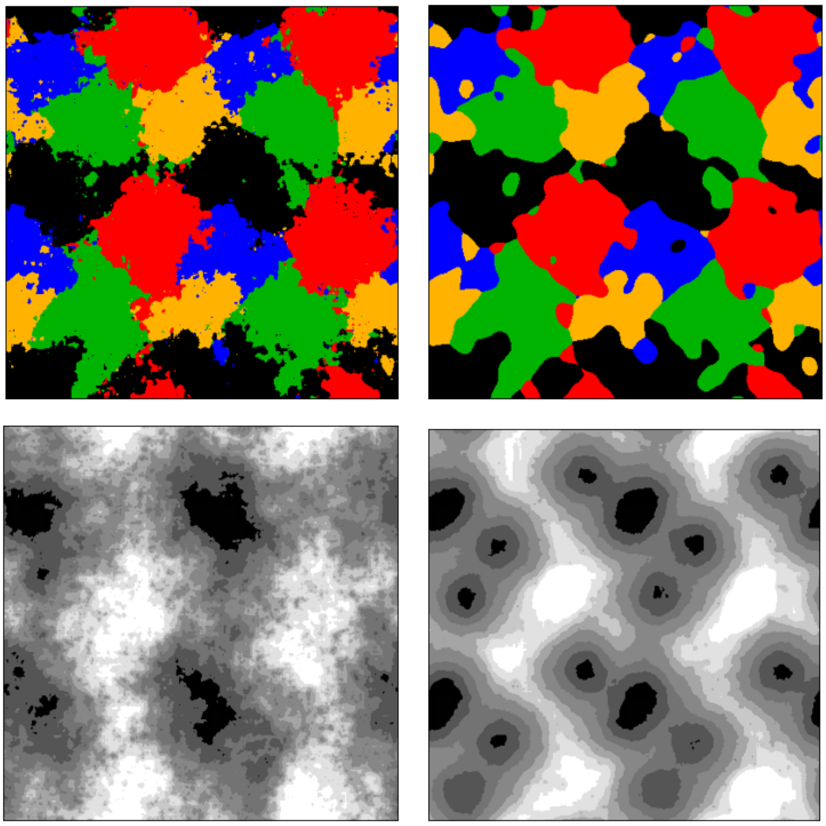
Intuitive Machine Learning



Vincent Granville, Ph.D. | www.MLTechniques.com | Version 1.0, September 2022

Preface

This book covers the foundations of machine learning, with modern approaches to solving complex problems. 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.

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, here.

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 upcoming 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), former VC-funded executive, author and patent owner. Vincent's past corporate experience includes Visa, Wells Fargo, eBay, NBC, Microsoft, CNET, InfoSpace. Vincent is also a former post-doc at Cambridge University, and the National Institute of Statistical Sciences (NISS).

Vincent published in *Journal of Number Theory*, *Journal of the Royal Statistical Society* (Series B), and *IEEE Transactions on Pattern Analysis and Machine Intelligence*. He is also the author of multiple books, available here. He lives in Washington state, and enjoys doing research on stochastic processes, dynamical systems, experimental math and probabilistic number theory.

Contents

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 44, 92, 126

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 32, 68, 139

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 31, 149

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 10, 91

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 7, 10, 13, 15, 24, 134, 137

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 10, 32, 88, 94, 139, 149

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 31, 32, 34, 36, 149, 150

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 7, 11, 150, 151

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 11, 91, 108

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 31, 78, 149

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 8, 64, 69, 78, 85

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 7, 10, 32, 89, 92, 130, 138, 149, 151

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 10, 51, 88, 89, 139, 149, 151

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 10, 26, 50, 84

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 65, 69, 142, 143

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 24, 51, 65, 70, 96, 150

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 8, 11, 150

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 11, 28, 31, 35, 149, 150

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 64, 68, 70, 78, 96, 149, 150

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 11.5 deals with creating a keyword taxonomy based on parsing Google search results pages. See pages 31, 141

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 7, 9, 54

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 10, 87, 96, 149, 151

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 33, 35, 39, 138, 140, 150

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 7, 10, 51, 85, 88, 90, 92, 99, 150, 151

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 24, 107, 114, 144

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 7, 8, 10, 11, 14, 22, 31, 35, 41, 44, 47, 51, 84, 90, 96, 103, 150, 151

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 151

Synthetic data

Artificial data simulated using a generative model, typically a mixture model, to enrich existed datasets and improve the quality of training sets. Called augmented data when blended with real data. See pages 7, 8, 10, 12, 22, 24, 28, 43, 50, 64, 65, 70, 83, 89, 100, 122, 135, 144, 149

Tensor

Matrix generalization with three of 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 64, 69

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 8, 10, 12, 15, 24, 31, 35, 51, 67, 83, 90, 96, 100, 139, 149, 150, 151

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 10, 22, 36, 51, 88, 96, 139, 149, 150, 151

Bibliography

[1] Weighted percentiles using numpy. *Forum discussion*, 2020. StackOverflow [Link]. 96

[2] Jan Ackmann et al. Machine-learned preconditioners for linear solvers in geophysical fluid flows. *Preprint*, pages 1–19, 2020. arXiv:2010.02866 [Link]. 88

[3] Rabi Bhattacharya and Edward Waymire. *Random Walk, Brownian Motion, and Martingales*. Springer, 2021. 121

[4] Barbara Bogacka. *Lecture Notes on Time Series*. 2008. Queen Mary University of London [Link]. 44

[5] Oliver Bröker and Marcus J. Groteb. Sparse approximate inverse smoothers for geometric and algebraic multigrid. *Applied Numerical Mathematics*, 41(1):61–80, 2002. 85

[6] Oliver Chikumbo and Vincent Granville. Optimal clustering and cluster identity in understanding high-dimensional data spaces with tightly distributed points. *Machine Learning and Knowledge Extraction*, 1(2):715–744, 2019. 145

[7] Keith Conrad. *L-functions and the Riemann Hypothesis*. 2018. 2018 CTNT Summer School [Link]. 110

[8] D.J. Daley and D. Vere-Jones. *An Introduction to the Theory of Point Processes*. Springer, second edition, 2002. Volume 1 – Elementary Theory and Methods. 125

[9] D.J. Daley and D. Vere-Jones. *An Introduction to the Theory of Point Processes*. Springer, second edition, 2014. Volume 2 – General Theory and Structure. 125

[10] Tilman M. Davies and Martin L. Hazelton. Assessing minimum contrast parameter estimation for spatial and spatiotemporal log-Gaussian Cox processes. *Statistica Neerlandica*, 67(4):355–389, 2013. 136

[11] Marc Deisenroth, A. Faisal, and Cheng Soon Ong. *Mathematics for Machine Learning*. Cambridge University Press, 2020. [Link]. 48

[12] Harold G. Diamond and Wen-Bin Zhang. *Beurling Generalized Numbers*. American Mathematical Society, 2016. Mathematical Surveys and Monographs, Volume 213 [Link]. 111

[13] Arash Farahmand. *Math 55 Lecture Notes*. 2021. University of Berkeley [Link]. 42, 48

[14] P. A. Van Der Geest. The binomial distribution with dependent Bernoulli trials. *Journal of Statistical Computation and Simulation*, pages 141–154, 2004. [Link]. 122

[15] Stamatia Giannarou and Tania Stathaki. Shape signature matching for object identification invariant to image transformations and occlusion. 2007. ResearchGate [Link]. 79

[16] B.V. Gnedenko and A. N. Kolmogorov. *Limit Distributions for Sums of Independent Random Variables*. Addison-Wesley, 1954. 126

[17] Manuel González-Navarrete and Rodrigo Lambert. Non-markovian random walks with memory lapses. *Preprint*, pages 1–14, 2018. arXiv [Link]. 121

[18] Ian Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep Learning*. MIT Press, 2016. [Link]. 48

[19] Vincent Granville. *Applied Stochastic Processes, Chaos Modeling, and Probabilistic Properties of Numeration Systems*. MLTechniques.com, 2018. [Link]. 111

[20] Vincent Granville. New perspective on the Riemann Hypothesis. *Preprint*, pages 1–23, 2022. MLTechniques.com [Link]. 20, 21

[21] Vincent Granville. *Stochastic Processes and Simulations: A Machine Learning Perspective*. MLTechniques.com, 2022. [Link]. 28, 46, 54, 65, 83, 85, 126, 134, 138, 147

[22] Vincent Granville, Mirko Krivanek, and Jean-Paul Rasson. Simulated annealing: A proof of convergence. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 16:652–656, 1996. 67

[23] Vincent Granville and Richard L Smith. Disaggregation of rainfall time series via Gibbs sampling. *NISS Technical Report*, pages 1–21, 1996. [Link]. 102

[24] Kristen Grauman. Shape matching. 2008. University of Texas, Austin [Link]. 82

[25] Radim Halir and Jan Flusser. Numerically stable direct least squares fitting of ellipses. *Preprint*, pages 1–8, 1998. [Link]. 12, 14

[26] Adam J. Harper. Moments of random multiplicative functions, II: High moments. *Algebra and Number Theory*, 13(10):2277–2321, 2019. [Link]. 107

[27] Adam J. Harper. Moments of random multiplicative functions, I: Low moments, better than squareroot cancellation, and critical multiplicative chaos. *Forum of Mathematics, Pi*, 8:1–95, 2020. [Link]. 107, 109

[28] Adam J. Harper. Almost sure large fluctuations of random multiplicative functions. *Preprint*, pages 1–38, 2021. arXiv [Link]. 109

[29] T. W. Hilberdink and M. L. Lapidus. Beurling Zeta functions, generalised primes, and fractal membranes. *Preprint*, pages 1–31, 2004. arXiv [Link]. 110, 111

[30] Christian Hill. *Learning Scientific Programming with Python*. Cambridge University Press, 2016. [Link]. 14

[31] Robert V. Hogg, Joseph W. McKean, and Allen T. Craig. *Introduction to Mathematical Statistics*. Pearson, eighth edition, 2016. [Link]. 48

[32] Zhiqiu Hu and Rong-Cai Yang. A new distribution-free approach to constructing the confidence region for multiple parameters. *PLOS One*, pages 1–13, 2013. [Link]. 135

[33] Chigozie Kelechi. Towards efficiency in the residual and parametric bootstrap techniques. *American Journal of Theoretical and Applied Statistics*, 5(5), 2016. [Link]. 92

[34] Yuk-Kam Lau, Gerald Tenenbaum, and Jie Wu. On mean values of random multiplicative functions. *Proceedings of the American Mathematical Society*, 142(2):409–420, 2013. [Link]. 107, 109

[35] Jing Lei et al. Distribution-free predictive inference for regression. *Journal of the American Statistical Association*, 113:1094–1111, 2018. [Link]. 92

[36] Christoph Molnar. *Interpretable Machine Learning*. ChristophMolnar.com, 2022. [Link]. 92

[37] Marc-Andreas Muendler. Linear difference equations and autoregressive processes. 2000. University of Berkeley [Link]. 44

[38] Peter Mörters and Yuval Peres. *Brownian Motion*. Cambridge University Press, 2010. Cambridge Series in Statistical and Probabilistic Mathematics, Volume 30 [Link]. 121, 125

[39] Jesper Møller. Introduction to spatial point processes and simulation-based inference. In *International Center for Pure and Applied Mathematics (Lecture Notes)*, Lomé, Togo, 2018. 136

[40] Guillermo Navas-Palencia. Optimal binning: mathematical programming formulation. *Preprint*, pages 1–21, 2020. arXiv:2001.08025 [Link]. 32

[41] Fred Park. Shape descriptor / feature extraction techniques. 2011. UCI iCAMP 2011 [Link]. 79

[42] Carl Rasmussen and Christopher Williams. *Gaussian Processes for Machine Learning*. MIT Press, 2006. [Link]. 47

[43] Kamron Saniee. A simple expression for multivariate Lagrange interpolation. *SIAM Undergraduate Research Online*, 2007. SIURO [Link]. 98

[44] Luuk Spreeuwers. *Image Filtering with Neural Networks: Applications and Performance Evaluation*. PhD thesis, University of Twente, 1992. 68

[45] E.C. Titchmarsh and D.R. Heath-Brown. *The Theory of the Riemann Zeta-Function*. Oxford Science Publications, second edition, 1987. 53, 110

[46] Chris Tofallis. Fitting equations to data with the perfect correlation relationship. *Preprint*, pages 1–11, 2015. Hertfordshire Business School Working Paper[Link]. 8

[47] D. Umbach and K.N. Jones. A few methods for fitting circles to data. *IEEE Transactions on Instrumentation and Measurement*, 52(6):1881–1885, 2003. [Link]. 9, 12

[48] D. A. Vaccari and H. K. Wang. Multivariate polynomial regression for identification of chaotic time series. *Mathematical and Computer Modelling of Dynamical Systems*, 13(4):1–19, 2007. [Link]. 12

[49] Yu Vizilter and Sergey Zheltov. Geometrical correlation and matching of 2D image shapes. 2012. ResearchGate [Link]. 81

[50] Lan Wua, Yongcheng Qi, and Jingping Yang. Asymptotics for dependent Bernoulli random variables. *Statistics and Probability Letters*, pages 455–463, 2012. [Link]. 121

[51] Shaohong Yan, Aimin Yang, et al. Explicit algorithm to the inverse of Vandermonde matrix. In *2009 International Conference on Test and Measurement*, 2009. IEEE [Link]. 42

Index