## **Texts in Computer Science**

**Series editors** 

David Gries Orit Hazzan Fred B. Schneider More information about this series at http://www.springer.com/series/3191

### Steven S. Skiena

# The Data Science Design Manual



Steven S. Skiena Computer Science Department Stony Brook University Stony Brook, NY USA

ISSN 1868-0941 ISSN 1868-095X (electronic)
Texts in Computer Science
ISBN 978-3-319-55443-3 ISBN 978-3-319-55444-0 (eBook)
https://doi.org/10.1007/978-3-319-55444-0

Library of Congress Control Number: 2017943201

This book was advertised with a copyright holder in the name of the publisher in error, whereas the author(s) holds the copyright.

#### © The Author(s) 2017

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.

Printed on acid-free paper

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

### **Preface**

Making sense of the world around us requires obtaining and analyzing data from our environment. Several technology trends have recently collided, providing new opportunities to apply our data analysis savvy to greater challenges than ever before.

Computer storage capacity has increased exponentially; indeed remembering has become so cheap that it is almost impossible to get computer systems to forget. Sensing devices increasingly monitor everything that can be observed: video streams, social media interactions, and the position of anything that moves. Cloud computing enables us to harness the power of massive numbers of machines to manipulate this data. Indeed, hundreds of computers are summoned each time you do a Google search, scrutinizing all of your previous activity just to decide which is the best ad to show you next.

The result of all this has been the birth of *data science*, a new field devoted to maximizing value from vast collections of information. As a discipline, data science sits somewhere at the intersection of statistics, computer science, and machine learning, but it is building a distinct heft and character of its own. This book serves as an introduction to data science, focusing on the skills and principles needed to build systems for collecting, analyzing, and interpreting data.

My professional experience as a researcher and instructor convinces me that one major challenge of data science is that it is considerably more subtle than it looks. Any student who has ever computed their grade point average (GPA) can be said to have done rudimentary statistics, just as drawing a simple scatter plot lets you add experience in data visualization to your resume. But meaningfully analyzing and interpreting data requires both technical expertise and wisdom. That so many people do these basics so badly provides my inspiration for writing this book.

#### To the Reader

I have been gratified by the warm reception that my book *The Algorithm Design Manual* [Ski08] has received since its initial publication in 1997. It has been recognized as a unique guide to using algorithmic techniques to solve problems that often arise in practice. The book you are holding covers very different material, but with the same motivation.

In particular, here I stress the following basic principles as fundamental to becoming a good data scientist:

• Valuing doing the simple things right: Data science isn't rocket science. Students and practitioners often get lost in technological space, pursuing the most advanced machine learning methods, the newest open source software libraries, or the glitziest visualization techniques. However, the heart of data science lies in doing the simple things right: understanding the application domain, cleaning and integrating relevant data sources, and presenting your results clearly to others.

Simple doesn't mean easy, however. Indeed it takes considerable insight and experience to ask the right questions, and sense whether you are moving toward correct answers and actionable insights. I resist the temptation to drill deeply into clean, technical material here just because it is teachable. There are plenty of other books which will cover the intricacies of machine learning algorithms or statistical hypothesis testing. My mission here is to lay the groundwork of what really matters in analyzing data.

• Developing mathematical intuition: Data science rests on a foundation of mathematics, particularly statistics and linear algebra. It is important to understand this material on an intuitive level: why these concepts were developed, how they are useful, and when they work best. I illustrate operations in linear algebra by presenting pictures of what happens to matrices when you manipulate them, and statistical concepts by examples and reducto ad absurdum arguments. My goal here is transplanting intuition into the reader.

But I strive to minimize the amount of formal mathematics used in presenting this material. Indeed, I will present exactly one formal proof in this book, an incorrect proof where the associated theorem is obviously false. The moral here is not that mathematical rigor doesn't matter, because of course it does, but that genuine rigor is impossible until after there is comprehension.

• Think like a computer scientist, but act like a statistician: Data science provides an umbrella linking computer scientists, statisticians, and domain specialists. But each community has its own distinct styles of thinking and action, which gets stamped into the souls of its members.

In this book, I emphasize approaches which come most naturally to computer scientists, particularly the algorithmic manipulation of data, the use of machine learning, and the mastery of scale. But I also seek to transmit the core values of statistical reasoning: the need to understand the application domain, proper appreciation of the small, the quest for significance, and a hunger for exploration.

No discipline has a monopoly on the truth. The best data scientists incorporate tools from multiple areas, and this book strives to be a relatively neutral ground where rival philosophies can come to reason together.

Equally important is what you will not find in this book. I do not emphasize any particular language or suite of data analysis tools. Instead, this book provides a high-level discussion of important design principles. I seek to operate at a conceptual level more than a technical one. The goal of this manual is to get you going in the right direction as quickly as possible, with whatever software tools you find most accessible.

#### To the Instructor

This book covers enough material for an "Introduction to Data Science" course at the undergraduate or early graduate student levels. I hope that the reader has completed the equivalent of at least one programming course and has a bit of prior exposure to probability and statistics, but more is always better than less

I have made a full set of lecture slides for teaching this course available online at http://www.data-manual.com. Data resources for projects and assignments are also available there to aid the instructor. Further, I make available online video lectures using these slides to teach a full-semester data science course. Let me help teach your class, through the magic of the web!

Pedagogical features of this book include:

- War Stories: To provide a better perspective on how data science techniques apply to the real world, I include a collection of "war stories," or tales from our experience with real problems. The moral of these stories is that these methods are not just theory, but important tools to be pulled out and used as needed.
- False Starts: Most textbooks present methods as a fait accompli, obscuring the ideas involved in designing them, and the subtle reasons why other approaches fail. The war stories illustrate my reasoning process on certain applied problems, but I weave such coverage into the core material as well.
- Take-Home Lessons: Highlighted "take-home" lesson boxes scattered through each chapter emphasize the big-picture concepts to learn from each chapter.
- Homework Problems: I provide a wide range of exercises for homework and self-study. Many are traditional exam-style problems, but there are also larger-scale implementation challenges and smaller-scale interview questions, reflecting the questions students might encounter when searching for a job. Degree of difficulty ratings have been assigned to all problems.

In lieu of an answer key, a Solution Wiki has been set up, where solutions to all even numbered problems will be solicited by crowdsourcing. A similar system with my *Algorithm Design Manual* produced coherent solutions,

or so I am told. As a matter of principle I refuse to look at them, so let the buyer beware.

- Kaggle Challenges: Kaggle (www.kaggle.com) provides a forum for data scientists to compete in, featuring challenging real-world problems on fascinating data sets, and scoring to test how good your model is relative to other submissions. The exercises for each chapter include three relevant Kaggle challenges, to serve as a source of inspiration, self-study, and data for other projects and investigations.
- Data Science Television: Data science remains mysterious and even threatening to the broader public. The Quant Shop is an amateur take on what a data science reality show should be like. Student teams tackle a diverse array of real-world prediction problems, and try to forecast the outcome of future events. Check it out at http://www.quant-shop.com.

A series of eight 30-minute episodes has been prepared, each built around a particular real-world prediction problem. Challenges include pricing art at an auction, picking the winner of the Miss Universe competition, and forecasting when celebrities are destined to die. For each, we observe as a student team comes to grips with the problem, and learn along with them as they build a forecasting model. They make their predictions, and we watch along with them to see if they are right or wrong.

In this book, *The Quant Shop* is used to provide concrete examples of prediction challenges, to frame discussions of the data science modeling pipeline from data acquisition to evaluation. I hope you find them fun, and that they will encourage you to conceive and take on your own modeling challenges.

• Chapter Notes: Finally, each tutorial chapter concludes with a brief notes section, pointing readers to primary sources and additional references.

#### **Dedication**

My bright and loving daughters Bonnie and Abby are now full-blown teenagers, meaning that they don't always process statistical evidence with as much alacrity as I would I desire. I dedicate this book to them, in the hope that their analysis skills improve to the point that they always just agree with me.

And I dedicate this book to my beautiful wife Renee, who agrees with me even when she doesn't agree with me, and loves me beyond the support of all creditable evidence.

#### Acknowledgments

My list of people to thank is large enough that I have probably missed some. I will try to do enumerate them systematically to minimize omissions, but ask those I've unfairly neglected for absolution.

First, I thank those who made concrete contributions to help me put this book together. Yeseul Lee served as an apprentice on this project, helping with figures, exercises, and more during summer 2016 and beyond. You will see evidence of her handiwork on almost every page, and I greatly appreciate her help and dedication. Aakriti Mittal and Jack Zheng also contributed to a few of the figures.

Students in my Fall 2016 Introduction to Data Science course (CSE 519) helped to debug the manuscript, and they found plenty of things to debug. I particularly thank Rebecca Siford, who proposed over one hundred corrections on her own. Several data science friends/sages reviewed specific chapters for me, and I thank Anshul Gandhi, Yifan Hu, Klaus Mueller, Francesco Orabona, Andy Schwartz, and Charles Ward for their efforts here.

I thank all the *Quant Shop* students from Fall 2015 whose video and modeling efforts are so visibly on display. I particularly thank Jan (Dini) Diskin-Zimmerman, whose editing efforts went so far beyond the call of duty I felt like a felon for letting her do it.

My editors at Springer, Wayne Wheeler and Simon Rees, were a pleasure to work with as usual. I also thank all the production and marketing people who helped get this book to you, including Adrian Pieron and Annette Anlauf.

Several exercises were originated by colleagues or inspired by other sources. Reconstructing the original sources years later can be challenging, but credits for each problem (to the best of my recollection) appear on the website.

Much of what I know about data science has been learned through working with other people. These include my Ph.D. students, particularly Rami al-Rfou, Mikhail Bautin, Haochen Chen, Yanqing Chen, Vivek Kulkarni, Levon Lloyd, Andrew Mehler, Bryan Perozzi, Yingtao Tian, Junting Ye, Wenbin Zhang, and postdoc Charles Ward. I fondly remember all of my Lydia project masters students over the years, and remind you that my prize offer to the first one who names their daughter Lydia remains unclaimed. I thank my other collaborators with stories to tell, including Bruce Futcher, Justin Gardin, Arnout van de Rijt, and Oleksii Starov.

I remember all members of the General Sentiment/Canrock universe, particularly Mark Fasciano, with whom I shared the start-up dream and experienced what happens when data hits the real world. I thank my colleagues at Yahoo Labs/Research during my 2015–2016 sabbatical year, when much of this book was conceived. I single out Amanda Stent, who enabled me to be at Yahoo during that particularly difficult year in the company's history. I learned valuable things from other people who have taught related data science courses, including Andrew Ng and Hans-Peter Pfister, and thank them all for their help.

If you have a procedure with ten parameters, you probably missed some.

#### Caveat

It is traditional for the author to magnanimously accept the blame for whatever deficiencies remain. I don't. Any errors, deficiencies, or problems in this book are somebody else's fault, but I would appreciate knowing about them so as to determine who is to blame.

Steven S. Skiena
Department of Computer Science
Stony Brook University
Stony Brook, NY 11794-2424
http://www.cs.stonybrook.edu/~skiena
skiena@data-manual.com
May 2017

# Contents

1	$\mathbf{W}\mathbf{h}$	at is I	Data Science?	1
	1.1 Computer Science, Data Science, and Real Science			2
	1.2	Askin	g Interesting Questions from Data	4
		1.2.1	The Baseball Encyclopedia	5
		1.2.2	The Internet Movie Database (IMDb)	7
		1.2.3	Google Ngrams	10
		1.2.4	New York Taxi Records	11
	1.3	Prope	erties of Data	14
		1.3.1	Structured vs. Unstructured Data	14
		1.3.2	Quantitative vs. Categorical Data	15
		1.3.3	Big Data vs. Little Data	15
	1.4	Classi	ification and Regression	16
	1.5		Science Television: The Quant Shop	17
		1.5.1	Kaggle Challenges	19
	1.6	About	t the War Stories	19
	1.7	War S	Story: Answering the Right Question	21
	1.8	Chapt	ter Notes	22
	1.9	Exerc	ises	23
2	Ma	thema	tical Preliminaries	27
	2.1	Proba	ability	27
		2.1.1	Probability vs. Statistics	29
		2.1.2	Compound Events and Independence	30
		2.1.3	Conditional Probability	31
		2.1.4	Probability Distributions	32
	2.2	Descr	iptive Statistics	34
		2.2.1	Centrality Measures	34
		2.2.2	Variability Measures	36
		2.2.3	Interpreting Variance	37
		2.2.4	Characterizing Distributions	39
	2.3	Corre	lation Analysis	40
		2.3.1	Correlation Coefficients: Pearson and Spearman Rank	41
		2.3.2	The Power and Significance of Correlation	43
		2 3 3	Correlation Does Not Imply Causation	45

xii CONTENTS

		2.3.4	Detecting Periodicities by Autocorrelation	46
	2.4	Logarith	hms	47
		2.4.1 1	Logarithms and Multiplying Probabilities	48
		2.4.2	Logarithms and Ratios	48
				49
	2.5			50
	2.6			52
	2.7			53
3	Dat	a Mung	ing 5	57
	3.1	Languag	ges for Data Science	57
		3.1.1	The Importance of Notebook Environments	59
		3.1.2	Standard Data Formats	31
	3.2	Collecti	ng Data	34
		3.2.1	Hunting	34
				37
				38
	3.3			39
				39
				72
			1 0	76
			~ ~ ~	78
	3.4			79
	3.5			30
				31
				32
				33
			00 0	34
				38
	3.6			90
	3.7	-		90
4	Sco	res and	Rankings 9	95
	4.1	The Bo	dy Mass Index (BMI)	96
	4.2	Develop	ing Scoring Systems	99
		4.2.1	Gold Standards and Proxies	99
		4.2.2	Scores vs. Rankings	00
		4.2.3	Recognizing Good Scoring Functions	)1
	4.3	Z-scores	s and Normalization	)3
	4.4	Advance	ed Ranking Techniques	)4
			Elo Rankings	)4
			Merging Rankings	)8
			Digraph-based Rankings	
			PageRank	
	4.5		ory: Clyde's Revenge	11
	4.6		Impossibility Theorem	14

CONTENTS xiii

	4.7	War Story: Who's Bigger?	15
	4.8	Chapter Notes	18
	4.9	Exercises	19
5	Stat	tistical Analysis	21
0	5.1	Statistical Distributions	
	0.1	5.1.1 The Binomial Distribution	
		5.1.2 The Normal Distribution	
		5.1.3 Implications of the Normal Distribution	
		5.1.4 Poisson Distribution	
		5.1.5 Power Law Distributions	
	5.2	Sampling from Distributions	
		5.2.1 Random Sampling beyond One Dimension	
	5.3	Statistical Significance	
		5.3.1 The Significance of Significance	
		5.3.2 The T-test: Comparing Population Means	
		5.3.3 The Kolmogorov-Smirnov Test	
		5.3.4 The Bonferroni Correction	
		5.3.5 False Discovery Rate	
	5.4	War Story: Discovering the Fountain of Youth?	
	5.5	Permutation Tests and P-values	45
		5.5.1 Generating Random Permutations	47
		5.5.2 DiMaggio's Hitting Streak	48
	5.6	Bayesian Reasoning	50
	5.7	Chapter Notes	51
	5.8	Exercises	51
6	Visi	ualizing Data	55
	6.1	Exploratory Data Analysis	
		6.1.1 Confronting a New Data Set	
		6.1.2 Summary Statistics and Anscombe's Quartet	
		6.1.3 Visualization Tools	
	6.2	Developing a Visualization Aesthetic	62
		6.2.1 Maximizing Data-Ink Ratio	63
		6.2.2 Minimizing the Lie Factor	64
		6.2.3 Minimizing Chartjunk	65
		6.2.4 Proper Scaling and Labeling	67
		6.2.5 Effective Use of Color and Shading	68
		6.2.6 The Power of Repetition	69
	6.3	<i>y</i> 1	70
			70
			74
			77
			79
		o .	83
		6.3.6 Data Maps	87

xiv CONTENTS

	6.4	Great Visualizations
		6.4.1 Marey's Train Schedule
		6.4.2 Snow's Cholera Map
		6.4.3 New York's Weather Year
	6.5	Reading Graphs
		6.5.1 The Obscured Distribution
		6.5.2 Overinterpreting Variance
	6.6	Interactive Visualization
	6.7	War Story: TextMapping the World
	6.8	Chapter Notes
	6.9	Exercises
7	Mat	chematical Models 201
	7.1	Philosophies of Modeling
		7.1.1 Occam's Razor
		7.1.2 Bias-Variance Trade-Offs
		7.1.3 What Would Nate Silver Do?
	7.2	A Taxonomy of Models
		7.2.1 Linear vs. Non-Linear Models 200
		7.2.2 Blackbox vs. Descriptive Models 200
		7.2.3 First-Principle vs. Data-Driven Models 207
		7.2.4 Stochastic vs. Deterministic Models 208
		7.2.5 Flat vs. Hierarchical Models 209
	7.3	Baseline Models
		7.3.1 Baseline Models for Classification 210
		7.3.2 Baseline Models for Value Prediction 212
	7.4	Evaluating Models
		7.4.1 Evaluating Classifiers
		7.4.2 Receiver-Operator Characteristic (ROC) Curves 218
		7.4.3 Evaluating Multiclass Systems
		7.4.4 Evaluating Value Prediction Models
	7.5	Evaluation Environments
		7.5.1 Data Hygiene for Evaluation
		7.5.2 Amplifying Small Evaluation Sets
	7.6	War Story: 100% Accuracy
	7.7	Simulation Models
	7.8	War Story: Calculated Bets
	7.9	Chapter Notes
		Exercises
8	Line	ear Algebra 237
	8.1	The Power of Linear Algebra
		8.1.1 Interpreting Linear Algebraic Formulae
		8.1.2 Geometry and Vectors
	8.2	Visualizing Matrix Operations
		8.2.1 Matrix Addition

CONTENTS xv

		8.2.2	Matrix Multiplication
		8.2.3	Applications of Matrix Multiplication 244
		8.2.4	Identity Matrices and Inversion
		8.2.5	Matrix Inversion and Linear Systems
		8.2.6	Matrix Rank
	8.3	Factor	ring Matrices
		8.3.1	Why Factor Feature Matrices?
		8.3.2	LU Decomposition and Determinants
	8.4	Eigen	values and Eigenvectors
		8.4.1	Properties of Eigenvalues
		8.4.2	Computing Eigenvalues
	8.5	Eigen	value Decomposition
		8.5.1	Singular Value Decomposition
		8.5.2	Principal Components Analysis
	8.6	War S	tory: The Human Factors
	8.7		er Notes
	8.8	-	ises
	0.0	211010	
9	Line		d Logistic Regression 267
	9.1	Linear	Regression
		9.1.1	Linear Regression and Duality
		9.1.2	Error in Linear Regression
		9.1.3	Finding the Optimal Fit
	9.2	Better	Regression Models
		9.2.1	Removing Outliers
		9.2.2	Fitting Non-Linear Functions
		9.2.3	Feature and Target Scaling
		9.2.4	Dealing with Highly-Correlated Features 277
	9.3	War S	tory: Taxi Deriver
	9.4	Regre	ssion as Parameter Fitting
		9.4.1	Convex Parameter Spaces
		9.4.2	Gradient Descent Search
		9.4.3	What is the Right Learning Rate?
		9.4.4	Stochastic Gradient Descent
	9.5	Simpl	ifying Models through Regularization
		9.5.1	Ridge Regression
		9.5.2	LASSO Regression
			Trade-Offs between Fit and Complexity 288
	9.6		fication and Logistic Regression
	0.0	9.6.1	Regression for Classification
		9.6.2	Decision Boundaries
		9.6.3	Logistic Regression
	9.7		in Logistic Classification
	0.1	9.7.1	Balanced Training Classes
		9.7.1	Multi-Class Classification
		9.7.2 $9.7.3$	Hierarchical Classification
		J.1.0	11101a101110a1 01a551110a11011

xvi CONTENTS

		9.7.4 Partition Functions and Multinor	nial Regression			299
	9.8	Chapter Notes				300
	9.9	Exercises				301
10		tance and Network Methods				303
	10.1	Measuring Distances				
		10.1.1 Distance Metrics				
		10.1.2 The $L_k$ Distance Metric				
		10.1.3 Working in Higher Dimensions .				
		10.1.4 Dimensional Egalitarianism				308
		10.1.5 Points vs. Vectors				309
		10.1.6 Distances between Probability Di	stributions			310
	10.2	Nearest Neighbor Classification				311
		10.2.1 Seeking Good Analogies				312
		10.2.2 k-Nearest Neighbors				313
		10.2.3 Finding Nearest Neighbors				315
		10.2.4 Locality Sensitive Hashing				317
	10.3	Graphs, Networks, and Distances				
		10.3.1 Weighted Graphs and Induced No				
		10.3.2 Talking About Graphs				
		10.3.3 Graph Theory				
	10.4	PageRank				
		Clustering				
		10.5.1 $k$ -means Clustering				
		10.5.2 Agglomerative Clustering				
		10.5.3 Comparing Clusterings				
		10.5.4 Similarity Graphs and Cut-Based				
	10.6	War Story: Cluster Bombing	_			
		Chapter Notes				
		Exercises				
11		chine Learning				351
	11.1	Naive Bayes				
		11.1.1 Formulation				354
		11.1.2 Dealing with Zero Counts (Discou	unting)			356
	11.2	Decision Tree Classifiers				357
		11.2.1 Constructing Decision Trees				359
		11.2.2 Realizing Exclusive Or				361
		11.2.3 Ensembles of Decision Trees				362
	11.3	Boosting and Ensemble Learning				363
		11.3.1 Voting with Classifiers				363
		11.3.2 Boosting Algorithms				364
	11.4	Support Vector Machines				366
		11.4.1 Linear SVMs				369
		11.4.2 Non-linear SVMs				369
		11.4.3 Kernels				371

CONTENTS	xvii

	11.5	Degrees of Supervision	372
		11.5.1 Supervised Learning	
			372
		11.5.3 Semi-supervised Learning	
			375
	11.6		377
	11.0	1 0	378
			382
		11.6.3 Word and Graph Embeddings	383
	11 7	•	385
			387
		Exercises	
	11.9	Exercises	300
12	Big	Data: Achieving Scale	391
		What is Big Data?	
	12.1	12.1.1 Big Data as Bad Data	
			394
	12.2		395
	12.2		397
	12.0		397
		12.3.2 Hashing	399
		12.3.3 Exploiting the Storage Hierarchy	401
			401
	19.4		402
	12.4	0 1 0	403
		1 0 0	404 $406$
	10.5	1 0	400
	12.5		
		, , ,	407
			409
			409
	10.0	1 0	410
	12.6	1	410
		1 0 0	412
		*	414
		1	416
		1	419
	12.9	Exercises	419
10	<i>a</i> .		400
13	Cod		423
		Get a Job!	
		Go to Graduate School!	
	13.3	Professional Consulting Services	425
14	Bibl	liography	427