adversarial Network . . . . .	439
10.4.2	Comparison with Variational Autoencoder . . . . .	442
10.4.3	Using GANs for Generating Image Data . . . . .	442
10.4.4	Conditional Generative Adversarial Networks . . . . .	444
10.5	Competitive Learning . . . . .	449
10.5.1	Vector Quantization . . . . .	450
10.5.2	Kohonen Self-Organizing Map . . . . .	450

10.6	Limitations of Neural Networks . . . . .	453
10.6.1	An Aspirational Goal: One-Shot Learning . . . . .	453
10.6.2	An Aspirational Goal: Energy-Efficient Learning . . . . .	455
10.7	Summary . . . . .	456
10.8	Bibliographic Notes . . . . .	457
10.8.1	Software Resources . . . . .	458
10.9	Exercises . . . . .	458
<b>Bibliography</b>		<b>459</b>
<b>Index</b>		<b>493</b>

**Computers connected to subscribing institutions download at:  
<https://rd.springer.com/book/10.1007/978-3-319-94463-0>**

---

## Author Biography

---

**Charu C. Aggarwal** is a Distinguished Research Staff Member (DRSM) at the IBM T. J. Watson Research Center in Yorktown Heights, New York. He completed his undergraduate degree in Computer Science from the Indian Institute of Technology at Kanpur in 1993 and his Ph.D. from the Massachusetts Institute of Technology in 1996.



He has worked extensively in the field of data mining. He has published more than 350 papers in refereed conferences and journals and authored over 80 patents. He is the author or editor of 18 books, including textbooks on data mining, recommender systems, and outlier analysis. Because of the commercial value of his patents, he has thrice been designated a Master Inventor at IBM. He is a recipient of an IBM Corporate Award (2003) for his work on bio-terrorist threat detection in data streams, a recipient of the IBM Outstanding Innovation Award (2008) for his scientific contributions to privacy technology, and a recipient of two IBM Outstanding

Technical Achievement Awards (2009, 2015) for his work on data streams/high-dimensional data. He received the EDBT 2014 Test of Time Award for his work on condensation-based privacy-preserving data mining. He is also a recipient of the IEEE ICDM Research Contributions Award (2015), which is one of the two highest awards for influential research contributions in the field of data mining.

He has served as the general co-chair of the IEEE Big Data Conference (2014) and as the program co-chair of the ACM CIKM Conference (2015), the IEEE ICDM Conference (2015), and the ACM KDD Conference (2016). He served as an associate editor of the IEEE Transactions on Knowledge and Data Engineering from 2004 to 2008. He is an associate editor of the IEEE Transactions on Big Data, an action editor of the Data Mining and Knowledge Discovery Journal, and an associate editor of the Knowledge and Information Systems Journal. He serves as the editor-in-chief of the ACM Transactions on Knowledge Discovery from Data as well as the ACM SIGKDD Explorations. He serves on the advisory board of the Lecture Notes on Social Networks, a publication by Springer. He has served as the vice-president of the SIAM Activity Group on Data Mining and is a member of the SIAM industry committee. He is a fellow of the SIAM, ACM, and the IEEE, for “contributions to knowledge discovery and data mining algorithms.”

**Computers connected to subscribing institutions download at:  
<https://rd.springer.com/book/10.1007/978-3-319-94463-0>**