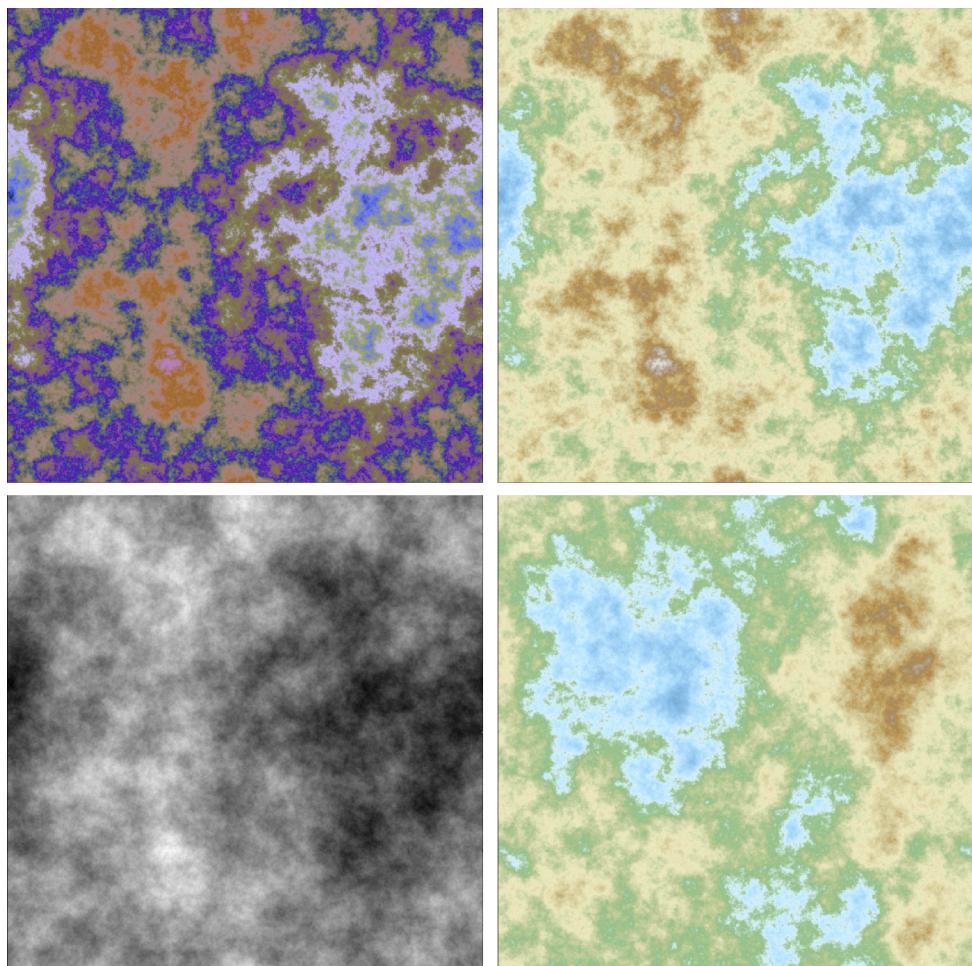

Synthetic Data



Preface

This book covers the foundations of machine learning, with modern approaches to solving complex problems and the systematic generation and use of synthetic data. Emphasis is on scalability, automation, testing, optimizing, and interpretability (explainable AI). For instance, regression techniques – including logistic and Lasso – are presented as a single method, without using advanced linear algebra. There is no need to learn 50 versions when one does it all and more. Confidence regions and prediction intervals are built using parametric bootstrap, without statistical models or probability distributions. Models (including generative models and mixtures) are mostly used to create rich synthetic data to test and benchmark various methods.

Topics covered include clustering and classification, GPU machine learning, ensemble methods including an original boosting technique, elements of graph modeling, deep neural networks, auto-regressive and non-periodic time series, Brownian motions and related processes, simulations, interpolation, random numbers, natural language processing (smart crawling, taxonomy creation and structuring unstructured data), computer vision (shapes generation and recognition), curve fitting, cross-validation, goodness-of-fit metrics, feature selection, curve fitting, gradient methods, optimization techniques and numerical stability. Chapters 12 and 13 focus on synthetic data applications: fractal-like terrain generation with the diamond-square algorithm, and synthetic star clusters evolving over time and bound by gravity. The latter provides great insights to explore the past and future of our universe or studying collision graphs. It also allows you to explore alternative universes, for instance with negative masses. Chapters 14 and 16 are more advanced and may be skipped in introductory classes. The former focuses on point process applications, while the later focuses on applications a machine learning methods to discover new insights in a famous mathematical conjecture: the Riemann Hypothesis.

Methods are accompanied by enterprise-grade Python code, replicable datasets and visualizations, including data animations (gifs, videos, even sound done in Python). The code uses various data structures and library functions sometimes with advanced options. It constitutes a Python tutorial in itself, and an introduction to scientific computing. Some data animations and chart enhancements are done in R. The code, datasets, spreadsheets and data visualizations are also on GitHub, spread across the following repositories: [Machine Learning](#), [Point Processes](#), [Visualizations](#), and [Experimental Math](#). Chapters are mostly independent from each other, allowing you to read in random order. A glossary, index and numerous cross-references make the navigation easy and unify all the chapters.

The style is very compact, getting down to the point quickly, and suitable to business professionals eager to learn a lot of useful material in a limited amount of time. Jargon and arcane theories are absent, replaced by simple English to facilitate the reading by non-experts, and to help you discover topics usually made inaccessible to beginners. While state-of-the-art research is presented in all chapters, the prerequisites to read this book are minimal: an analytic professional background, or a first course in calculus and linear algebra. The original presentation avoids all unnecessary math and statistics, yet without eliminating advanced topics. Finally, this book is the main reference for my course on intuitive machine learning. For details about the classes, see [here](#).

About the Author

Vincent Granville is a pioneering data scientist and machine learning expert, co-founder of Data Science Central (acquired by a publicly traded company in 2020), founder of [MLTechniques.com](#), former VC-funded executive, author and patent owner. Vincent's past corporate experience includes Visa, Wells Fargo, eBay, NBC, Microsoft, and CNET.



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Contents

List of Figures	9
List of Tables	11
1 Machine Learning Cloud Regression and Optimization	12
1.1 Introduction: circle fitting	12
1.1.1 Previous versions of my method	13
1.2 Methodology, implementation details and caveats	14
1.2.1 Solution, R-squared and backward compatibility	14
1.2.2 Upgrades to the model	15
1.3 Case studies	16
1.3.1 Logistic regression, two ways	16
1.3.2 Ellipsoid and hyperplane fitting	17
1.3.2.1 Curve fitting: 250 examples in one video	17
1.3.2.2 Confidence region for the fitted ellipse: application to meteorite shapes	18
1.3.2.3 Python code	19
1.3.3 Non-periodic sum of periodic time series: ocean tides	25
1.3.3.1 Numerical instability and how to fix it	26
1.3.3.2 Python code	27
1.3.4 Fitting a line in 3D, unsupervised clustering, and other generalizations	28
1.3.4.1 Example: confidence region for the cluster centers	29
1.3.4.2 Exact solution and caveats	30
1.3.4.3 Comparison with K-means clustering	31
1.3.4.4 Python code	33
1.4 Connection to synthetic data: meteorites, ocean tides	35
2 A Simple, Robust and Efficient Ensemble Method	36
2.1 Introduction	36
2.2 Methodology	37
2.2.1 How hidden decision trees (HDT) work	37
2.2.2 NLP case study: summary and findings	38
2.2.3 Parameters	39
2.2.4 Improving the methodology	39
2.3 Implementation details	39
2.3.1 Correcting for bias	39
2.3.1.1 Time-adjusted scores	40
2.3.2 Excel spreadsheet	40
2.3.3 Python code and dataset	40
2.4 Model-free confidence intervals and perfect nodes	44
2.4.1 Interesting asymptotic properties of confidence intervals	44
3 Gentle Introduction to Linear Algebra	46
3.1 Power of a matrix	46
3.2 Examples, generalization, and matrix inversion	47
3.2.1 Example with a non-invertible matrix	48
3.2.2 Fast computations	48
3.2.3 Square root of a matrix	48
3.3 Application to machine learning problems	49
3.3.1 Markov chains	49
3.3.2 Time series: auto-regressive processes	49
3.3.3 Linear regression	49

3.4	Mathematics of auto-regressive time series	50
3.4.1	Simulations: curious fractal time series	50
3.4.1.1	White noise: Fréchet, Weibull and exponential cases	51
3.4.1.2	Illustration	51
3.4.2	Solving Vandermonde systems: a numerically stable method	52
3.5	Math for Machine Learning: Must-Read Books	53
4	The Art of Visualizing High Dimensional Data	54
4.1	Introduction	54
4.2	Applications	55
4.2.1	Spatial time series	55
4.2.2	Prediction intervals in any dimensions	55
4.2.3	Supervised classification of an infinite dataset	56
4.2.3.1	Machine learning perspective	56
4.2.3.2	Six challenging problems	57
4.2.3.3	Mathematical background: the Riemann Hypothesis	57
4.2.3.4	Partial solutions to the six challenging problems	58
4.2.4	Algorithms with chaotic convergence	59
4.3	Python code	59
4.3.1	Path simulation	59
4.3.2	Visual convergence analysis in 2D	62
4.3.3	Supervised classification	63
4.4	Visualizations	66
5	Fast Classification and Clustering via Image Convolution Filters	69
5.1	Introduction	69
5.2	Generating the synthetic data	70
5.2.1	Simulations with logistic distribution	70
5.2.2	Mapping the raw observations onto an image bitmap	71
5.3	Classification and unsupervised clustering	71
5.3.1	Supervised classification based on convolution filters	72
5.3.2	Clustering based on histogram equalization	72
5.3.3	Fractal classification: deep neural network analogy	73
5.3.4	Generalization to higher dimensions	74
5.3.5	Towards a very fast implementation	74
5.4	Python code	75
5.4.1	Fractal classification	76
5.4.2	GPU classification and clustering	78
5.4.3	Home-made graphic library	80
6	Shape Classification via Explainable AI	83
6.1	Introduction	83
6.2	Mathematical foundations	83
6.3	Shape signature	84
6.3.1	Weighted centroid	84
6.3.2	Computing the signature	85
6.3.3	Example	86
6.4	Shape comparison	86
6.4.1	Shape classification	87
6.5	Application	87
6.6	Exercises	88
7	Synthetic Data, Interpretable Regression, and Submodels	89
7.1	Introduction	89
7.2	Synthetic data sets and the spreadsheet	90
7.2.1	Correlation structure	90
7.2.2	Standardized regression	91
7.2.3	Initial conditions	91
7.2.4	Simulations and Excel spreadsheet	91
7.3	Damping schedule and convergence acceleration	92
7.3.1	Spreadsheet implementation	92
7.3.2	Interpretable regression with no overfitting	93
7.3.3	Adaptive damping	93

7.4	Performance assessment on synthetic data	93
7.4.1	Results	94
7.4.2	Distribution-free confidence intervals	96
7.4.2.1	Parametric bootstrap	97
7.5	Feature selection	97
7.5.1	Combinatorial approach	97
7.5.2	Stepwise approach	98
7.6	Conclusion	99
8	From Interpolation to Fuzzy Regression	101
8.1	Introduction	101
8.2	Original version	102
8.3	Full, non-linear model in higher dimensions	102
8.3.1	Geometric proximity, weights, and numerical stability	103
8.3.2	Predicted values and prediction intervals	103
8.3.3	Illustration, with spreadsheet	104
8.3.3.1	Output fields	105
8.4	Results	105
8.4.1	Performance assessment	105
8.4.2	Visualization	106
8.4.3	Amplitude restoration	106
8.5	Exercises	107
8.6	Python source code and datasets	108
9	Detecting Subtle Departures from Randomness	112
9.1	Introduction	112
9.2	Pseudo-random numbers	113
9.2.1	Strong pseudo-random numbers	113
9.2.1.1	New test of randomness for PRNGs	114
9.2.1.2	Theoretical background: the law of the iterated logarithm	114
9.2.1.3	Connection to the Generalized Riemann Hypothesis	114
9.2.2	Testing well-known sequences	115
9.2.2.1	Reverse-engineering a pseudo-random sequence	116
9.2.2.2	Illustrations	117
9.3	Python code	119
9.3.1	Fixes to the faulty random function in Python	119
9.3.2	Prime test implementation to detect subtle flaws in PRNG's	119
9.3.3	Special formula to compute 10 million digits of $\sqrt{2}$	122
10	Some Unusual Random Walks	126
10.1	Symmetric unbiased constrained random walks	126
10.1.1	Three fundamental properties of pure random walks	126
10.1.2	Random walks with more entropy than pure random signal	127
10.1.2.1	Applications	127
10.1.2.2	Algorithm to generate quasi-random sequences	128
10.1.2.3	Variance of the modified random walk	128
10.1.3	Random walks with less entropy than pure random signal	129
10.2	Related stochastic processes	130
10.2.1	From Brownian motions to clustered Lévy flights	130
10.2.2	Integrated Brownian motions and special auto-regressive processes	131
10.3	Python code	132
10.3.1	Computing probabilities and variances attached to S_n	132
10.3.2	Path simulations	133
11	Empirical Optimization with Divergent Fixed Point Algorithm	135
11.1	Introduction	135
11.1.1	The problem, with illustration	136
11.2	Non-converging fixed-point algorithm	137
11.2.1	Trick leading to intuitive solution	137
11.2.2	Root detection: method and parameters	137
11.2.3	Case study: factoring a product of two large primes	138
11.3	Generalization with synthetic random functions	138
11.3.1	Example	140

11.3.2	Connection to the Poisson-binomial distribution	141
11.3.2.1	Location of next root: guesstimate	141
11.3.2.2	Integer sequences with high density of primes	141
11.3.3	Python code: finding the optimum	142
11.4	Smoothing highly chaotic curves	143
11.4.1	Python code: smoothing	143
11.5	Connection to synthetic data: random functions	146
12	Synthetic Terrain Generation and AI-generated Art	147
12.1	Introduction	147
12.2	Terrain generation and the evolutionary process	149
12.2.1	Morphing and non-linear palette operations	149
12.2.2	The diamond-square algorithm	149
12.2.3	The evolutionary process	150
12.2.4	Finding optimum parameters	150
12.2.5	Mimicking real terrain: the synthesis step	150
12.3	Python code	151
12.3.1	Producing data videos with four sub-videos in parallel	151
12.3.2	Main program	152
12.4	AI-generated art with 3D contours	156
12.4.1	Python code using Matplotlib	157
12.4.2	Python code using Plotly	158
12.4.3	Tips to quickly solve new problems	159
13	Synthetic Star Clusters Generation with Collision Graphs	160
13.1	Introduction	160
13.2	Model parameters and simulation results	161
13.2.1	Explanation of color codes	161
13.2.2	Detailed description of top parameters	161
13.2.3	Interesting parameter sets	162
13.3	Analysis of star collisions and collision graph	163
13.3.1	Weighted directed graphs: visualization with NetworkX	164
13.3.2	Interesting findings: how the universe got started	164
13.4	Animated data visualizations	165
13.5	Python code and computational issues	166
13.5.1	Simulating the real and synthetic universes	166
13.5.2	Visualizing collision graphs	170
14	Perturbed-Lattice Point Process: Inference, Nearest Neighbor Graph	172
14.1	Perturbed lattices: definition and properties	172
14.1.1	Point counts distribution	173
14.1.2	Periodicity and amplitude of point count expectations	173
14.1.3	Testing the independence of point counts	174
14.1.3.1	Results and Interpretation	175
14.1.3.2	About the Spreadsheet	176
14.2	Cluster processes and nearest neighbor graphs	176
14.2.1	Synthetic, semi-rigid cluster structures	176
14.2.2	Python code to generate cluster processes	178
14.2.3	References on cluster processes	178
14.2.4	Superimposed perturbed lattices: an alternative to mixture models	179
14.2.4.1	Hexagonal lattice, nearest neighbors	180
14.2.4.2	Exercises: nearest neighbor graphs, size of connected components	181
14.2.4.3	Python code to compute connected components	182
14.3	Statistical inference for point processes	184
14.3.1	Estimation of Core Parameters	184
14.3.1.1	Intensity	185
14.3.1.2	Scaling factor	185
14.3.1.3	Alternative estimation method	185
14.3.2	Spatial statistics, nearest neighbors, clustering	186
14.3.2.1	Inference for two-dimensional processes	186
14.3.2.2	Other possible tests	186
14.3.2.3	Rayleigh test	187

14.3.2.4	Exercises	188
14.4	Special topics	189
14.4.1	Minimum contrast estimation and explainable AI	189
14.4.2	Model identifiability, hard-to-detect patterns	190
14.4.2.1	Stochastic residues	190
14.4.3	Hidden model and random permutations	190
14.4.4	Retrieving the F distribution	192
14.4.4.1	Theoretical values obtained by simulations	192
14.4.4.2	Retrieving F from the interarrival times distribution	193
14.4.5	Record distances between an observed point and its vertex	193
14.4.5.1	Distribution of records	194
14.4.5.2	Distribution of arrival times for records	195
15	New Perspective on the Riemann Hypothesis	196
15.1	Introduction	196
15.1.1	Key concepts and terminology	197
15.1.2	Orbits and holes	197
15.1.3	Industrial Applications	197
15.2	Euler products	198
15.2.1	Finite Euler Products	198
15.2.1.1	Generalization using Dirichlet characters	199
15.2.2	Infinite Euler products	200
15.2.2.1	Special products	200
15.2.2.2	Probabilistic properties and conjectures	201
15.3	Finite Dirichlet series and generalizations	202
15.3.1	Finite Dirichlet series	202
15.3.2	Non-trivial cases with infinitely many primes and a hole	204
15.3.2.1	Sums of two cubes, or cuban primes	204
15.3.2.2	Primes associated to elliptic curves	204
15.3.2.3	Analytic continuation, convergence, and functional equation	205
15.3.2.4	Hybrid Dirichlet-Taylor series	205
15.3.3	Riemann Hypothesis with cosines replaced by wavelets	206
15.3.4	Riemann Hypothesis for Beurling primes	207
15.3.5	Stochastic Euler products	208
15.4	Exercises	209
15.5	Python code	212
15.5.1	Computing the orbit of various Dirichlet series	212
15.5.2	Creating videos of the orbit	215
16	Miscellaneous Topics	218
16.1	The sound that data makes	218
16.1.1	From data visualizations to videos to data music	218
16.1.2	References	219
16.1.3	Python code	219
16.2	Data videos and enhanced visualizations in R	220
16.2.1	Cairo library to produce better charts	220
16.2.2	AV library to produce videos	221
16.3	Dual confidence regions	222
16.3.1	Case study	222
16.3.2	Standard confidence region	222
16.3.3	Dual confidence region	223
16.3.4	Simulations	223
16.3.5	Original problem with minimum contrast estimators	224
16.3.6	General shape of confidence regions	225
16.4	Fast feature selection based on predictive power	226
16.4.1	How cross-validation works	227
16.4.2	Measuring the predictive power of a feature	227
16.4.3	Efficient implementation	228
16.5	Natural language processing: taxonomy creation	229
16.5.1	Designing a keyword taxonomy	229
16.5.2	Fast clustering algorithm for keyword data	230
16.5.2.1	Computational complexity	230

16.5.2.2	Smart crawling of the whole Internet and a bit of graph theory	230
16.6	Automated detection of outliers and number of clusters	232
16.6.1	Black-box elbow rule to detect outliers	232
16.7	New developments in explainable AI	233
16.7.1	Sensitivity analysis and imputation method based on synthetic data	234
16.8	Advice to beginners	234
16.8.1	Getting started and learning how to learn	234
16.8.1.1	Getting help	234
16.8.1.2	Beyond Python	235
16.8.2	Automated data cleaning and exploratory analysis	235
16.8.3	Example of simple analysis: marketing attribution	236
16.8.4	Upcoming books and courses	236
Glossary		237
Bibliography		240
Index		245

List of Figures

1.1	Fitted ellipse (blue), given the training set (red) distributed around a partial arc	18
1.2	Confidence region in blue, $n = 30$ training set points; 50 training sets (left) vs 150 (right)	19
1.3	Three non-periodic time series made of periodic terms (see section 15.2.2.1)	25
1.4	Training set (red), validation set (orange), fitted curve (blue) and model (gray)	26
1.6	Biased confidence region for (θ_A^*, θ_B^*) ; same example as in Figure 1.5; true value is $(0.5, 1.0)$	29
1.5	Finding the two centers θ_A^*, θ_B^* in sample 39; $n = 1000$	30
1.7	Challenging mixture, requiring $p_A = 3, p_B = 1$ to identify the two cluster centers	31
2.1	Output from the Excel version of HDT	41
3.1	AR models, classified based on the types of roots of the characteristic polynomial	52
4.1	Scatterplot observations vs. predicted values, with prediction intervals (in any dimension)	66
4.2	Comets orbiting the sun: simulation	66
4.3	Comets orbiting the sun: snapshot in time	67
4.4	Three orbits of $\eta(\sigma + it)$: $\sigma = 0.5$ (red), 0.75 (blue) and 1.25 (yellow)	67
4.5	Sample orbit points of $\eta(\sigma + it)$: $\sigma = 0.5$ (red), 0.75 (blue) and 1.25 (yellow)	67
4.6	Sample orbit points of $\eta(\sigma + it)$: $\sigma = 0.5$ (red), 0.75 (blue) and 1.25 (yellow)	68
4.7	Raw orbit points of $\eta(\sigma + it)$: $\sigma = 0.5$ (red), 0.75 (blue) and 1.25 (yellow)	68
4.8	Convergence of partial sums of $\eta(z)$, for six $z = \sigma + it$ in the complex plane	68
5.1	Special interlacing of 4 lattice processes with $s = 0$	71
5.2	Classification of left dataset; $s = 0.15, w = 10$. One loop (middle) vs 3 (right).	72
5.3	Clustering of left dataset; $s = 0.15$, 3 loops, $w = 10$ (middle) vs 20 (right).	73
5.4	Classification ($w = 10$) and clustering ($w = 20$); $s = 0.05$, three loops.	73
5.5	Fractal classification, $s = 0.15$. Loop 6, 250 and 400.	74
5.6	Fractal classification, $s = 0.05$.Loop: 6 and 60.	74
5.7	Fast (left) vs standard method (right), 3 loops, $s = 0.15, w = 10$	75
5.8	Fast method, $s = 0.05, w = 20$. Three loops (middle), one loop (right).	75
6.1	Comparing two shapes	84
6.2	Weighted centroid, shape signature	85
6.3	Weight function used in Figure 6.2	86
6.4	Another interesting shape	87
7.1	Regression coefficients oscillating when using adaptive damping	94
7.2	Convergence of regression coefficients (left) and distribution of residual error (right)	95
7.3	Goodness-of-fit: training set (right) versus validation set (left)	95
8.1	Fuzzy regression with prediction intervals, original version, 1D	102
8.2	Fuzzy regression with prediction intervals, full model, 2D	104
8.3	Scatterplots: median vs weighted method, on validation (left) vs training set (right)	106
8.4	Dirichlet eta function (real part, bottom) and interpolation error (top)	108
9.1	Orbit of $L(z, \chi)$ at $\sigma = \frac{1}{2}$, with $0 < t < 200$ and $\chi = \chi_4$ (left) versus pseudo-random χ (right) . .	115
9.2	$L_3^*(n)$ test statistic for four sequences: Python[200] and SQRT[90,91] fail	117
9.3	$ L_3(n) $ test statistic for four sequences: Python[200] and SQRT[90,91] fail	117
10.1	Typical path S_n with $0 \leq n \leq 50,000$ for four types of random walks	127
10.2	$\delta_n = 1 - \text{Var}[S_{n+1}] + \text{Var}[S_n]$ for four types of random walks, with $0 \leq n \leq 5000$	128

10.3	Same as Figure 10.2, using a more aesthetic but less meaningful chart type	129
10.4	Clustered Brownian process	131
10.5	AR models, classified based on the types of roots of the characteristic polynomial	132
11.1	Function $f(b)$ as a better alternative to $g(b)$ in Figure 11.2. Root at $b = 3083$.	136
11.2	Function $g(b) = 2 - \cos(2\pi b) - \cos(2\pi a/b)$, with $a = 3083 \times 7919$.	136
11.3	Transformed function f_3 , amplifying the root at $b = 3083$.	137
11.4	Signal strength ρ_n , first 130 fixed-point iterations; $n = 31$ leads to a root.	140
11.5	(b_n, ρ_n) plot. Yellow and orange dots linked to roots.	140
11.6	Signal strength ρ_n , first 130 fixed-point iterations; $n = 87$ leads to a root.	140
11.7	Random function from section 11.3.1, with root at $b = 5646$.	143
12.1	Six frames from the terrain video, each one containing four images	148
12.2	Contour plot, 3D mixture model, produced with Plotly	156
12.3	Same as Figure 12.2, produced with Matplotlib	157
13.1	Collisions graph for the biggest star eater (star 47) in video 7	164
13.2	Summary statistics for the whole collision structure: the X axis represents the time	165
13.3	Snapshots of universe 4 (left) and universe 7 (right)	166
14.1	Period and amplitude of $\phi_\tau(t)$; here $\tau = 1, \lambda = 1.4, s = 0.3$	174
14.2	A new test of independence (R-squared version)	174
14.3	Radial cluster process ($s = 0.2, \lambda = 1$) with centers in blue; zoom in on the left	177
14.4	Radial cluster process ($s = 2, \lambda = 1$) with centers in blue; zoom in on the left	177
14.5	Manufactured marble lacking true lattice randomness (left)	177
14.6	Four superimposed Poisson-binomial processes: $s = 0$ (left), $s = 5$ (right)	180
14.7	Rayleigh test to assess if a point distribution matches that of a Poisson process	188
14.8	Realization of a 5-interlacing with $s = 0.15$ and $\lambda = 1$: original (left), modulo $2/\lambda$ (right)	191
14.9	Locally random permutation σ ; $\tau(k)$ is the index of X_k 's closest neighbor to the right	191
14.10	Each arrow links a point (blue) to its vertex (red): $s = 0.2$ (left), $s = 1$ (right)	194
14.11	Distance between a point and its vertex ($\lambda = s = 1$)	195
15.1	Three orbits ($\sigma = 0.5, 0.75, 1.25$) with finite Euler product: $P = \{2, 3\}$ (left) vs $\{2, 3, 5\}$ (right)	199
15.2	Distance between orbit and location $(c, 0)$ depending on t on the X-axis	201
15.3	Distance between orbit and location $(c, 0)$ depending on t on the X-axis	201
15.4	Distance between orbit and location $(c, 0)$ depending on t on the X-axis	201
15.5	Four orbits where the “hole” (repulsion basin) is apparent	203
15.6	Three orbits with “hole” closer to the origin, showing impact of $\beta > \frac{1}{2}$ and larger n	203
15.7	Orbit of Dirichlet eta $\eta(z)$ when cosines are replaced by other periodic functions	207
16.1	Data linked to the melody: red curve for note frequencies, blue curve for note durations	219
16.2	R plot before Cairo (left), and after (right)	220
16.3	Intermediate (left) and last frame (right) of the video	221
16.4	Example of 90% dual confidence region for (p, q)	223
16.5	Minimum contrast estimation for (λ, s) using (p, q) as proxy stats	224
16.6	Non-elliptic confidence regions with various confidence levels	225
16.7	Elbow rule (right) finds $m = 3$ clusters in Brownian motion (left)	233

List of Tables

1.1	Estimated ellipse parameters vs true values ($n = 30$), for shape in Figure 1.2	19
1.2	First and last step of <code>curve_fitting</code> , approaching the model.	27
1.3	MSE for different methods and θ s, same data set as in Figure 1.5	32
1.4	MSE for different methods and θ s, same data set as in Figure 1.7	32
2.1	List of potential features to use in the model	37
2.2	Statistics for selected HDT nodes (Excel version)	40
2.3	Order of magnitude for the expectation and standard deviation of the range R_n	44
3.1	Characteristic polynomials used in the simulations	51
7.1	Regression coefficients and performance metrics r, s based on methodology	96
7.2	Correlation matrix	96
7.3	Best performance given m (number of features)	97
7.4	Feature comparison table (top 32 feature combinations)	99
7.5	Feature comparison table (bottom 31 feature combinations)	100
8.1	R -squared ρ^2 and slope β , on training and validation sets, median vs weighted	106
9.1	$L_3^*(n)$, for various sequences ($n = 20,000$); “Fail” means failing the prime test	118
11.1	High ρ_n at iterations $n = 31$ and $n = 127$ points to roots 3083 and 7919	139
13.1	Description of top parameters used in the star cluster simulator	162
13.2	Eight selected parameter sets covering various situations	163
14.1	Variance attached to F_s , as a function of s	173
14.2	Poisson process ($s = \infty$) versus $s = 39.85$	193
16.1	Extract of the mapping table used to recover (λ, s) from (p, q)	225
16.2	Eight bins: 2 features (A, B) times 2 outcomes (Good/Bad)	227
16.3	Amount of data collected at each level, when crawling the Internet	231

Glossary

Autoregressive process	Auto-correlated time series, as described in section 3.4. Time-continuous versions include Gaussian processes and Brownian motions, while random walks are a discrete example; two-dimensional versions exist. These processes are essentially integrated white noise. See pages 49, 97, 131
Binning	Feature binning consists of aggregating the values of a feature into a small number of bins, to avoid overfitting and reduce the number of nodes in methods such as naive Bayes, neural networks, or decision trees. Binning can be applied to two or more features simultaneously. I discuss optimum binning in this book. See pages 37, 73, 227
Boosted model	Blending of several models to get the best of each one, also referred to as ensemble methods. The concept is illustrated with hidden decision trees in this book. Other popular examples are gradient boosting and AdaBoost. See pages 36, 237
Bootstrapping	A data-driven, model-free technique to estimate parameter values, to optimize goodness-of-fit metrics. Related to resampling in the context of cross-validation. In this book, I discuss parametric bootstrap on synthetic data that mimics the actual observations. See pages 15, 96, 188, 237
Confidence Region	A confidence region of level γ is a 2D set of minimum area covering a proportion γ of the mass of a bivariate probability distribution. It is a 2D generalization of confidence intervals. In this book, I also discuss dual confidence regions – the analogous of credible regions in Bayesian inference. See pages 12, 15, 18, 20, 29, 185, 186, 222, 225
Cross-validation	Standard procedure used in bootstrapping, and to test and validate a model, by splitting your data into training and validation sets. Parameters are estimated based on training set data. An alternative to cross-validation is testing your model on synthetic data with known response. See pages 15, 37, 93, 99, 163, 227, 237
Decision trees	A simple, intuitive non-linear modeling techniques used in classification problems. It can handle missing and categorical data, as well as a large number of features, but requires appropriate feature binning. Typically one blends multiple binary trees each with a few nodes, to boost performance. See pages 36, 37, 39, 41, 237, 238
Dimension reduction	A technique to reduce the number of features in your dataset while minimizing the loss in predictive power. The most well known are principal component analysis and feature selection to maximize goodness-of-fit metrics. See pages 12, 16, 238, 239
Empirical distribution	Cumulative frequency histogram attached to a statistic (for instance, nearest neighbor distances), and based on observations. When the number of observations tends to infinity and the bin sizes tend to zero, this step function tends to the theoretical cumulative distribution function of the statistic in question. See pages 16, 96, 113, 172, 175, 181, 187, 192, 194, 206
Ensemble methods	A technique consisting of blending multiple models together, such as many decision trees with logistic regression, to get the best of each method and outperform each method taken separately. Examples include boosting, bagging, and AdaBoost. In this book, I discuss hidden decision trees. See pages 36, 83, 237
Explainable AI	Automated machine learning techniques that are easy to interpret are referred to as interpretable machine learning or explainable artificial intelligence. As much as possible, the methods discussed in this book belong to that category. The goal is to design black-box systems less likely to generate unexpected results with unintended consequences. See pages 13, 35, 69, 74, 83, 90, 135, 151, 189, 233

Feature selection	Features – as opposed to the model response – are also called independent variables or predictors. Feature selection, akin to dimensionality reduction , aims at finding the minimum subset of variables with enough predictive power . It is also used to eliminate redundant features and find causality (typically using hierarchical Bayesian models), as opposed to mere correlations. Sometimes, two features have poor predictive power when taken separately, but provide improved predictions when combined together. See pages 12 , 15 , 37 , 94 , 97 , 218 , 226 , 237 , 239
Generative model	Bayesian Gaussian mixtures (GMM) combined with kernel density estimation and the EM algorithm is a classic modeling tool. In this book, I used <i>m</i>-interlacings instead. Generative adversarial networks (GAN) work as follows: the generator creates new observations and the discriminator tests whether the new observations are statistically indistinguishable from training set data. When this goal is achieved, the new observations is your synthetic data. In this book, new observations are generated with parametric bootstrap instead. See pages 35 , 52 , 146 , 147 , 149 , 156 , 163 , 239
Goodness-of-fit	A model fitting criterion or metric to assess how a model or sub-model fits to a dataset, or to measure its predictive power on a validation set . Examples include R-squared , Chi-squared, Kolmogorov-Smirnov, error rate such as false positives and other metrics discussed in this book. See pages 15 , 56 , 93 , 94 , 227 , 237 , 239
Gradient methods	Iterative optimization techniques to find the minimum of maximum of a function, such as the maximum likelihood . When there are numerous local minima or maxima, use swarm optimization . Gradient methods (for instance, stochastic gradient descent or Newton's method) assume that the function is differentiable. If not, other techniques such as Monte Carlo simulations or the fixed-point algorithm can be used. Constrained optimization involves using Lagrange multipliers . See pages 15 , 31 , 55 , 89
Graph structures	Graphs are found in decision trees , in neural networks (connections between neurons), in nearest neighbors methods (NN graphs), in hierarchical Bayesian models , and more. See pages 70 , 74 , 164 , 230 , 231
Hyperparameter	An hyperparameter is used to control the learning process: for instance, the dimension, the number of features, parameters, layers (neural networks) or clusters (clustering problem), or the width of a filtering window in image processing. By contrast, the values of other parameters (typically node weights in neural networks or regression coefficients) are derived via training. See pages 29 , 56 , 70 , 75 , 101 , 150 , 238
Link function	A link function maps a nonlinear relationship to a linear one so that a linear model can be fit, and then mapped back to the original form using the inverse function. For instance, the logit link function is used in logistic regression . Generalizations include quantile functions and inverse sigmoids in neural network to work with additive (linear) parameters. See pages 13 , 16 , 238
Logistic regression	A generalized linear regression method where the binary response (fraud/non-fraud or cancer/non-cancer) is modeled as a probability via the logistic link function. Alternatives to the iterative maximum likelihood solution are discussed in this book. See pages 16 , 33 , 36 , 40 , 237 , 238
Neural network	A blackbox system used for predictions, optimization, or pattern recognition especially in computer vision. It consists of layers, neurons in each layer, link functions to model non-linear interactions, parameters (weights associated to the connections between neurons) and hyperparameters . Networks with several layers are called deep neural networks . Also, neurons are sometimes called nodes. See pages 69 , 73 , 75 , 83 , 101 , 237 , 238
NLP	Natural language processing is a set of techniques to deal with unstructured text data, such as emails, automated customer support, or webpages downloaded with a crawler. The example discussed in section 16.5 deals with creating a keyword taxonomy based on parsing Google search results pages. See pages 36 , 229
Numerical stability	This issue occurring in unstable optimization problems typically with multiple minima or maxima, is frequently overlooked and leads to poor predictions or high volatility. It is sometimes referred to as ill-conditioned problems . I explain how to fix it in several examples in this book, for instance in section 3.4.2 . Not to be confused with numerical precision. See pages 12 , 14 , 59

Overfitting	Using too many unstable parameters resulting in excellent performance on the training set , but poor performance on future data or on the validation set . It typically occurs with numerically unstable procedures such as regression (especially polynomial regression) when the training set is not large enough, or in the presence of wide data (more features than observations) when using a method not suited to this situation. The opposite is underfitting. See pages 15, 92, 101, 234, 237, 239
Predictive power	A metric to assess the goodness-of-fit or performance of a model or subset of features, for instance in the context of dimensionality reduction or feature selection . Typical metrics include R-squared , or confusion matrices in classification. See pages 38, 40, 44, 226, 228, 233, 238
R-squared	A goodness-of-fit metric to assess the predictive power of a model, measured on a validation set . Alternatives include adjusted R-squared, mean absolute error and other metrics discussed in this book. See pages 12, 15, 35, 56, 90, 93, 95, 97, 104, 238, 239
Random number	Pseudo-random numbers are sequences of binary digits, usually grouped into blocks, satisfying properties of independent Bernoulli trials. In this book, the concept is formally defined, and strong pseudo-number generators are built and used in computer-intensive simulations. See pages 29, 112, 119, 232
Regression methods	I discuss a unified approach to all regression problems in chapter 1. Traditional techniques include linear, logistic, Bayesian, polynomial and Lasso regression (to deal with numerical instability and overfitting), solved using optimization techniques, maximum likelihood methods, linear algebra (eigenvalues and singular value decomposition) or stepwise procedures. See pages 12, 13, 15, 16, 19, 27, 36, 40, 46, 49, 52, 56, 89, 95, 101, 108, 238, 239
Supervised learning	Techniques dealing with labeled data (classification) or when the response is known (regression). The opposite is unsupervised learning , for instance clustering problems. In-between, you have semi-supervised learning and reinforcement learning (favoring good decisions). The technique described in chapter 1 fits into unsupervised regression. Adversarial learning is testing your model against extreme cases intended to make it fail, to build better models. See pages 239
Synthetic data	Artificial data simulated using a generative model , typically a mixture model , to enrich existing datasets and improve the quality of training sets . Called augmented data when blended with real data. See pages 12, 13, 15, 17, 27, 29, 33, 35, 48, 52, 55, 69, 70, 75, 88, 94, 105, 127, 135, 149, 156, 163, 223, 232, 234, 237
Tensor	Matrix generalization with three or more dimensions. A matrix is a two-dimensional tensor. A triple summation with three indices is represented by a three-dimensional tensor, while a double summation involves a standard matrix. See pages 69, 74
Training set	Dataset used to train your model in supervised learning . Typically, a portion of the training set is used to train the model, the other part is used as validation set . See pages 13, 15, 17, 20, 29, 36, 40, 56, 72, 88, 95, 101, 105, 163, 227, 237, 239
Validation set	A portion of your training set , typically 20%, used to measure the actual performance of your predictive algorithm outside the training set. In cross-validation and bootstrapping, the training and validation sets are split into multiple subsets to get a better sense of variations in the predictions. See pages 15, 27, 41, 56, 93, 101, 163, 227, 234, 237, 238, 239

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Index

- α -compositing, 57
 m -interlacing, 71, 179, 187, 190, 238
- A/B testing, 236
AdaBoost, 36, 237
additive number theory, 204, 211
adversarial learning, 234, 239
AI-art, 156
algebraic number, 117
analytic continuation, 198, 205
analytic function, 115
anisotropy, 165, 186, 192
anti-aliasing, 55, 59, 215, 220
association rule, 228
attraction (point process), 177
attraction basin, 58
attractor distribution, 131, 181, 187, 194
augmented data, 35, 88, 147, 149, 239
auto-correlation, 49, 116
auto-regressive process, 49, 131, 237
- Bailey–Borwein–Plouffe formulas, 117
Bayesian classification, 74
Bayesian inference, 44
 - hierarchical models, 238
 - naive Bayes, 228Bernoulli trials, 222
Berry-Esseen inequality, 113
Bessel function, 193
Beurling primes, 116, 208
binning, 227
 - optimum binning, 37, 237binomial distribution, 187
bisection method (root finding), 138
bootstrapping, 15, 96, 188
 - percentile method, 101boundary effect, 174, 175, 180, 181, 185–187, 191
Brownian motion, 51, 126, 130, 147, 148, 163, 232, 237
 - Lévy flight, 131Brun's theorem, 204
- Cauchy distribution, 131
Cauchy-Riemann equations, 115
causality, 238
Cayley-Hamilton theorem, 47
CDF regression, 17
censored data, 180
central limit theorem, 131, 172, 222
chaotic dynamical system, 147, 163
character
 - principal, 200
- characteristic function, 193
characteristic polynomial, 47, 49, 50, 132
Chebyshev's bias (prime numbers), 115, 200
checksum, 235
Chi-squared test, 174
Chowla conjecture, 202
classification, 239
clique (graph theory), 182
cluster process, 176, 180, 187
clustering, 239
Collatz conjecture, 123
collision graph, 163
color model
 - RGB, 55, 221
 - RGBA, 55, 56, 76, 221color opacity, 157
color transparency, 20, 149, 221
complex random variable, 112, 208
computational complexity, 229
computer vision, 12, 83
confidence band, 188
confidence interval, 44, 185, 237
confidence level, 222, 225
confidence region, 15, 29, 185, 186, 222
 - dual region, 44, 223, 237conformal map, 14
confusion matrix, 227, 239
connected components, 164, 180–182, 186, 187, 230
contour level, 156, 225
contour plot, 225
convergence
 - abscissa, 200, 205
 - absolute, 197, 198
 - alternating series, 198
 - conditional, 114, 200
 - Dirichlet test, 198convergence acceleration, 59
convex linear combination, 108
convolution of distributions, 193
counting measure, 173
covariance matrix, 90, 222
covering (stochastic), 189
covering problem, 188
credible interval, 44
credible region (Bayesian), 223, 237
cross-validation, 15, 163, 227
cuban primes, 204
curve fitting, 26
- data video, 147, 156

decision tree, 36
 Dedekind zeta function, 115, 208
 deep neural network, 73, 238
 dense set (topology), 202
 density estimation, 179
 diamond-square algorithm, 148
 Diehard tests of randomness, 114
 dimensionality reduction, 16
 Dirichlet character, 115, 116, 199, 204
 modulo 4, 200, 205, 206
 Dirichlet eta function, 212
 Dirichlet functional equation, 115, 205, 206
 Dirichlet series, 112
 Dirichlet's theorem, 115, 200, 202, 206
 Dirichlet-*L* function, 115, 199, 206
 dissimilarity metric, 229
 distributed architecture, 226
 distribution
 Cauchy, 131
 Fréchet, 51, 131
 Gaussian, 222
 generalized logistic, 90, 176
 Hotelling, 223
 Laplace, 193
 logistic, 16
 Lévy, 131
 modified Bessel, 193
 Poisson-binomial, 141, 195
 Poisson-exponential, 172
 Rademacher, 112, 113
 Rayleigh, 187, 188, 194
 Weibull, 51, 131, 187
 domain of attraction, 181
 dot product, 14
 dummy variable, 36
 dyadic map, 116
 dynamical systems, 116, 181
 chaotic systems, 147, 163
 dyadic map, 116
 ergodicity, 116
 logistic map, 116
 shift map, 116
 stochastic, 148
 edge effect (statistics), 180
 eigenvalue, 13, 52, 90, 239
 power iteration, 92
 elbow rule, 135, 180, 187, 232
 elliptic curve, 204
 EM algorithm, 35, 238
 empirical distribution, 16, 96, 172, 175, 181, 187, 192, 194, 206
 multivariate, 113
 empirical quantiles, 101
 ensemble methods, 36, 83
 entropy, 166, 192, 228
 equidistribution modulo 1, 119
 equilibrium distribution, 148
 Erdős–Rényi model, 182
 ergodicity, 116, 148, 185, 187, 193
 Euler product, 112, 198, 205
 random, 208
 Euler's transform, 212
 evolutionary process, 147
 experimental design, 236
 experimental math, 56, 196
 explainable AI, 13, 35, 74, 83, 90, 135, 151, 189, 233
 exploratory analysis, 235
 exponential decay, 40
 exponential sums, 205
 extrapolation, 108
 extreme value theory, 131, 194
 feature attribution, 233
 feature importance, 233
 feature selection, 15, 97, 226
 Fermat's last theorem, 205
 fixed-point algorithm, 59, 89, 135, 238
 flag vector, 228, 236
 Fourier transform, 193
 fractal dimension, 51
 fractional part function, 118
 Frobenius norm, 90
 Fruchterman and Rheingold algorithm, 230
 Fréchet distribution, 51, 131
 fuzzy classification, 56
 Gamma function, 51, 131
 GAN (generative adversarial networks), 35, 238
 Gaussian circle problem, 211
 Gaussian distribution, 222
 Gaussian mixture, 35, 70
 Gaussian primes, 115, 207
 Gaussian process, 49, 237
 general linear model, 13
 generalized linear model, 13, 48
 generalized logistic distribution, 90, 186
 generative adversarial networks, 35, 151, 234, 238
 generative model, 35, 52, 146, 147, 149, 156, 163, 239
 geostatistics, 102
 Glivenko–Cantelli theorem, 206
 GMM (Gaussian mixture model), 35, 238
 Goldbach's conjecture, 204
 goodness-of-fit, 56, 227
 GPU-based clustering, 71
 gradient (optimization), 135
 gradient boosting, 237
 gradient operator, 15
 graph, 180
 collision graph, 163
 connected components, 164, 186, 230
 directed, 164
 edge, 180
 Fruchterman-Reingold, 164
 nearest neighbor graph, 182, 186
 node, 180, 182
 random graph, 181
 random nearest neighbor graph, 181
 tree, 164
 undirected, 180–182, 187
 vertex, 180
 graph database, 230

graph theory, 180
GraphViz, 164
greedy algorithm, 211
grid search, 135, 150
half-tone (music), 218
Hartman–Wintner theorem, 126
hash table, 166, 191, 228, 229
sparse, 228
Hausdorff distance, 87
hexagonal lattice, 180
hidden decision trees, 36, 37, 237
hidden layer, 73
hidden process, 172, 190, 194
hierarchical clustering, 73, 229
Hilbert primes, 207
histogram equalization, 71, 73
Hoeffding inequality, 129
homogeneity (point process), 141, 179
Hotelling distribution, 223
Hurst exponent, 51
hyperparameter, 29, 56, 103, 150
identifiability, 190, 192
ill-conditioned problem, 26, 52, 92, 238
image segmentation, 73
imputation (missing values), 234
index
 index discrepancy, 192
intensity (stochastic process), 172, 179, 186
interarrival times, 130, 172, 181, 185, 192
 standardized, 193
interlaced processes, 179
Internet of Things, 172
inverse distance weighting, 104
inverse square law, 160
iterated logarithm, 113, 114, 126
Itô integral, 52
K-means clustering, 31, 32
key-value pair, 37, 228
Kolmogorov-Smirnov test, 113, 174, 181
Kronecker's theorem, 202, 210
Lagrange interpolation, 52
Lagrange multiplier, 15, 238
Laplace distribution, 193
Lasso regression, 15, 239
lattice, 178
 perturbed lattice, 172
 shifted, 180
 stretched, 180
law of the iterated logarithm, 113, 114, 126, 202, 208
Le Cam's theorem, 141, 173
least absolute residuals, 101
link function, 13, 16
Liouville function, 199, 210
log-polar map, 14
logistic distribution, 16, 179
logistic map, 116
logistic regression, 16
 unsupervised, 33
logit function, 238
Lévy distribution, 131
Lévy flight, 131
Map-reduce, 226
marketing attribution, 236
Markov chain, 49
 MCMC, 112
Mathematica, 225
MaxCliqueDyn algorithm, 182
maximum likelihood estimation, 224, 238, 239
mean squared error, 15, 30
medoid, 31
Mersenne twister, 29, 116, 119, 128
Mertens function, 199
minimum contrast estimation, 150, 189, 192, 224
mixture model, 29, 45, 148, 156, 172, 179, 180, 187, 225, 239
 blending, 148
model fitting, 56, 238
model identifiability, 15
modulus (complex number), 132, 198
Monte Carlo simulations, 112, 238
morphing (computer vision), 147
moving average, 137
multiplicative function
 completely multiplicative, 112, 114, 199, 200, 211
 Rademacher, 112
Möbius function, 199
N-body problem, 160
n-gram (NLP), 229
naive Bayes, 228, 237
natural language processing, 36, 229
nearest neighbor interpolation, 101, 104
nearest neighbors, 172, 182, 188, 238
 nearest neighbor distances, 186–188, 190, 194
 nearest neighbor graph, 186
NetworkX, 164
neural network, 73
 hidden layer, 73
 hyperparameter, 75
 neuron, 73, 238
 seq2seq, 146
 sparse, 69
 very deep, 73
Newton's method, 135
node (decision tree), 37, 237
 perfect node, 44
 usable node, 38
normal number, 113, 202, 206
 strongly normal, 114
numerical stability, 47
Omega function, 199, 205
order statistics, 194
ordinary least squares, 49, 101
outliers, 194, 232
overfitting, 15, 192, 234, 237
palette, 147, 221
parametric bootstrap, 20, 29, 35, 97, 188, 237, 238

partial least squares, 13
 path (graph theory), 180
 percentile bootstrap, 101
 permutation
 entropy, 192
 random permutation, 191
 perturbed lattices, 172
 Plotly, 156
 point count distribution, 173, 186, 189
 point process
 attractive, 187
 cluster process
 Matérn, 178
 Neyman-Scott, 178
 non-homogeneous, 141, 179
 perturbed lattice process, 178
 radial, 179
 renewal process, 178
 repulsive, 177
 Poisson point process, 130, 141, 172, 186
 Poisson-binomial distribution, 141, 172, 195
 Poisson-exponential distribution, 172
 positive semidefinite (matrix), 48, 91
 power iteration, 92
 preconditioning, 92
 prediction interval, 15, 96, 101
 predictive power, 37, 44, 227, 228, 233
 prime test (of randomness), 114, 127
 principal component analysis, 47, 233, 237
 probability generating function, 127
 proxy space, 225
 pseudo-inverse matrix, 48
 pseudo-random numbers, 128, 232
 congruential generator, 119
 Diehard tests, 114
 Mersenne twister, 119, 128, 149
 prime test, 114, 127
 strongly random, 114, 117
 TestU01, 114
 Pólya conjecture, 201
 quadratic irrational, 116, 119
 quantile, 223, 238
 empirical, 101
 weighted, 101
 quantile function, 172, 176, 187
 quantile regression, 15
 R-squared, 15, 35, 150
 Rademacher distribution, 113
 Rademacher function, 112, 202, 208
 random, 114
 random function, 140
 random graph, 181, 182
 random multiplicative function, 112
 Rademacher, 114
 random permutation, 191
 random variable
 complex, 112
 random walk, 126, 150, 237
 first hitting time, 127, 130
 zero crossing, 126
 Rayleigh distribution, 187, 188, 194
 Rayleigh test, 187
 records, 194
 regression splines, 13
 regular expression, 229, 235
 reinforcement learning, 239
 renewal process, 178
 repulsion (point process), 177, 188
 repulsion basin, 198
 resampling, 96, 188
 Riemann Hypothesis, 107
 Generalized, 114, 200, 204, 206
 Riemann zeta function, 112, 115, 206, 208
 root mean squared error, 56
 scaling factor, 186, 194
 seed (random number generator), 149
 semi-supervised learning, 239
 shape signature, 84
 Shapley value, 233
 Shepard's method, 104
 shift map, 116
 sigmoid function, 238
 simplex, 209
 singular value decomposition, 13, 239
 singularity, 166
 six degrees of separation, 231
 smoothing parameter, 103
 spatial statistics, 102, 178
 spectral domain, 148
 square root (matrix), 48, 91
 square-free integer, 113, 202
 stable distribution, 131, 149, 193
 state space, 148
 stationary distribution, 52
 stationary process, 49, 131, 148, 163, 174, 179, 186
 stepwise regression, 98
 stochastic convergence, 148
 stochastic function, 51
 stochastic geometry, 189
 stochastic process, 172
 stochastic residues, 190
 stop word (NLP), 229
 stretching (point process), 180
 superimposition (point processes), 179
 supervised classification, 71
 surface plot, 156
 swarm optimization, 27, 238
 synthetic data, 13, 27, 29, 52, 88, 90, 127, 135, 149, 156, 163, 196, 223, 234
 synthetic metric, 228
 Tarjan's algorithm, 230
 tensor, 74
 text normalization, 229
 Theil-Sen estimator, 101
 time series, 50
 auto-regressive, 50, 131
 disaggregation, 107
 Hurst exponent, 51

non-periodic, 25
total least squares, 13
training set, 101, 163, 227
transcendental number, 117
transformer, 73, 146
tree (graph theory), 164
twin primes, 204

universality property, 198, 202, 204
unsupervised clustering, 71
unsupervised learning, 33, 239

validation set, 15, 56, 101, 163, 227, 234
Vandermonde matrix, 47, 52
vertex, 172, 180, 181, 194
video compression
 FFmpeg, 55, 59

Waring's problem, 204
Watts and Strogatz model, 231
Weibull distribution, 51, 131, 187, 194
weighted least squares, 13
weighted quantiles, 101
weighted regression, 16
white noise, 27, 49, 131, 237
wide data, 239

XOR operator, 119