## Introduction to Machine Learning with Python

A Guide for Data Scientists

Andreas C. Müller and Sarah Guido



## Introduction to Machine Learning with Python

by Andreas C. Müller and Sarah Guido

Copyright © 2017 Sarah Guido, Andreas Müller. 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 (<a href="http://safaribooksonline.com">http://safaribooksonline.com</a>). For more information, contact our corporate/institutional sales department: 800-998-9938 or <a href="mailto:corporate@oreilly.com">corporate@oreilly.com</a>.

Editor: Dawn Schanafelt
Production Editor: Kristen Brown
Copyeditor: Rachel Head
Proofreader: Jasmine Kwityn

Indexer: Judy McConville
Interior Designer: David Futato
Cover Designer: Karen Montgomery
Illustrator: Rebecca Demarest

October 2016: First Edition

**Revision History for the First Edition** 2016-09-22: First Release

See http://oreilly.com/catalog/errata.csp?isbn=9781449369415 for release details.

The O'Reilly logo is a registered trademark of O'Reilly Media, Inc. *Introduction to Machine Learning with Python*, the cover image, and related trade dress are trademarks of O'Reilly Media, Inc.

While the publisher and the authors have used good faith efforts to ensure that the information and instructions contained in this work are accurate, the publisher and the authors 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.

## **Table of Contents**

Pre	Prefacevii		
1.	Introduction		
	Why Machine Learning?	1	
	Problems Machine Learning Can Solve	2	
	Knowing Your Task and Knowing Your Data	4	
	Why Python?	5	
	scikit-learn	5	
	Installing scikit-learn	6	
	Essential Libraries and Tools	7	
	Jupyter Notebook	7	
	NumPy	7	
	SciPy	8	
	matplotlib	9	
	pandas	10	
	mglearn	11	
	Python 2 Versus Python 3	12	
	Versions Used in this Book	12	
	A First Application: Classifying Iris Species	13	
	Meet the Data	14	
	Measuring Success: Training and Testing Data	17	
	First Things First: Look at Your Data	19	
	Building Your First Model: k-Nearest Neighbors	20	
	Making Predictions	22	
	Evaluating the Model	22	
	Summary and Outlook	23	

2.	Supervised Learning	. 25
	Classification and Regression	25
	Generalization, Overfitting, and Underfitting	26
	Relation of Model Complexity to Dataset Size	29
	Supervised Machine Learning Algorithms	29
	Some Sample Datasets	30
	k-Nearest Neighbors	35
	Linear Models	45
	Naive Bayes Classifiers	68
	Decision Trees	70
	Ensembles of Decision Trees	83
	Kernelized Support Vector Machines	92
	Neural Networks (Deep Learning)	104
	Uncertainty Estimates from Classifiers	119
	The Decision Function	120
	Predicting Probabilities	122
	Uncertainty in Multiclass Classification	124
	Summary and Outlook	127
3.	Unsupervised Learning and Preprocessing	131
	Types of Unsupervised Learning	131
	Challenges in Unsupervised Learning	132
	Preprocessing and Scaling	132
	Different Kinds of Preprocessing	133
	Applying Data Transformations	134
	Scaling Training and Test Data the Same Way	136
	The Effect of Preprocessing on Supervised Learning	138
	Dimensionality Reduction, Feature Extraction, and Manifold Learning	140
	Principal Component Analysis (PCA)	140
	Non-Negative Matrix Factorization (NMF)	156
	Manifold Learning with t-SNE	163
	Clustering	168
	k-Means Clustering	168
	Agglomerative Clustering	182
	DBSCAN	187
	Comparing and Evaluating Clustering Algorithms	191
	Summary of Clustering Methods	207
	Summary and Outlook	208
4.	Representing Data and Engineering Features	211
	Categorical Variables	212
	One-Hot-Encoding (Dummy Variables)	213

	Numbers Can Encode Categoricals	218
	Binning, Discretization, Linear Models, and Trees	220
	Interactions and Polynomials	224
	Univariate Nonlinear Transformations	232
	Automatic Feature Selection	236
	Univariate Statistics	236
	Model-Based Feature Selection	238
	Iterative Feature Selection	240
	Utilizing Expert Knowledge	242
	Summary and Outlook	250
5.	Model Evaluation and Improvement	251
	Cross-Validation	252
	Cross-Validation in scikit-learn	253
	Benefits of Cross-Validation	254
	Stratified k-Fold Cross-Validation and Other Strategies	254
	Grid Search	260
	Simple Grid Search	261
	The Danger of Overfitting the Parameters and the Validation Set	261
	Grid Search with Cross-Validation	263
	Evaluation Metrics and Scoring	275
	Keep the End Goal in Mind	275
	Metrics for Binary Classification	276
	Metrics for Multiclass Classification	296
	Regression Metrics	299
	Using Evaluation Metrics in Model Selection	300
	Summary and Outlook	302
6.	Algorithm Chains and Pipelines	305
	Parameter Selection with Preprocessing	306
	Building Pipelines	308
	Using Pipelines in Grid Searches	309
	The General Pipeline Interface	312
	Convenient Pipeline Creation with make_pipeline	313
	Accessing Step Attributes	314
	Accessing Attributes in a Grid-Searched Pipeline	315
	Grid-Searching Preprocessing Steps and Model Parameters	317
	Grid-Searching Which Model To Use	319
	Summary and Outlook	320
7.	Working with Text Data	323
	Types of Data Represented as Strings	323

	Example Application: Sentiment Analysis of Movie Reviews	325
	Representing Text Data as a Bag of Words	327
	Applying Bag-of-Words to a Toy Dataset	329
	Bag-of-Words for Movie Reviews	330
	Stopwords	334
	Rescaling the Data with tf-idf	336
	Investigating Model Coefficients	338
	Bag-of-Words with More Than One Word (n-Grams)	339
	Advanced Tokenization, Stemming, and Lemmatization	344
	Topic Modeling and Document Clustering	347
	Latent Dirichlet Allocation	348
	Summary and Outlook	355
8.	Wrapping Up	357
	Approaching a Machine Learning Problem	357
	Humans in the Loop	358
	From Prototype to Production	359
	Testing Production Systems	359
	Building Your Own Estimator	360
	Where to Go from Here	361
	Theory	361
	Other Machine Learning Frameworks and Packages	362
	Ranking, Recommender Systems, and Other Kinds of Learning	363
	Probabilistic Modeling, Inference, and Probabilistic Programming	363
	Neural Networks	364
	Scaling to Larger Datasets	364
	Honing Your Skills	365
	Conclusion	366
lne	Nov	267