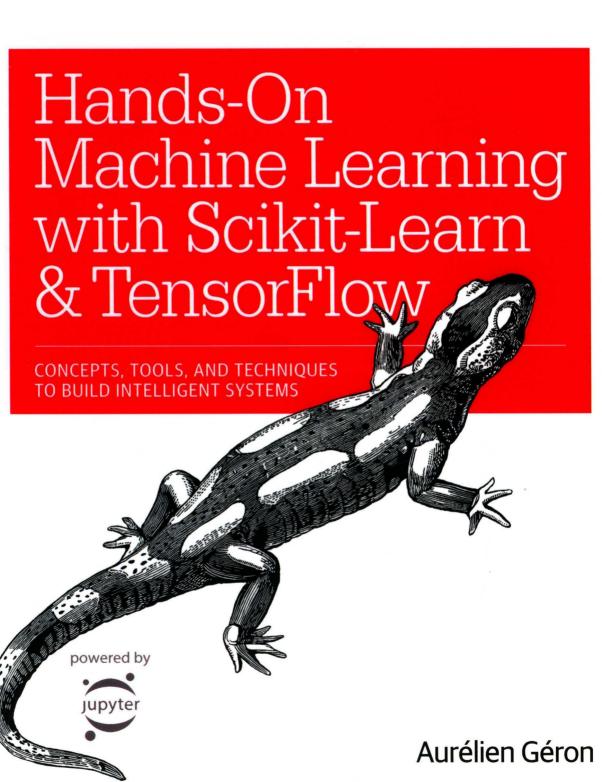
O'REILLY'



# Hands-On Machine Learning with Scikit-Learn and TensorFlow

Concepts, Tools, and Techniques to Build Intelligent Systems

Aurélien Géron



### Hands-On Machine Learning with Scikit-Learn and TensorFlow

by Aurélien Géron

Copyright © 2017 Aurélien Géron. All rights reserved.

Printed in the United States of America.

Published by O'Reilly Media, Inc., 1005 Gravenstein Highway North, Sebastopol, CA 95472.

O'Reilly books may be purchased for educational, business, or sales promotional use. Online editions are also available for most titles (http://oreilly.com/safari). For more information, contact our corporate/institutional sales department: 800-998-9938 or corporate@oreilly.com.

Editor: Nicole Tache Production Editor: Nicholas Adams Copyeditor: Rachel Monaghan Proofreader: Charles Roumeliotis

Indexer: Wendy Catalano
Interior Designer: David Futato
Cover Designer: Randy Comer
Illustrator: Rebecca Demarest

March 2017:

First Edition

#### **Revision History for the First Edition**

2017-03-10: First Release 2017-06-09: Second Release

See http://oreilly.com/catalog/errata.csp?isbn=9781491962299 for release details.

The O'Reilly logo is a registered trademark of O'Reilly Media, Inc. *Hands-On Machine Learning with Scikit-Learn and TensorFlow*, the cover image, and related trade dress are trademarks of O'Reilly Media, Inc.

While the publisher and the author have used good faith efforts to ensure that the information and instructions contained in this work are accurate, the publisher and the author disclaim all responsibility for errors or omissions, including without limitation responsibility for damages resulting from the use of or reliance on this work. Use of the information and instructions contained in this work is at your own risk. If any code samples or other technology this work contains or describes is subject to open source licenses or the intellectual property rights of others, it is your responsibility to ensure that your use thereof complies with such licenses and/or rights

# The Machine Learning Tsunami

In 2006, Geoffrey Hinton et al. published a paper¹ showing how to train a deep neural network capable of recognizing handwritten digits with state-of-the-art precision (>98%). They branded this technique "Deep Learning." Training a deep neural net was widely considered impossible at the time,² and most researchers had abandoned the idea since the 1990s. This paper revived the interest of the scientific community and before long many new papers demonstrated that Deep Learning was not only possible, but capable of mind-blowing achievements that no other Machine Learning (ML) technique could hope to match (with the help of tremendous computing power and great amounts of data). This enthusiasm soon extended to many other areas of Machine Learning.

Fast-forward 10 years and Machine Learning has conquered the industry: it is now at the heart of much of the magic in today's high-tech products, ranking your web search results, powering your smartphone's speech recognition, and recommending videos, beating the world champion at the game of Go. Before you know it, it will be driving your car.

# **Machine Learning in Your Projects**

So naturally you are excited about Machine Learning and you would love to join the party!

Perhaps you would like to give your homemade robot a brain of its own? Make it recognize faces? Or learn to walk around?

<sup>1</sup> Available on Hinton's home page at http://www.cs.toronto.edu/~hinton/.

<sup>2</sup> Despite the fact that Yann Lecun's deep convolutional neural networks had worked well for image recognition since the 1990s, although they were not as general purpose.

Or maybe your company has tons of data (user logs, financial data, production data, machine sensor data, hotline stats, HR reports, etc.), and more than likely you could unearth some hidden gems if you just knew where to look; for example:

- · Segment customers and find the best marketing strategy for each group
- · Recommend products for each client based on what similar clients bought
- · Detect which transactions are likely to be fraudulent
- · Predict next year's revenue
- And more (https://www.kaggle.com/wiki/DataScienceUseCases)

Whatever the reason, you have decided to learn Machine Learning and implement it in your projects. Great idea!

# **Objective and Approach**

This book assumes that you know close to nothing about Machine Learning. Its goal is to give you the concepts, the intuitions, and the tools you need to actually implement programs capable of *learning from data*.

We will cover a large number of techniques, from the simplest and most commonly used (such as linear regression) to some of the Deep Learning techniques that regularly win competitions.

Rather than implementing our own toy versions of each algorithm, we will be using actual production-ready Python frameworks:

- Scikit-Learn (http://scikit-learn.org/) is very easy to use, yet it implements many Machine Learning algorithms efficiently, so it makes for a great entry point to learn Machine Learning.
  - TensorFlow (http://tensorflow.org/) is a more complex library for distributed numerical computation using data flow graphs. It makes it possible to train and run very large neural networks efficiently by distributing the computations across potentially thousands of multi-GPU servers. TensorFlow was created at Google and supports many of their large-scale Machine Learning applications. It was open-sourced in November 2015.

The book favors a hands-on approach, growing an intuitive understanding of Machine Learning through concrete working examples and just a little bit of theory. While you can read this book without picking up your laptop, we highly recommend you experiment with the code examples available online as Jupyter notebooks at <a href="https://github.com/ageron/handson-ml">https://github.com/ageron/handson-ml</a>.

# **Prerequisites**

This book assumes that you have some Python programming experience and that you are familiar with Python's main scientific libraries, in particular NumPy (http:// numpy.org/), Pandas (http://pandas.pydata.org/), and Matplotlib (http://matplot lib.org/).

Also, if you care about what's under the hood you should have a reasonable understanding of college-level math as well (calculus, linear algebra, probabilities, and statistics).

If you don't know Python yet, http://learnpython.org/ is a great place to start. The official tutorial on python.org (https://docs.python.org/3/tutorial/) is also quite good.

If you have never used Jupyter, Chapter 2 will guide you through installation and the basics: it is a great tool to have in your toolbox.

If you are not familiar with Python's scientific libraries, the provided Jupyter notebooks include a few tutorials. There is also a quick math tutorial for linear algebra.

# Roadmap

This book is organized in two parts. Part I, The Fundamentals of Machine Learning, covers the following topics:

- · What is Machine Learning? What problems does it try to solve? What are the main categories and fundamental concepts of Machine Learning systems?
- The main steps in a typical Machine Learning project.
- · Learning by fitting a model to data.
- · Optimizing a cost function.
- · Handling, cleaning, and preparing data.
- Selecting and engineering features.
- Selecting a model and tuning hyperparameters using cross-validation.
- The main challenges of Machine Learning, in particular underfitting and overfitting (the bias/variance tradeoff).
- · Reducing the dimensionality of the training data to fight the curse of dimensionality.
- The most common learning algorithms: Linear and Polynomial Regression, Logistic Regression, k-Nearest Neighbors, Support Vector Machines, Decision Trees, Random Forests, and Ensemble methods.

Part II, Neural Networks and Deep Learning, covers the following topics:

- What are neural nets? What are they good for?
- · Building and training neural nets using TensorFlow.
- · The most important neural net architectures: feedforward neural nets, convolutional nets, recurrent nets, long short-term memory (LSTM) nets, and autoencoders.
- Techniques for training deep neural nets.
- Scaling neural networks for huge datasets.
- · Reinforcement learning.

The first part is based mostly on Scikit-Learn while the second part uses TensorFlow.



Don't jump into deep waters too hastily: while Deep Learning is no doubt one of the most exciting areas in Machine Learning, you should master the fundamentals first. Moreover, most problems can be solved quite well using simpler techniques such as Random Forests and Ensemble methods (discussed in Part I). Deep Learning is best suited for complex problems such as image recognition, speech recognition, or natural language processing, provided you have enough data, computing power, and patience.

### Other Resources

Many resources are available to learn about Machine Learning. Andrew Ng's ML course on Coursera (https://www.coursera.org/learn/machine-learning/) and Geoffrey Hinton's course on neural networks and Deep Learning (https://www.coursera.org/ course/neuralnets) are amazing, although they both require a significant time investment (think months).

There are also many interesting websites about Machine Learning, including of Scikit-Learn's exceptional User Guide (http://scikit-learn.org/stable/ user\_guide.html). You may also enjoy Dataquest (https://www.dataquest.io/), which provides very nice interactive tutorials, and ML blogs such as those listed on Quora (http://goo.gl/GwtU3A). Finally, the Deep Learning website (http://deeplearning.net/) has a good list of resources to learn more.

Of course there are also many other introductory books about Machine Learning, in particular:

• Joel Grus, Data Science from Scratch (O'Reilly). This book presents the fundamentals of Machine Learning, and implements some of the main algorithms in pure Python (from scratch, as the name suggests).

- · Stephen Marsland, Machine Learning: An Algorithmic Perspective (Chapman and Hall). This book is a great introduction to Machine Learning, covering a wide range of topics in depth, with code examples in Python (also from scratch, but using NumPy).
- Sebastian Raschka, Python Machine Learning (Packt Publishing). Also a great introduction to Machine Learning, this book leverages Python open source libraries (Pylearn 2 and Theano).
- Yaser S. Abu-Mostafa, Malik Magdon-Ismail, and Hsuan-Tien Lin, Learning from Data (AMLBook). A rather theoretical approach to ML, this book provides deep insights, in particular on the bias/variance tradeoff (see Chapter 4).
- Stuart Russell and Peter Norvig, Artificial Intelligence: A Modern Approach, 3rd Edition (Pearson). This is a great (and huge) book covering an incredible amount of topics, including Machine Learning. It helps put ML into perspective.

Finally, a great way to learn is to join ML competition websites such as Kaggle.com this will allow you to practice your skills on real-world problems, with help and insights from some of the best ML professionals out there.

### Conventions Used in This Book

The following typographical conventions are used in this book:

Italic

Indicates new terms, URLs, email addresses, filenames, and file extensions.

#### Constant width

Used for program listings, as well as within paragraphs to refer to program elements such as variable or function names, databases, data types, environment variables, statements and keywords.

### Constant width bold

Shows commands or other text that should be typed literally by the user.

#### Constant width italic

Shows text that should be replaced with user-supplied values or by values determined by context.



This element signifies a tip or suggestion.



This element signifies a general note.



This element indicates a warning or caution.

# **Using Code Examples**

Supplemental material (code examples, exercises, etc.) is available for download at https://github.com/ageron/handson-ml.

This book is here to help you get your job done. In general, if example code is offered with this book, you may use it in your programs and documentation. You do not need to contact us for permission unless you're reproducing a significant portion of the code. For example, writing a program that uses several chunks of code from this book does not require permission. Selling or distributing a CD-ROM of examples from O'Reilly books does require permission. Answering a question by citing this book and quoting example code does not require permission. Incorporating a significant amount of example code from this book into your product's documentation does require permission.

We appreciate, but do not require, attribution. An attribution usually includes the title, author, publisher, and ISBN. For example: "Hands-On Machine Learning with Scikit-Learn and TensorFlow by Aurélien Géron (O'Reilly). Copyright 2017 Aurélien Géron, 978-1-491-96229-9."

If you feel your use of code examples falls outside fair use or the permission given above, feel free to contact us at permissions@oreilly.com.

# O'Reilly Safari



Safari (formerly Safari Books Online) is a membership-based Safari training and reference platform for enterprise, government, educators, and individuals.

Members have access to thousands of books, training videos, Learning Paths, interactive tutorials, and curated playlists from over 250 publishers, including O'Reilly Media, Harvard Business Review, Prentice Hall Professional, Addison-Wesley Professional, Microsoft Press, Sams, Que, Peachpit Press, Adobe, Focal Press, Cisco Press,

John Wiley & Sons, Syngress, Morgan Kaufmann, IBM Redbooks, Packt, Adobe Press, FT Press, Apress, Manning, New Riders, McGraw-Hill, Jones & Bartlett, and Course Technology, among others.

For more information, please visit http://oreilly.com/safari.

### How to Contact Us

Please address comments and questions concerning this book to the publisher:

O'Reilly Media, Inc. 1005 Gravenstein Highway North Sebastopol, CA 95472 800-998-9938 (in the United States or Canada) 707-829-0515 (international or local) 707-829-0104 (fax)

We have a web page for this book, where we list errata, examples, and any additional information. You can access this page at http://bit.ly/hands-on-machine-learningwith-scikit-learn-and-tensorflow.

To comment or ask technical questions about this book, send email to bookquestions@oreilly.com.

For more information about our books, courses, conferences, and news, see our website at http://www.oreilly.com.

Find us on Facebook: http://facebook.com/oreilly

Follow us on Twitter: http://twitter.com/oreillymedia

Watch us on YouTube: http://www.youtube.com/oreillymedia

# Acknowledgments

I would like to thank my Google colleagues, in particular the YouTube video classification team, for teaching me so much about Machine Learning. I could never have started this project without them. Special thanks to my personal ML gurus: Clément Courbet, Julien Dubois, Mathias Kende, Daniel Kitachewsky, James Pack, Alexander Pak, Anosh Raj, Vitor Sessak, Wiktor Tomczak, Ingrid von Glehn, Rich Washington, and everyone at YouTube Paris.

I am incredibly grateful to all the amazing people who took time out of their busy lives to review my book in so much detail. Thanks to Pete Warden for answering all my TensorFlow questions, reviewing Part II, providing many interesting insights, and of course for being part of the core TensorFlow team. You should definitely check out his blog (https://petewarden.com/)! Many thanks to Lukas Biewald for his very thorough review of Part II: he left no stone unturned, tested all the code (and caught a few errors), made many great suggestions, and his enthusiasm was contagious. You should check out his blog (https://lukasbiewald.com/) and his cool robots (https://goo.gl/Eu5u28)! Thanks to Justin Francis, who also reviewed Part II very thoroughly, catching errors and providing great insights, in particular in Chapter 16. Check out his posts (https://goo.gl/28ve8z) on TensorFlow!

Huge thanks as well to David Andrzejewski, who reviewed Part I and provided incredibly useful feedback, identifying unclear sections and suggesting how to improve them. Check out his website (http://www.david-andrzejewski.com/)! Thanks to Grégoire Mesnil, who reviewed Part II and contributed very interesting practical advice on training neural networks. Thanks as well to Eddy Hung, Salim Sémaoune, Karim Matrah, Ingrid von Glehn, Iain Smears, and Vincent Guilbeau for reviewing Part I and making many useful suggestions. And I also wish to thank my father-in-law, Michel Tessier, former mathematics teacher and now a great translator of Anton Chekhov, for helping me iron out some of the mathematics and notations in this book and reviewing the linear algebra Jupyter notebook.

And of course, a gigantic "thank you" to my dear brother Sylvain, who reviewed every single chapter, tested every line of code, provided feedback on virtually every section, and encouraged me from the first line to the last. Love you, bro!

Many thanks as well to O'Reilly's fantastic staff, in particular Nicole Tache, who gave me insightful feedback, always cheerful, encouraging, and helpful. Thanks as well to Marie Beaugureau, Ben Lorica, Mike Loukides, and Laurel Ruma for believing in this project and helping me define its scope. Thanks to Matt Hacker and all of the Atlas team for answering all my technical questions regarding formatting, asciidoc, and LaTeX, and thanks to Rachel Monaghan, Nick Adams, and all of the production team for their final review and their hundreds of corrections.

Last but not least, I am infinitely grateful to my beloved wife, Emmanuelle, and to our three wonderful kids, Alexandre, Rémi, and Gabrielle, for encouraging me to work hard on this book, asking many questions (who said you can't teach neural networks to a seven-year-old?), and even bringing me cookies and coffee. What more can one dream of?

# **Table of Contents**

Preface	xiii
Part I. The Fundamentals of Machine Learning	134
1. The Machine Learning Landscape	3
What Is Machine Learning?	4
Why Use Machine Learning?	4
Types of Machine Learning Systems	7
Supervised/Unsupervised Learning	8
Batch and Online Learning	14
Instance-Based Versus Model-Based Learning	17
Main Challenges of Machine Learning	
Insufficient Quantity of Training Data	22
Nonrepresentative Training Data	24
Poor-Quality Data	25
Irrelevant Features	25
Overfitting the Training Data	
Underfitting the Training Data	-
Stepping Back Total Ba	
Testing and Validating	29
Exercises	31
2. End-to-End Machine Learning Project	33
Working with Real Data nother the and the season of the se	33
Look at the Big Picture	35
901 Frame the Problem noite of the Problem	00
Select a Performance Measure modification in the select a performance Measure	37

Check the Assumptions	40
Get the Data	40
Create the Workspace	40
Download the Data	43
Take a Quick Look at the Data Structure	45
Create a Test Set	49
Discover and Visualize the Data to Gain Insights	53
Visualizing Geographical Data	53
Looking for Correlations	56
Experimenting with Attribute Combinations	59
Prepare the Data for Machine Learning Algorithms	60
Data Cleaning	61
Handling Text and Categorical Attributes	63
Custom Transformers	65
Feature Scaling	66
Transformation Pipelines	66
Select and Train a Model	68
Training and Evaluating on the Training Set	69
Better Evaluation Using Cross-Validation	70
Fine-Tune Your Model	72
Grid Search Springer Learnings	72
Randomized Search	75
Ensemble Methods	75
Analyze the Best Models and Their Errors and Best Models and Their Errors	75
Evaluate Your System on the Test Set	76
Launch, Monitor, and Maintain Your System	77
Try It Out!	77
Exercises and a supplied to a supplied the supplied to a s	78
an Somrepresentative Transing Data a reads to place virgory has been allowed to the Classification	70
Classification.	79
Trailerant Features	79
Training a Binary Classifier and games and gam	82
Performance Measures and gaining and gaini	82 83
Measuring Accuracy Using Cross-Validation	
Confusion Matrix  President and Basell	84
Precision and Recall Precision/Recall Tradeoff	86 87
The ROC Curve	91
Multiclass Classification and Analysis	
Error Analysis  Multilabel Classification	96
Multilabel Classification muldory adjument	100
Multioutput Classification	101

	Exercises		102
4.	Training Models	Training and Visualizing a Decision T	105
7.			
			106
	The Normal Equation		108
	Computational Complexity		110
	Gradient Descent		111
			114
	Stochastic Gradient Descent		17
	Mini-batch Gradient Descent		119
	Polynomial Regression		121
	Learning Curves		123
			127
	Ridge Regression		127
	Lasso Regression		130
			132
	Early Stopping		133
			134
	Estimating Probabilities		134
	Training and Cost Function	1 / Extra-Trees	135
	Decision Boundaries	Feature importance	136
	Softmax Regression	Boosting breeds as I made as I	139
	Exercises	1 AdaBoost	142
5.	Support Vector Machines		145
	Linear SVM Classification	1 Exercises	145
	Soft Margin Classification		146
	Nonlinear SVM Classification	Digrensionality Reduction	149
			150
	Adding Similarity Features		151
	Gaussian RBF Kernel	I Projection	152
	Computational Complexity		153
	SVM Regression		154
	Under the Hood	Preserving the Variance CA level dig	156
	Decision Function and Predictions		156
			157
	Quadratic Programming		159
	The Dual Problem		160
			161
	Online SVMs		164
	Exercises		165
		A STATE OF THE PARTY OF THE PAR	

6.	Decision Trees	Pretrives	167
	Training and Visualizing a Decision Tree		167
	Making Predictions		169
	Estimating Class Probabilities		171
	The CART Training Algorithm		171
	Computational Complexity		172
	Gini Impurity or Entropy?		172
	Regularization Hyperparameters		173
	Regression		175
	Instability		177
	Exercises		178
7.	Ensemble Learning and Random Forests	Regularizati Libert Madalla Libertal	181
	Voting Classifiers		181
	Bagging and Pasting		185
	Bagging and Pasting in Scikit-Learn		186
	Out-of-Bag Evaluation		187
	Random Patches and Random Subspaces		188
	Random Forests		189
	Extra-Trees		190
	Feature Importance		190
	Boosting		191
	AdaBoost		192
	Gradient Boosting		195
	Stacking		200
	Exercises		202
8.	Dimensionality Reduction	Madinest Stat Cheditoring	205
	The Curse of Dimensionality		206
	Main Approaches for Dimensionality Rec		207
	Projection		207
	Manifold Learning		210
	PCA		211
	Preserving the Variance		211
	Principal Components		212
	Projecting Down to d Dimensions		213
	Using Scikit-Learn		214
	Explained Variance Ratio		214
	Choosing the Right Number of Dimens		215
	PCA for Compression		216
	Incremental PCA		217
	Randomized PCA		218

Kernel PCA	218
Selecting a Kernel and Tuning Hyperparameters	219
	push good pantial 221
Other Dimensionality Reduction Techniques	
Exercises Consolination Consolination Incident	
Part II. Neural Networks and Deep Learning	115 Butch Normalizat 116 Gradient Chppin
9. Up and Running with TensorFlow	
ram Other Frameworks abrovement radio mor	PelabaM galaus H 232
Creating Your First Graph and Running It in a Session	wolladayawaari 232
그 이 내는 내가 있으면 살이 사람들이 많아 가게 보이는 그가 하고 무슨 아이지 않는데 보기 때문에 바다 이 주민을 모여 있어 내가 있는데 나를 했다.	234 Caching the From
Lifecycle of a Node Value	growth guldrend 235
Linear Regression with TensorFlow	200X labol4 235
Implementing Gradient Descent	ng besivisquenil 237
Manually Computing the Gradients	no no saintavera 237
Using autodiff	238 Faster Optimizers
Using an Optimizer	ingO minimemoM 239
Feeding Data to the Training Algorithm	releva A vonetseM 239
Saving and Restoring Models	barOsbA 241
Visualizing the Graph and Training Curves Using Tensor	Board 242
Name Scopes	ms/mbqO msbA 245
Modularity gnilyke	12 ole A grima sal 246
Sharing Variables and Sharing Variables	military galbiova 248
Exercises	251 Early Stopping
	253
From Biological to Artificial Neurons	бувя втоИ-хиМ 254
Biological Neurons	Mannemge A staff 255
Logical Computations with Neurons	control to to a 256
The Perceptron	essions 257
Multi-Layer Perceptron and Backpropagation	261
Training an MLP with TensorFlow's High-Level API	264
Training a DNN Using Plain TensorFlow	to apply all aliquida A 265
Construction Phase	nofishinant 265
Execution Phase MARI	9D sili prigensi/ 269
	rolling Operation 269
71 1	northografiells ung 270
	sbasgott lossato 270
Number of Neurons per Hidden Layer	
Activation Functions	obase2 a palnegO 272

	Exercises  Selection and Vanadalana and another another and another another and another anothe	212
11.		275
22		275
	Xavier and He Initialization	277
	Nonsaturating Activation Functions	279
	Batch Normalization	282
	Gradient Clipping	286
	Reusing Pretrained Layers	287
	Reusing a TensorFlow Model	287
	Reusing Models from Other Frameworks	289
	Freezing the Lower Layers	290
	Caching the Frozen Layers	291
	Tweaking, Dropping, or Replacing the Upper Layers	292
	Model Zoos Manual Tensor low	292
	Unsupervised Pretraining	293
	Pretraining on an Auxiliary Task	294
	Faster Optimizers Mb6tus gald/	295
	Momentum Optimization	295
	Nesterov Accelerated Gradient	297
	AdaGrad AdaGra	298
	Visualizing the Graph and Training Curves Using Tener Board on Tener Street	300
	Adam Optimization	300
	Learning Rate Scheduling	303
	Avoiding Overfitting Through Regularization	305
	Early Stopping	305
	$\ell_1$ and $\ell_2$ Regularization	305
	Dropout 25 25 25 25 25 25 25 25 25 25 25 25 25	307
	Max-Norm Regularization	309
	Data Augmentation	311
	Practical Guidelines anomal dilw anomal gmod langed	312
	Exercises	313
12.	Distributing TonsorFlow Across Devices and Servers	315
12.		
	Multiple Devices on a Single Machine Machine Installation	316 316
	Installation  Managing the GPU RAM	319
	Placing Operations on Devices  Parallel Execution	320
	Parallel Execution  Control Dependencies	323 325
	Multiple Devices Across Multiple Servers	325
	어느 보고 있다. 그는 그는 그는 그는 그는 그는 그는 그는 그는 그들이 되었다. 그들이 그는 그들은 그들은 그를 가지 않는 것이 없는 것이 없는 것이 없는 것이 없는 것이 없다.	
	Opening a Session	327