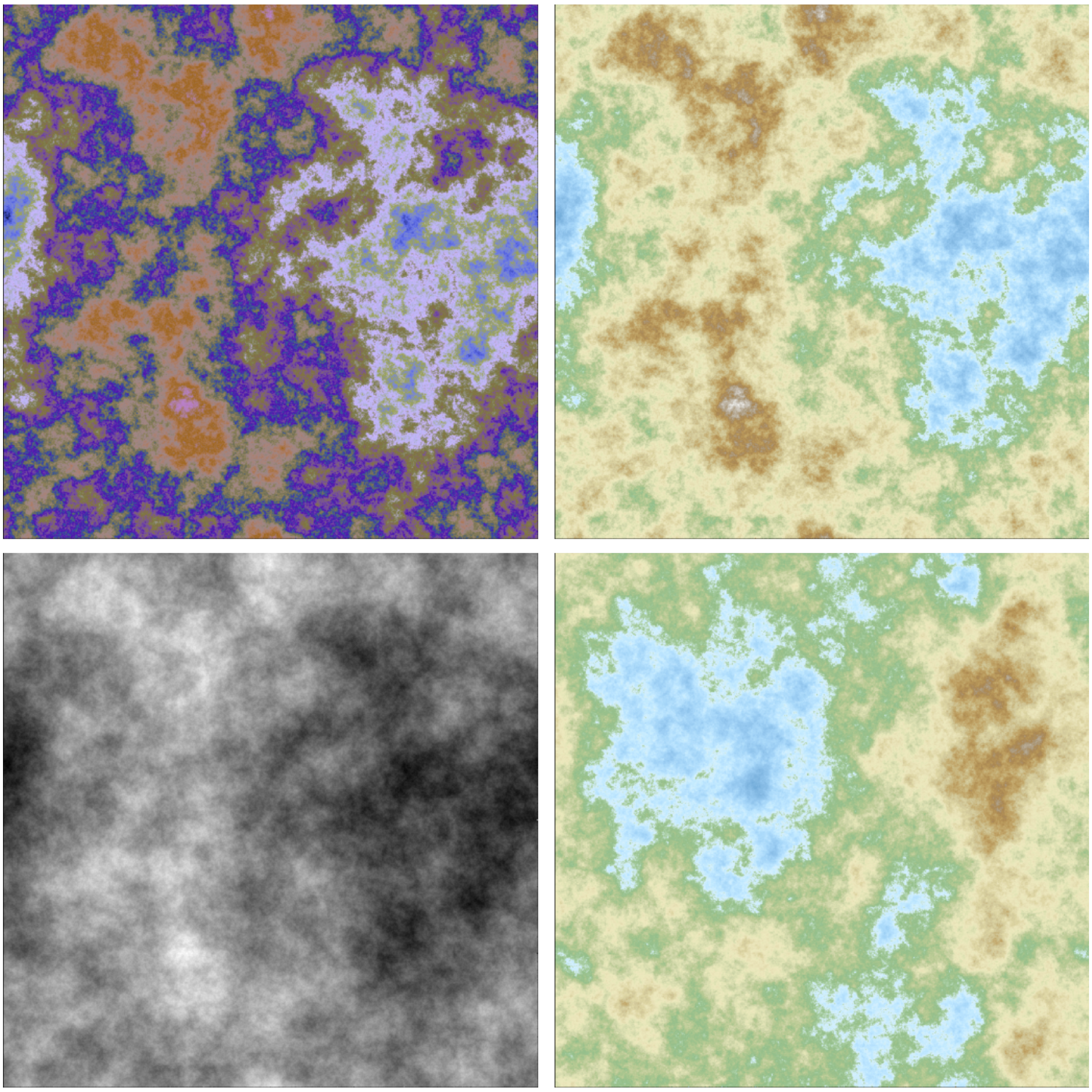
Synthetic Data and Generative AI



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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.

Several chapters focus on synthetic data, agent-based modeling and GIS applications: fractal-like terrain generation with the diamond-square algorithm, disaggregation of of ocean tides time series, geospatial interpolation of temperatures in the Chicago area, 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 15 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. Section 17.7.2 illustrates the use of copulas to produce synthetic data, applied to a well-known insurance dataset.

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 solid introduction to scientific programming. 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. 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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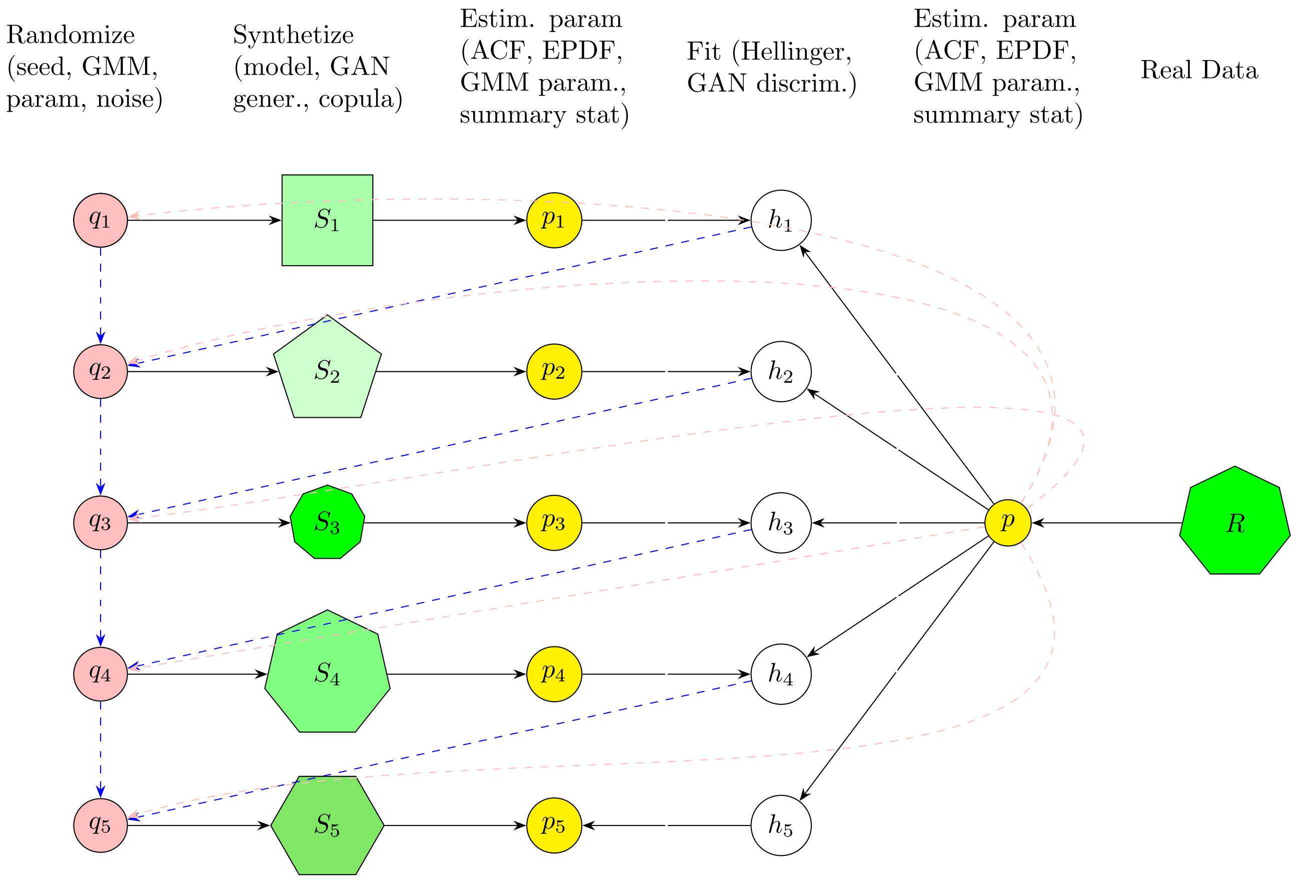
Data synthetization explained in one picture

The diagram is organized as follows. Dashed blue lines are associated to GANs (generative adversarial networks), where the goal is to produce a sequence of synthetic datasets that get better and better at mimicking the structure present in the real data, over successive iterations. The diagram features 5 such iterations, with the synthetized datasets denoted as $S_1, S_2, \ldots, S_5$. Typically, GANs follow the gradient of h to reach an optimum configuration q that can not be classified as non-real anymore. Synthetic data that gets closer to the real data gets rewarded in this reinforcement learning technique. Like any simulation-intensive method, training the neural network can be time-consuming, and this black-box approach may lack explainability.

Dashed pink lines are associated to modeling techniques (generative model, GMM) where synthetic data is obtained by simulating the underlying model using the parameter values estimated on the real data, that is, $q_k = p$ for all k. In case of GMM (Gaussian mixture models), the parameters are the cluster centers, the covariance matrix attached to each cluster, and the proportions of the mixture. For stationary time series, the parameter is typically the autocorrelation function (ACF). In some applications including when using copulas, the EDPD (empirical probability density function) is used instead.

The goal is to mimic the structure in the real data, not the real data itself. The structure is represented by a parametric configuration denoted as p in the real data. I use the notation $p_1, \ldots, p_5$ for the structures found in the 5 synthetic data sets. The quality h_k of the synthetic data set k is the distance between p_k and p, based on the Hellinger metric or some discriminating function in the case of GAN. It is assumed that the real data has been normalized (transformed) before synthesizing. “Estim. param.” stands for estimated parameters in the diagram, though sometimes the parameters can be a function or matrix rather than a set of elements.



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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 50, 98, 152
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 38, 74, 248
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 37, 261
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 16, 97, 209, 261
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 13, 16, 19, 21, 30, 206, 207, 243, 246
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 16, 38, 94, 100, 184, 248, 261
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 37, 38, 40, 42, 261, 262
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 13, 17, 262, 263
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 17, 97, 121, 130, 193, 196, 202, 208, 213, 215, 227, 255
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 37, 84, 261
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 14, 36, 70, 75, 84, 91, 156, 172, 210, 254

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 13, 16, 38, 95, 98, 239, 247, 261, 263

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 m-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 3, 36, 53, 100, 167, 168, 170, 177, 184, 263

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 16, 57, 94, 95, 248, 261, 263

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 16, 32, 56, 90

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 71, 75, 185, 251, 252

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 30, 57, 71, 76, 102, 171, 262

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 14, 17, 262

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 17, 34, 37, 41, 261, 262

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 70, 74, 76, 84, 102, 261, 262

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 17.5 deals with creating a keyword taxonomy based on parsing Google search result pages. Text generation is referred to as NLG or natural language generation, using large language models (LLM). See pages 37, 250

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 13, 15, 60
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 16, 93, 102, 255, 256, 261, 263
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 39, 41, 45, 247, 249, 254, 262
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 13, 16, 36, 57, 91, 94, 96, 98, 105, 262, 263
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 30, 129, 136, 253
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 13, 14, 16, 17, 20, 28, 37, 41, 47, 51, 53, 57, 90, 96, 102, 109, 262, 263
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 263
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 13, 14, 16, 18, 28, 30, 34, 36, 49, 53, 56, 70, 71, 76, 89, 95, 106, 113, 119, 129, 142, 148, 156, 170, 177, 184, 244, 253, 255, 261
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 70, 75
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 14, 16, 18, 21, 30, 37, 41, 57, 73, 89, 96, 102, 106, 184, 248, 261, 263
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 16, 28, 42, 57, 94, 102, 184, 248, 255, 256, 261, 262, 263

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