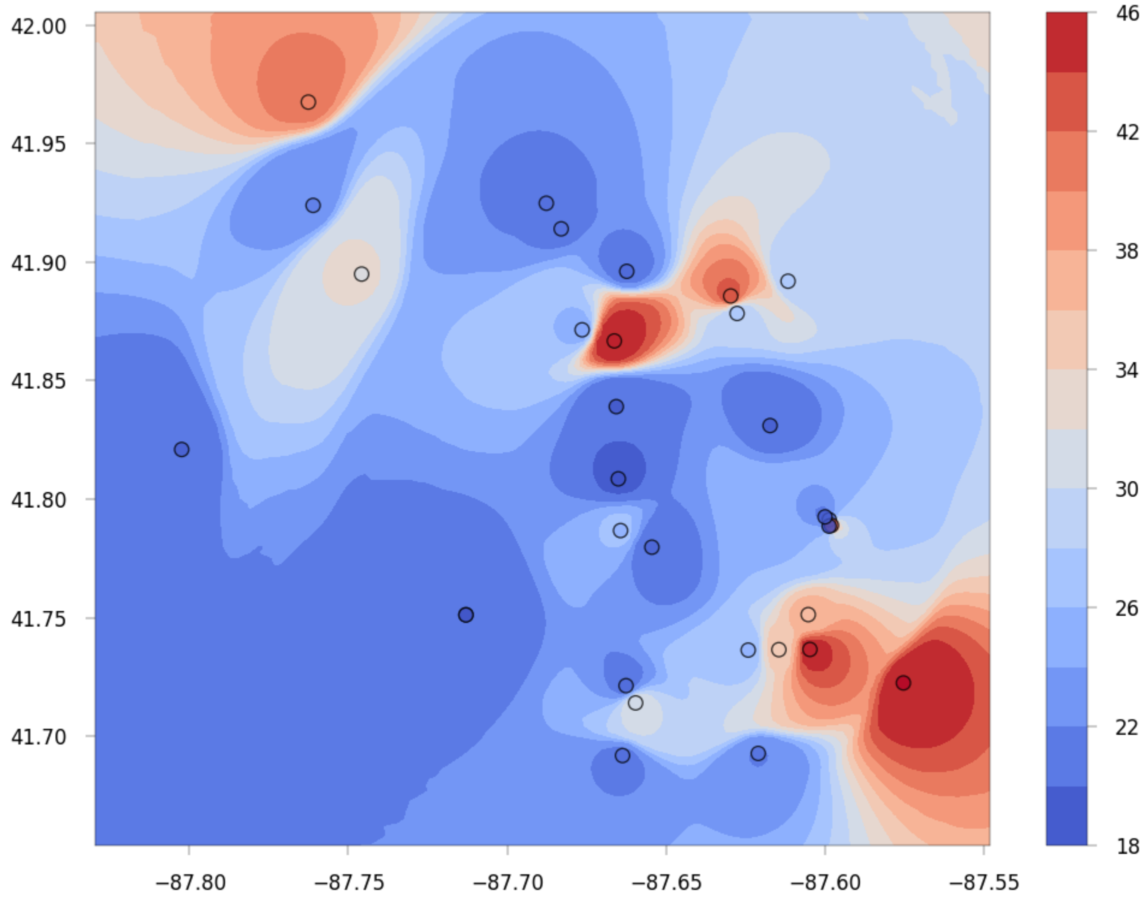
Statistical Optimization for AI and Machine Learning



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Preface

This book covers optimization techniques pertaining to machine learning and generative AI, with an emphasis on producing better synthetic data with faster methods, some not even involving neural networks. NoGAN for tabular data is described in detail, along with full Python code, and case studies in healthcare, insurance, cybersecurity, education, and telecom. This low-cost technique is a game changer: it runs 1000x faster than generative adversarial networks (GAN) while consistently producing better results. Also, it leads to replicable results and auto-tuning.

Many evaluation metrics fail to detect defects in synthesized data, not because they are bad, but because they are poorly implemented: due to the complexity, the full multivariate version is absent from vendor solutions. In this book, I describe an implementation of the full version, tested on numerous examples. Known as the multivariate Kolmogorov-Smirnov distance (KS), it is based on the joint empirical distributions attached to the datasets, and work in any dimension on categorical and numerical features. Python libraries, both for NoGAN and KS, are now available and presented in this book.

A very different synthesizer also discussed, namely NoGAN2, is based on resampling, model-free hierarchical methods, auto-tuning, and explainable AI. It minimizes a particular loss function, also without gradient descent. While not based on neural networks, it nevertheless shares many similarities with GAN. Thus you can use it as a sandbox to quickly test various features and hyperparameters before adding the ones that work best, to GAN. Even though NoGAN and NoGAN2 don't use traditional optimization, gradient descent is the topic of the first chapter. Applied to data rather than math functions, there is no assumption of differentiability, no learning parameter, and essentially no math. The second chapter introduces a generic class of regression methods covering all existing ones and more, whether your data has a response or not, for supervised or unsupervised learning. I use gradient descent in this case.

One chapter is devoted to NLP, featuring an efficient technique to process large amounts of text data: hidden decision trees, presenting some similarities with XGBoost. A similar technique is used in NoGAN. Then I discuss other GenAI methods and various optimization techniques, including feature clustering, data thinning, smart grid search and more. Multivariate interpolation is used for time series and geospatial data, while agent-based modeling applies to complex systems.

Methods are accompanied by enterprise-grade Python code, also available on GitHub. Chapters are mostly independent from each other, allowing you to read in random order. The style is very compact, and suitable to business professionals with little 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.

About the author

Vincent Granville is a pioneering GenAI scientist and machine learning expert, co-founder of Data Science Central (acquired by a publicly traded company in 2020), Chief AI Scientist at MLTechniques.com, former VC-funded executive, author and patent owner – one related to LLM. 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 the author of multiple books, available here, including "Synthetic Data and Generative AI" (Elsevier, 2024). Vincent lives in Washington state, and enjoys doing research on stochastic processes, dynamical systems, experimental math and probabilistic number theory. He recently launched a GenAI certification program, offering state-of-the-art, enterprise grade projects to participants. The program, based on his books, is discussed here.

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replicability	A replicable neural network is one that can produce the exact same results when run multiple times on the same data, regardless of the platform. Usually controlled by a seed parameter: using the same seed leads to the same results.
scaling	A transformation that keeps the values of each feature within the same range, or with the same variance in the real data, before using GAN. A measurement, whether in yards or miles, will be scale-free after the transformation. It can dramatically improve the quality of the generated data. Inverse scaling is then applied to the generated data, after the GAN synthetization.
seed	Parameter used to initialize the various random number generators involved in the GAN architecture, typically one for each Python library that generates random numbers. It produces replicable results, at least with CPU implementations. In GPU, the problem is different.
stopping rule	A criterion to decide when to stop training a GAN, typically when an epoch produces an unusually good synthetization, based on quality evaluation metrics such as the KS distance. It produces much better results than stopping after a fixed number of epochs.
synthetization	Production of generated observations, also called synthetic data, with statistical properties mimicking those computed on a pre-specified real data set.
tabular data	Data arranged in tables, where columns represent features, and rows represent observations. Typically used for transactional data. Time series are treated with specific algorithms.
training set	The portion of your real data used to train your synthesizer. The other part is called the validation set, and used to evaluate the quality of the synthetic data (how well it mimics real data). This setting known as holdout allows you to test you synthetisizer on future data and avoid overfitting.
transform	Similar to transformers in large language models. Consists of using an invertible transform on your real data prior to GAN processing, to improve GAN performance. You need to apply the inverse transform on the generated data, after GAN. Example of transforms: scaling, PCA, standardization (transformed features having the same variance and zero mean), and normalization (to eliminate skewness).
validation set	See training set.
vanishing gradient	When the gradient gets close to zero in a gradient descent algorithm, it can prevent further progress towards locating the optimum. In the worst case, this may completely stop the neural network from further training.
Wasserstein loss	The GAN Wasserstein loss function seeks to increase the gap between the scores for real and generated data. It is one of the many loss functions to improve the gradient descent algorithm, avoiding mode collapse and similar problems in some synthetizations.
WGAN	Wasserstein GAN, based on the Wasserstein loss function.

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