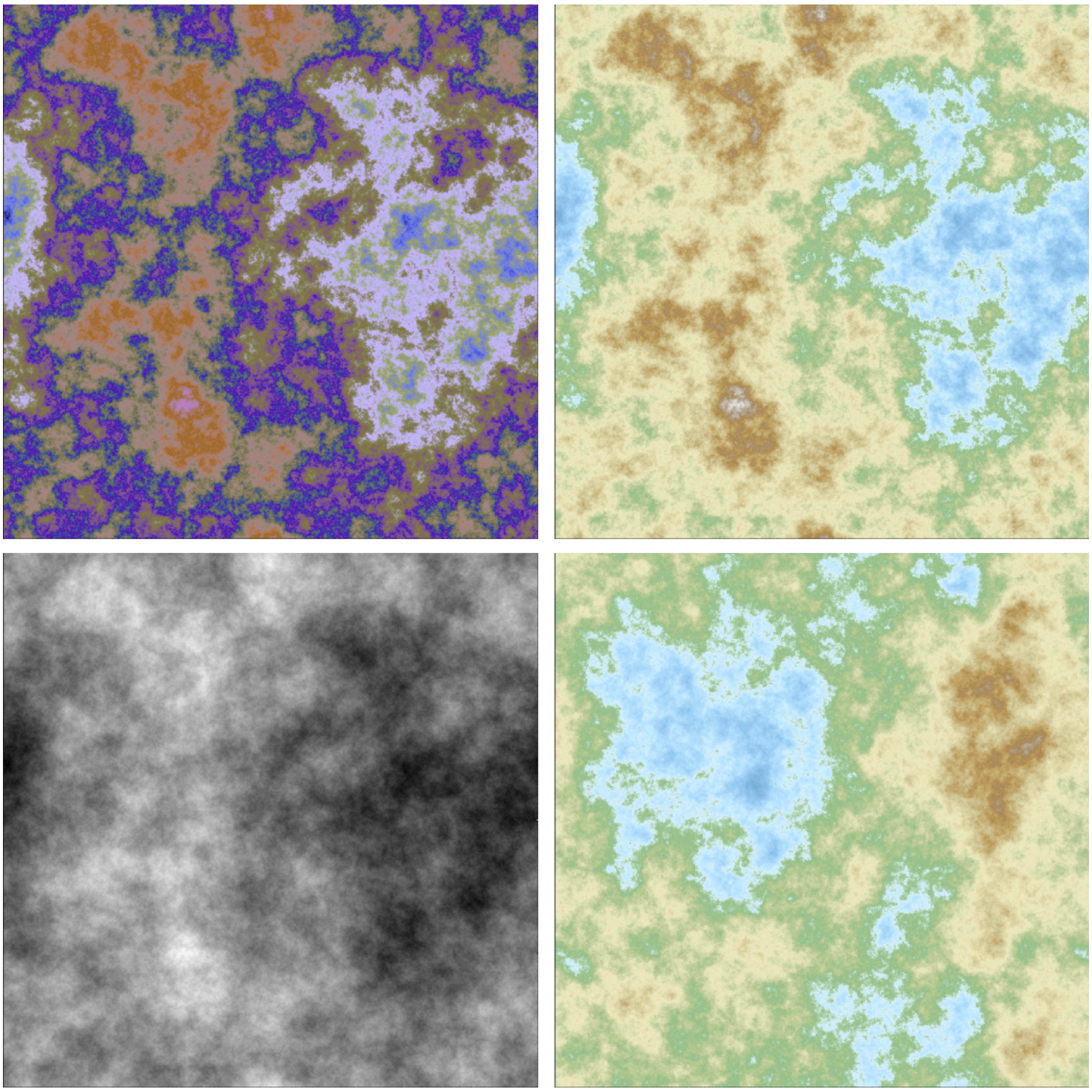
Synthetic Data and Generative AI



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Preface

This book was first started in December 2022 and has been revised and augmented multiple times since the first writing. It now covers all the modern techniques on the subject as well as efficient proprietary methods developed by the author, with real industry use cases and Python implementations. The goal is to quickly help you pick up the right tool and run the code on your own dataset, in very little time. Yet the author provides enough background so that the reader understands all the aspects and interconnections of the methods involved, their strengths and weaknesses, potential enhancements, rule of thumbs, and best practices. Research-level material is also present throughout the book, and explained in simple English.

What is synthetic data and why use it?

Synthetic data is more than simulations, mimicking real data, fake (gibberish) data or noise injection to add variations to real data. It is defined by its usage and purpose. Four broad areas include:

- Data augmentation to produce richer training sets for predictive modeling; it leads to more robust predictions and reduced overfitting. For instance, to produce a better version of ChatGPT or better detection of cancer from medical images or tabular data.
- Generation of diversified data to test and benchmark machine learning algorithms, to identify their limits or to understand and improve black-box systems. Sensitivity testing fits in this category.
- Increasing security and compliance with data protection laws by strongly anonymizing data (especially for data sharing purposes), as well as reduction of algorithm bias impacting minorities.
- Data re-balancing in the presence of small segments (fraud / non-fraud, minority group), and smart data imputation. It is also useful in the presence of small samples with many features, when the data is difficult to obtain: for instance, clinical trials.

The data can be tabular (transactional), time series, graphs or consisting of images, videos, sound, text, spatial information or the result of agent-based systems. The goal is to identify and reproduce the structure (such as the autocorrelation function, shape, or correlation structure) rather than replicating the original data itself. In some instances (benchmarking), no real data is even needed.

Several techniques can be used for synthetization: GAN (generative adversarial networks), GMM (Gaussian mixture models) and other statistical models, interpolation, parametric noise with a target correlation structure, and more. Many metrics are available to assess the quality, be it cross-validation, ROC curves, statistical summaries, or Hellinger and related distances. All this material is reviewed in this book. In particular, chapter 10 discusses a GAN with replicable output especially designed for synthetization, illustrated on tabular data.

Book contents and target audience

This book covers the foundations of generative models and data synthetization. Emphasis is on scalability, automation, testing, optimizing, and interpretability (explainable AI). Models (including GMM, GAN and copulas) are often used to create rich synthetic data, augment real data, or to test and benchmark various methods. Many machine learning algorithms are revisited, simplified, unified, and generalized. 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: it shows another usage of synthetization, with an application to meteorites shapes, for instance when the goal is to classify these celestial bodies.

With a focus on applications, synthetization and simulations, the book also covers 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, strong 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.

Chapter 10 illustrates the use of copulas to produce synthetic data, applied to a well-known insurance dataset. It also features both GAN (generative adversarial networks) and copulas applied to an health industry data set, comparing results and showing how both methods can be blended for better synthetization and predictions, or even for data compression. Agent-based modeling and GIS applications are also covered, with interpolation techniques used for synthetization: fractal-like terrain generation with the diamond-square algorithm, disaggregation of of ocean tides time series, and geospatial interpolation of temperatures in the Chicago area.

Image and video generation include star clusters evolving over time and bound by gravity, providing potential scenarios about the past and future of our universe, or to synthesize collision graphs. It also allows you to explore alternative universes, for instance with negative masses. Chapters 16 and 17 are more advanced and may be skipped in introductory classes. The former focuses on point processes as a simple alternative to GMM. The later features synthetic multiplicative functions to discover new insights about 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 solid introduction to scientific programming. 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. 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 synthetic data and generative AI.

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.

Vincent is also a former post-doc at Cambridge University, and the National Institute of Statistical Sciences (NISS). He 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.

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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, 175
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, 271
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, 280
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, 232, 280
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, 229, 230, 266, 269
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, 138, 207, 271, 280
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, 280, 281
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, 281, 282
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, 153, 216, 219, 225, 231, 236, 238, 250
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, 280

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, 129, 141, 179, 195, 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 13, 16, 38, 95, 98, 262, 270, 280, 282

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. New observations can also be generated via parametric bootstrap. See pages 36, 53, 100, 147, 190, 191, 193, 200, 207, 282

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, 271, 280, 282

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, 208, 274, 275

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, 136, 194, 281

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, 281

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, 280, 281

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, 280, 281

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 18.5 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, 273

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, 130, 136, 280, 282

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, 129, 270, 272, 281

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, 281, 282

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, 152, 159, 276

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, 281, 282

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 282

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, 130, 152, 165, 171, 179, 193, 200, 207, 267, 276, 280

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, 207, 271, 280, 282

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, 130, 207, 271, 280, 281, 282

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