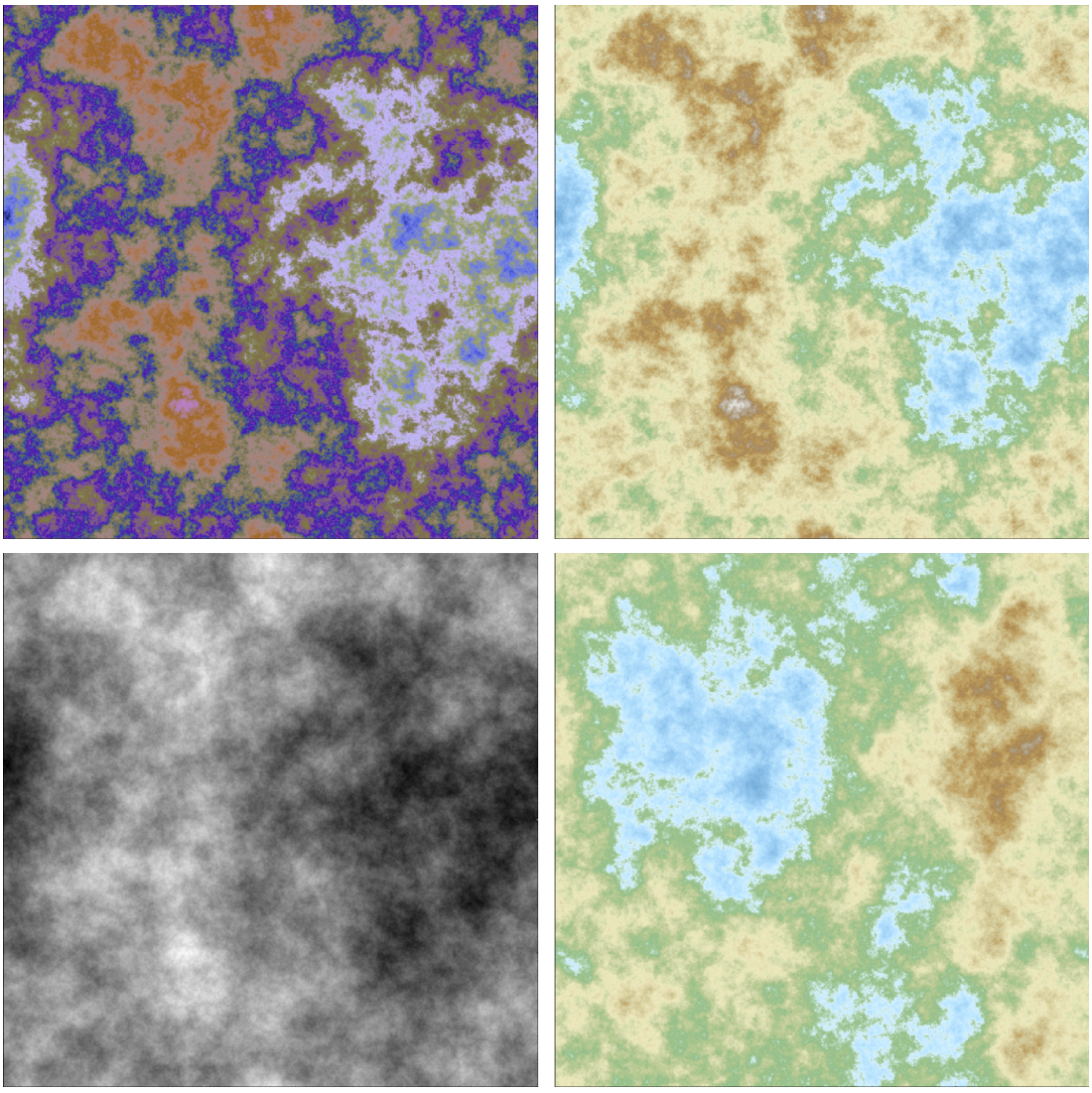
Synthetic Data and Generative AI



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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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implementation can be found here. Start by computing the correlation matrix attached to your real data. Rank all pairs of features $\{A, B\}$ by correlation between A and B, starting with the largest correlation in absolute value, down to the lowest one that is statistically significant and/or at least above (say) 0.30. The top pair constitutes your first group of features. Look at the second pair. If it contains a feature from the first group, merge the two groups to obtain a single group with 3 features. If not, you have two groups of features at this stage, each containing 2 features. Proceed iteratively until all pairs of features have been visited.

However, the correlation structure may not always represent all the dependencies in the data: points distributed on a circle are not correlated, yet they are highly dependent! In this case, use 1 dimension (the angular position) rather than the 2 Cartesian coordinates. More generally, appropriate data transformations and reduction can fix the issue.

10.4 Deep dive into generative adversarial networks (GAN)

In this section I discuss GAN in details, with a Python implementation to synthesize tabular data. Unlike many neural networks, my code can generate replicable outputs. Other solutions and references are provided in section 10.4.1. Later on, I discuss enhancements to the original model. Finally, I show how to blend GAN with copulas to get the best of both worlds.

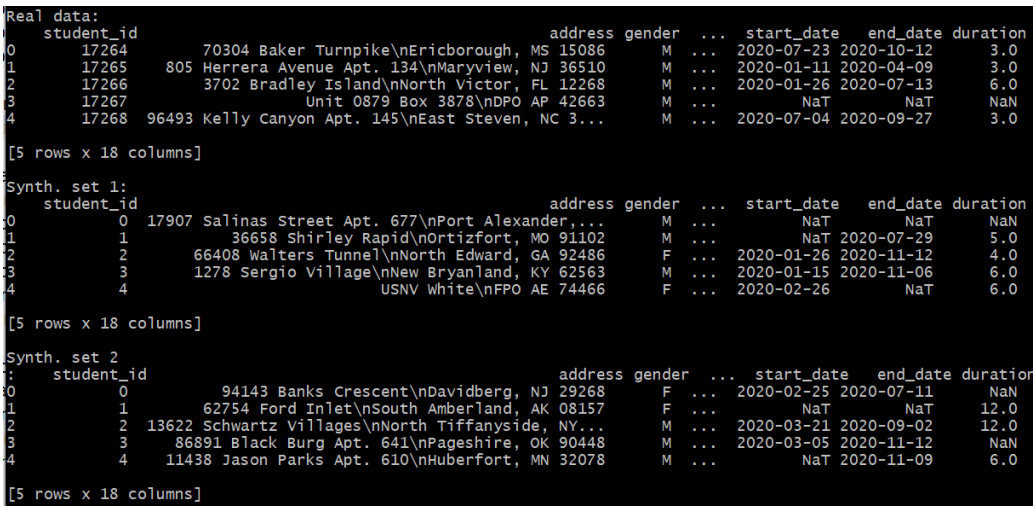

Figure 10.1: Synthetic versus real data, produced by SDV GAN + copula

10.4.1 Open source libraries and references

One of the most popular libraries for synthetization is SDV, which stands for synthetic data vault. You can check it out on GitHub, here. For sample code, see here. and here. SDV comes with 28 real-life datasets. To see the list, with the number of tables, rows and columns for each data set, run the code below.

```
from sdv.demo import get_available_demos
from sdv.demo import load_tabular_demo
from sdv.tabular import CopulaGAN

demos = get_available_demos()
print(demos) # show list of demo datasets

metadata, real_data = load_tabular_demo('student_placements_pii',metadata=True)
print("\nReal data:\n",real_data.head())
model = CopulaGAN()
model = CopulaGAN(primary_key='student_id',anonymize_fields={'address': 'address' })
model.fit(real_data)
synth_data1 = model.sample(200)
print("\nSynth. set 1:\n",synth_data1.head())

model.save('my_model.pkl')      # this shows how to save the model
loaded = CopulaGAN.load('my_model.pkl') # load the model, and
synth_data2 = loaded.sample(200) # get new set of synth. data
print("\nSynth. set 2\n:",synth_data2.head())
```

The first example is a YouTube dataset with 2 tables, 2735 rows and 10 columns. The number of rows ranges from 83 to over 6 million, and some datasets have over 300 features. The code in question also loads one dataset (`'student_placements_pii'`), and shows how to use a GAN model based on Gaussian copulas. See output in Figure 10.1. The code is on GitHub, here. Some of the fields such as the address are anonymized rather than synthesized. This is performed by implicitly calling the Python library Faker, described here. Also, you can choose the option `FAST_ML` for the optimizer (the gradient descent algorithm), for faster processing but with lower accuracy. This is done using the instruction `TabularPreset(name='FAST_ML', metadata=metadata)` as explained here.

SDV is a black-box, so to illustrate the various steps of GAN in details, I use an implementation based on the Keras library instead. Keras is easier to use than Tensorflow [Wiki], though it requires Tensorflow to be installed on your system. Another black-box alternative, allowing you to implement GAN for tabular data synthetization with just 3 lines of code, is TabGAN, available here. See [6] for a discussion. I had to install the most recent version of Numpy to get it to work. More generally, installing these libraries may also require the most recent version of pip, which you can get via the command `pip install --upgrade pip`. TabGAN uses LightGBM [Wiki], a fast version of gradient boosting, and it is thus a bit faster than my step-by-step version in section 10.7.

Another implementation very similar to mine and illustrated on time series, is discussed here. Mine includes a new version of correlation matrix distance to assess quality; see here and [64] for a standard definition. It also uses a seed for every single source of randomness in the algorithm, allowing for full replicability, as well as other specific features. If you run the code in GPU, there might be additional sources of randomness that you can't control. You can run the code (say `mycode.py`) with the following command line in that case, if replicability is important for your application:

```
> CUDA_VISIBLE_DEVICES="" PYTHONHASHSEED=0 python mycode.py
```

Finally, there are various libraries to assess the quality of the synthetized data. I use TableEvaluator in my code in section 10.7, along with home-made metrics that are more useful to me. TableEvaluator is described here. There is not much documentation about it, but you can check out the full source code on GitHub, here. That is how I found out that the output metric called "Base Statistics" is a correlation distance between the real versus synthesized data, computed on various bivariate indicators as data points (mean, median, correlation between features and so on both for real and synthesized).

Additional reading on the subject includes the book "Synthetic Data for Deep Learning" [97], "Pros and Cons of GAN Evaluation Measures" [15], "Survey on Synthetic Data Generation, Evaluation Methods and GANs" [40], and "Are GANs Created Equal? A Large-Scale Study" by Google Brain [80]. See also Lei Xu's master thesis (MIT, 2017) available here and the related article on ArXiv [120], as well as this article. For the Keras models used in my implementation, see here.

10.4.2 Synthesizing medical data with GAN

Here I summarize my implementation of GAN applied to the Kaggle diabetes data set. First, I discuss the hyperparameters, then the main steps in the methodology. The data is processed "as is", without normalization or transformation. Possible transformations (preprocessing) are discussed in section 10.5.1. However, I removed all the observations with missing values, for better comparison with the copula method. Anyway, it makes sense to treat these observations separately, as a different segment, by re-running GAN on them only. Indeed, it produces better results when they are separated from the complete observations. After removing observations with missing values, we are left with 392 rows.

The dataset has 9 features. One of them called `Outcome` is the response: it indicates whether or not the patient had cancer. Thus the problem is predicting – based on the remaining 8 features – the chance of getting cancer. It is a supervised classification problem with two groups: cancer versus non-cancer.

The first part of the code (section 10.7.1) imports the libraries, reads the data and removes observations with missing values, and then performs the classification with the random forest algorithm [Wiki]. It also defines some global variables such as the learning rate [Wiki] in the Adam gradient descent, and `seed` which allows for replicability by using the same value in each run. The quality of the classification is displayed on the screen, as the `Base Accuracy` metric.

The last part of the code (section 10.7.3) evaluates the quality of the synthetic data. It also performs the classification on the synthetic data, for comparison with the results obtained on the real data. It would be interesting to augment the real data by adding the synthetic data into it, and see if we get more robust predictions. The augmented data is not expected to increase accuracy; instead it is expected to increase robustness and reduce overfitting.

The dataset `diabetes.csv` is on my GitHub directory, here. The original can be found on Kaggle, here. It should be noted that all the features are treated as continuous, even the binary `Outcome`. Thus

the number of pregnancies (an integer) or the "outcome" generated by GAN are real numbers, that must be mapped onto integers to make sense. Other implementations such as copulas or copula-based GANs do not have this limitation. An alternative is to use one GAN for `Outcome==0`, and another one for `Outcome==1`. Also, categorical features (absent here except for Outcome) can be replaced by dummy variables [Wiki].

10.4.2.1 Hyperparameters

There is a surprisingly large number of hyperparameters that can be fine-tuned. This is one of the reasons why these systems take a lot of time to train and optimize. In addition, the gradient descent present in all GANs (with its own parameters), is the bottleneck. Self-identification of good parameters by the algorithm itself – and possibly adjusted over time – is one way to at least automate the process. But it can lead to overfitting. The best solution is to use standard hyperparameters that work well in many contexts, without trying to over-adjust.

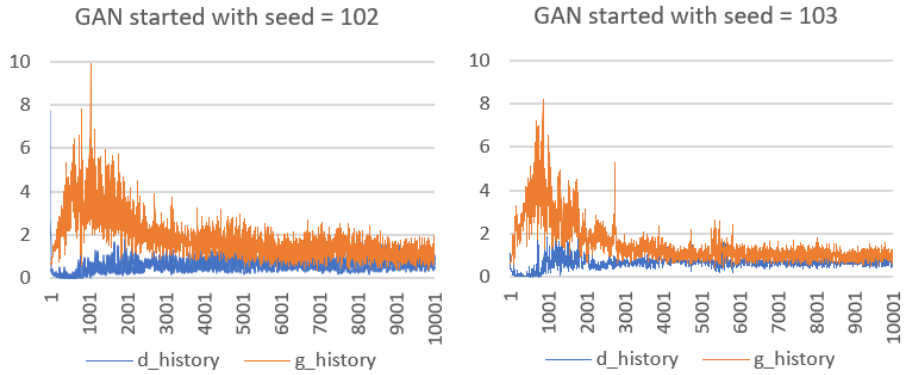

Figure 10.2: Loss function (in orange) for 10^4 successive epochs; enhanced GAN on the right plot

All these parameters are set and used in the GAN part of the code, in section 10.7.2. The only exception is the learning rate parameter.

- Epochs: One iteration of GAN consists of processing the full data set: this is done using a number of small samples (batches), one at a time. The number of iterations is the number of epochs, set to `n_epochs=10000` (a typical value) in the `train` function used to train the GAN.
- Batch size: see Epochs. Here it is set to `n_batch=128` in the `train` function. Half of the batch is used to sample from the real data, and the other half to generate latent data.
- Latent data: here latent variables [Wiki] are univariate random Gaussian deviates with zero mean and unit variance; typically their number matches the number of features. Their role is similar to the Gaussian deviates in the copula method. However, using a uniform distribution on $[-1, 1]$ is worth exploring as many GAN functions (for instance ReLU) return values between 0 and 1. Such restrictions are also used in Fourier regression in section 9.3.3.
- Activation function: in neural network, the activation function [Wiki] decides whether a neuron should be activated or not. Classic examples used in the code are ReLU [Wiki] and sigmoid [Wiki].
- Kernel initializer: defines the way to set the initial random weights of Keras layers. See documentation here.
- Number of layers: the neural networks (both the generator and discriminator) use 3 layers. A layer is added via the instruction `model.add`, with a number of options: activation function, kernel initializer, and so on. See `define_generator`, `define_discriminator` and `define_gan` (the combination of both) in the code. With 3 layers, we are dealing with a deep neural network.
- Learning rate: attached to the gradient descent. I tried 0.01 and 0.001, and settled for the latter. Small values result in quite chaotic, faster behavior (at the beginning) and somewhat reduced accuracy. Large values result in slow steady progress but you can end up stuck in a bad local optimum. Think of it as the cooling schedule in a simulated annealing algorithm.
- Gradient descent method: I use `Adam`. The alternative `SGD` (stochastic gradient descent [Wiki]) did no do well here, but does well in computer vision.
- Loss function: in gradient descent or any optimization problem, the loss function [Wiki] specifies the type of distance to the optimum vector, used for minimization. Think of it as a regression problem solved by least squares – the loss function being quadratic in this case. It is sometimes called the error function.

- Accuracy: calculates how often predictions equal labels in the context of classification. In this context, classification means assigning an observation to either real (truly real or excellent synthetization) or fake (poor synthetic data not close to the reality). See Keras documentation here. There are various options to choose from, to measure accuracy.
- Architecture: the type of neural network. In this example, set to `Sequential`.

10.4.2.2 GAN: Main steps

The steps in this section corresponds to the actual GAN procedure in section 10.7.2. It does not include the pre-processing step: checking how good the real training set is at predicting cancer in a cross-validation framework (section 10.7.1). It does not cover the post-processing step either: GAN evaluation and how good the synthesized training set is at predicting cancer in the same cross-validation framework. This part of the code is covered in section 10.7.3. It is assumed that all the GAN models have been created and compiled, with the hyperparameters discussed in section 10.4.2.1. So this section only covers the `train` function used to train GAN. That said, it is the most important part of the code.

		Pregnanci	Glucose	BloodPres	SkinThickr	Insulin	BMI	DiabetesP	Age	Outcome
AVG	synth 1	1.82	119.34	68.49	27.25	141.86	33.52	1.53	30.40	0.46
	synth 2	3.00	124.20	73.55	28.89	137.10	35.70	1.54	34.26	0.42
	copula	3.07	121.30	70.64	29.30	153.85	33.29	0.50	30.13	0.33
	real	3.30	122.63	70.66	29.15	156.06	33.09	0.52	30.86	0.33
MIN	synth 1	-5.01	26.22	13.35	4.04	14.41	7.72	0.20	2.29	0.00
	synth 2	-3.08	16.41	14.94	7.16	1.69	9.15	-0.71	8.03	0.00
	copula	0.00	62.37	28.42	7.48	17.49	18.76	0.09	21.00	0.00
	real	0.00	56.00	24.00	7.00	14.00	18.20	0.09	21.00	0.00
MAX	synth 1	13.31	355.83	194.77	86.79	662.69	95.30	4.22	75.99	1.00
	synth 2	15.67	304.61	154.16	91.65	745.49	89.84	3.63	87.25	1.00
	copula	14.83	197.93	110.00	60.03	602.11	58.01	2.30	72.57	1.00
	real	17.00	198.00	110.00	63.00	846.00	67.10	2.42	81.00	1.00
Stdev	synth 1	2.85	56.02	35.53	16.54	115.73	17.46	0.63	13.74	0.50
	synth 2	3.37	46.89	25.06	13.88	96.11	13.36	0.73	14.99	0.49
	copula	2.85	31.57	11.52	10.41	112.60	7.13	0.32	9.22	0.47
	real	3.21	30.86	12.50	10.52	118.84	7.03	0.35	10.20	0.47
p.25	synth 1	0.04	79.11	42.47	14.71	58.77	20.15	1.09	20.40	0.00
	synth 2	0.62	88.09	55.71	18.13	66.24	25.77	1.02	23.42	0.00
	copula	1.00	97.75	64.00	21.00	76.00	28.70	0.27	23.00	0.00
	real	1.00	99.00	62.00	21.00	76.75	28.40	0.27	23.00	0.00
p.75	synth 1	3.64	149.07	88.13	36.65	187.51	43.08	1.88	38.94	1.00
	synth 2	4.94	156.80	88.59	38.04	185.61	44.81	2.01	42.15	1.00
	copula	4.02	142.25	78.00	36.37	192.27	37.22	0.67	35.03	1.00
	real	5.00	143.00	78.00	37.00	190.00	37.10	0.69	36.00	1.00

Figure 10.3: Summary statistics, medical dataset (synth 1 and 2 correspond to GAN)

The following steps are repeated for each epoch in the `train` function:

- Step 1: update the discriminator: get a new sample (half batch) from the real data and assign these points to `label=1`; get a new latent data sample (half batch, random Gaussian vectors) to generate fake data and assign these points to `label=0`. The fake sampling function also maps the latent data into the space of the real data via the instruction `X=generator.predict(x_input)`. Here `x_input` represents the latent data, and `X` the mapped version. The `train_on_batch` function (one call for the real sample, one call for the fake one) also returns the losses for each data label (fake / real). Note that the discriminator is set to "non-trainable".
- Step 2: update the generator: get a full sample (full batch) of latent data, assigned this time to `label=1` to train the generator. Training aims at minimizing over time (on average) the loss function `g_loss` (an average of the `d_loss` values returned by the discriminator) until an equilibrium is reached: a local minimum in all likelihood. Note that `g_loss` oscillates over time in order to not get stuck too quickly in a local minimum. The steepest gradient descent can result in this problem. So we use the Adam gradient descent (adaptive moment estimation) instead to avoid this issue.
- Step 3: If the epoch iteration is a multiple of 200, output the summary statistics to show progress, in particular how `g_loss` is decreasing over time, on average.

Note that the output layer of the discriminator is activated by the sigmoid function to discriminate between real and fake samples.

Correl	Pregnanci	1.00	0.38	0.20	0.23	0.17	0.32	0.14	0.82	0.17
synth 2	Glucose	0.38	1.00	0.64	0.63	0.72	0.75	0.82	0.67	0.67
	BloodPres	0.20	0.64	1.00	0.48	0.35	0.75	0.52	0.70	0.51
	SkinThickr	0.23	0.63	0.48	1.00	0.45	0.92	0.18	0.44	0.44
	Insulin	0.17	0.72	0.35	0.45	1.00	0.55	0.63	0.43	0.66
	BMI	0.32	0.75	0.75	0.92	0.55	1.00	0.37	0.68	0.55
	DiabetesP	0.14	0.82	0.52	0.18	0.63	0.37	1.00	0.43	0.56
	Age	0.82	0.67	0.70	0.44	0.43	0.68	0.43	1.00	0.46
	Outcome	0.17	0.67	0.51	0.44	0.66	0.55	0.56	0.46	1.00

		Pregnanci	Glucose	BloodPres	SkinThickr	Insulin	BMI	DiabetesP	Age	Outcome
Correl	Pregnanci	1.00	0.13	0.22	0.05	0.00	-0.06	-0.02	0.56	0.25
copula	Glucose	0.13	1.00	0.27	0.25	0.62	0.25	0.20	0.36	0.57
	BloodPres	0.22	0.27	1.00	0.23	0.15	0.29	-0.02	0.26	0.21
	SkinThickr	0.05	0.25	0.23	1.00	0.22	0.67	0.13	0.15	0.26
	Insulin	0.00	0.62	0.15	0.22	1.00	0.25	0.21	0.16	0.33
	BMI	-0.06	0.25	0.29	0.67	0.25	1.00	0.13	0.12	0.25
	DiabetesP	-0.02	0.20	-0.02	0.13	0.21	0.13	1.00	0.05	0.22
	Age	0.56	0.36	0.26	0.15	0.16	0.12	0.05	1.00	0.36
	Outcome	0.25	0.57	0.21	0.26	0.33	0.25	0.22	0.36	1.00

		Pregnanci	Glucose	BloodPres	SkinThickr	Insulin	BMI	DiabetesP	Age	Outcome
Correl	Pregnanci	1.00	0.20	0.21	0.09	0.08	-0.03	0.01	0.68	0.26
real	Glucose	0.20	1.00	0.21	0.20	0.58	0.21	0.14	0.34	0.52
	BloodPres	0.21	0.21	1.00	0.23	0.10	0.30	-0.02	0.30	0.19
	SkinThickr	0.09	0.20	0.23	1.00	0.18	0.66	0.16	0.17	0.26
	Insulin	0.08	0.58	0.10	0.18	1.00	0.23	0.14	0.22	0.30
	BMI	-0.03	0.21	0.30	0.66	0.23	1.00	0.16	0.07	0.27
	DiabetesP	0.01	0.14	-0.02	0.16	0.14	0.16	1.00	0.09	0.21
	Age	0.68	0.34	0.30	0.17	0.22	0.07	0.09	1.00	0.35
	Outcome	0.26	0.52	0.19	0.26	0.30	0.27	0.21	0.35	1.00

Figure 10.4: Correlation matrix, real vs synthetic: GAN (synth 2) and copula-based

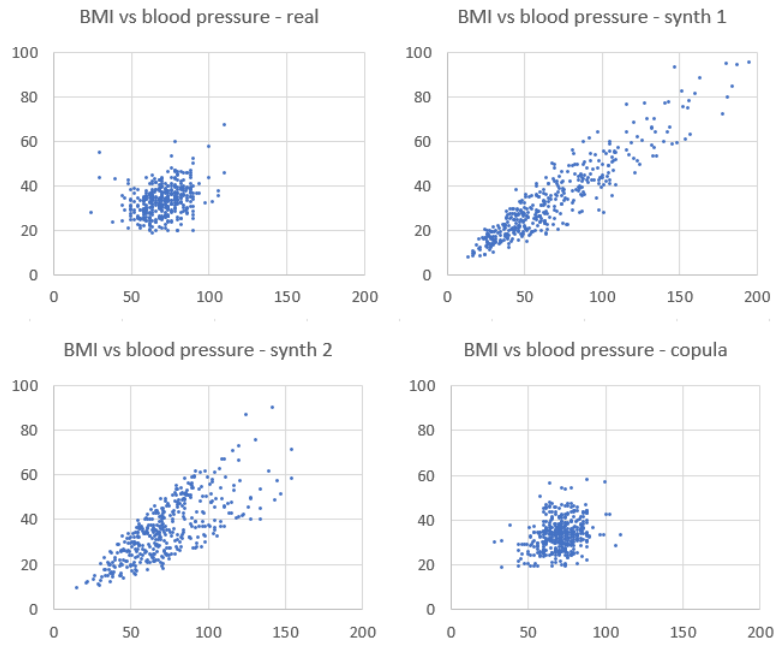

Figure 10.5: Copulas superior to GANs (synth 1, 2) to capture correlations in real data

10.4.3 Initial results

The first synthetized data using GAN on the medical dataset was disappointing. While GAN was able to replicate the mean, variance, and percentiles attached to each of the 9 features, it failed at replicating the

correlation structure. In addition, GAN was very sensitive to the seed (denoted as `seed` in the code). Also, even for a single gradient path started with a specific seed, the oscillations in the loss function over successive epochs, and thus the quality of the synthetized data, were still volatile even after 5000 epochs. I present the initial results here. It originates from a piece of code widely distributed over the Internet. I show in section 10.4.5 how to significantly improve the algorithm using front-end modifications, with little changes to the hyperparameters.

The left plot in Figure 10.2 shows the volatility in the loss function – the orange curve. In the same figure, the contrast between the left and right plot shows the huge impact of the seed on the final results. In Figures 10.3, 10.4 and 10.5, "synth 1" represents the initial version of GAN, while "synth 2" corresponds to the enhanced version. Even the enhanced version is inferior to copulas to reconstruct the correlation structure. However, GAN, even with the initial version, does a decent job at reconstructing the statistical summaries of most features (mean, variance, percentiles $p_{.25}$ and $p_{.75}$). More results are in the spreadsheet `diabetes_synthetic.xlsx`, available here on GitHub.

10.4.4 Fine-tuning the hyperparameters

You can use a back-end or front-end approach to fine-tune the hyperparameters and other GAN components, or a combination of both. The back-end strategy consists of modifying components that are buried more deeply in the architecture, such as the loss function, the number and type of layers, the type of neural network (sequential here), the gradient descent method (Adam here), the size of the batches and the ratio when splitting batches into real versus fake, the dimension and type of random deviates for the latent variables (Gaussian here, with dimension about the same as the number of features), the Keras metric used in the compile step, the learning rate, the type of activation function, and so on. I kept the original settings as found here and elsewhere, except for the learning rate and number of epochs.

Instead, I focused on front-end modifications. In particular, the enhanced version of my implementation produces a full synthetic dataset at each epoch, and computes the fit with the real data each time. It barely increases the amount of time needed to run a full GAN cycle. The fit is measured as the correlation matrix distance between the real and synthesized data. This metric is always between 0 and 1, with 0 being best. The goal was to replicate the correlation structure in the real dataset, thus the choice of this particular metric. The final synthetic data is the one obtained at the epoch where the correlation matrix distance is best (minimum). In addition, it must not come from an early epoch. For instance if the number of epochs id 10,000, I check the correlation matrix distance starting at epoch 7500.

In addition, the seed is an integral and important part of my algorithm. I made the results replicable, so if you run the program twice with the same seed, you will get the same results, unlike in most other implementations. Then, I test various seeds and pick up the one that produces the best results.

10.4.5 Enhanced GAN: methodology and results

To achieve better results, I explained how to process missing data separately, or applying a different GAN to specific segments of your population. Or a different Gan for each group of features resulting from feature clustering, as discussed in section 7.2.1.

Transforming or normalizing your data (for instance, decorrelate) may also lead to better synthetization. For instance, say your real data X is an $n \times m$ array with n rows – the observations – and m columns – the features. Assume that all the features have been normalized, thus having zero mean and unit variance. You can transform X to obtain $Y = XW$, where $\text{Cov}[Y] = W^T C_X W$ is a $m \times m$ diagonal matrix, ^{T} denotes the transposition operator, $C_X = \text{Cov}[X]$ and W has size $m \times m$. The transformed data Y consists of uncorrelated features. To achieve this goal take $W = C^{-1/2}$. There are multiple possible square roots, and this transformation is discussed in section 10.3.2. You can use an iterative algorithm to compute the matrix square root. Then synthesize Y (instead of X) and let Z be the resulting data. Your final (un-transformed) synthesized data is $X' = ZW^{-1}$, with the exact same correlation matrix as your real data X. This procedure is known as decorrelation [Wiki], followed by recorrelation.

However, the easiest solution is as follows. The GAN algorithm is very sensitive to the seed, which determines the initial configuration. In Figure 10.2, I compare two trajectories of the gradient descent based on two different seeds. Clearly, `seed=103` does a much better job than `seed=102`, attaining and staying in regions of lower loss much faster than `seed=102`. Thus the solution consists in trying different seeds. Not only that, but even with a same seed, the iterates (called epochs) oscillate wildly. In short, you could get a much better synthetization if you stop after 9800 epochs rather than (say) 10,000. The problem is further compounded by the fact that the loss function may achieve an optimization goal different from what you are looking for.

I address these issues in my enhanced version of GAN. To use it, set `mode='Enhanced'` in the Python code in section 10.7.2. Given one instance of GAN corresponding to a specific seed, it will retain the best

synthetic data (in other words, the best model produced by Keras) based on a distance function of your choice, rather than the one obtained at the last epoch and very dependent on the loss function. In my code, I was interested in synthetic data good a mimicking the correlation structure present in the real dataset, so I wrote my own function `gan_distance`, measuring the correlation distance between real and synthetic data at each epoch. It is based on the correlation matrix distance. Of course, you can modify that function to meet your own needs.

The enhancement techniques described so far are front-end: they do not modify the internal components of GAN. They are also easy to understand and implement, contributing to explainable AI. But you can also dig into the GAN black-box internals and modify some of the low-level components. This is facilitated to some extend by the Keras library, which offers some tools, for instance to customize the loss function. These back-end enhancements require more knowledge about how GANs work. You can write your own function `custom_distance` and have Keras "digest" it by choosing the option `model.compile(metrics=[custom_distance])` in your GAN model. See additional documentation here and here. Another possibility is to use an adaptive learning rate: see how to do it here. Finally, being able with reinforcement learning [Wiki] to reward configurations minimizing your own front-end distance function (rather than the default loss function) would be helpful, see [126]. By configuration, I mean the updated model and its set of updated weights obtained at the end of each epoch.

To summarize, the enhanced version of my implementation has the following upgrades:

- Replicable results
- Missing data treated separately
- Run multiple versions each with a different seed, use the best version
- Binary data: 0 and 1 processed with two different GANs (available in future version)
- Stop when your customized distance between real and synthetic data is minimum

The last feature requires `mode='Enhanced'` in the Python code. The increased performance of the enhanced version can be seen in the Figure 10.2, comparing standard (left) with enhanced mode (right). Also, the GAN synthetization in Figure 10.6 (right plot) uses the enhanced mode. It features an example on tabular data where GAN outperforms copulas. An additional upgrade is to blend copula methods with GAN. This is done in the SDV library: see code in section 10.4.1. Finally, applying GAN on decorrelated data (followed by a re-correlation step) as discussed at the beginning of this section, is guaranteed to preserve the exact correlation structure in the real data. This operation is fully reversible.

10.5 Comparing GANs with the copula method

On the medical data set, the copula method performs better as illustrated in Figures 10.3 and 10.4, and it is a lot faster. Unlike my copula method in section 10.2.1, many GAN implementations do not produce replicable results. However, this problem is solved in my implementation in section 10.7. Also GAN is very sensitive to the initial configuration (the seed), and oscillations from one epoch to the next one are rather large, even after 10,000 epochs. This latter issue may actually be an advantage: trying different seeds and/or using a stopping rule based on the quality of the synthetisation in any given epoch, leads to substantial improvements.

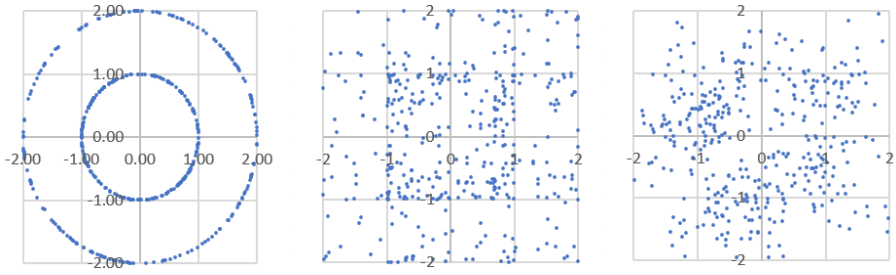

Figure 10.6: Real data (left), copula (middle) and GAN synthetization (right)

GAN has many hyperparameters that can be fine-tuned, even the loss function. This can lead to overfitting and makes the method less suitable as a black-box, compared to the parameter-free copula technique. Copulas are also less sensitive to outliers and small modifications of the real data, at least in this context (tabular data) and when using a parameter-free method based on empirical quantiles. But unlike GAN, they may not be able to generate synthetic data outside the range of observations. There are solutions to this problem: noise injection, or using parametric rather than empirical quantiles. Parametric quantiles are obtained by fitting a

feature or pair of features to a known probability distribution such as a mixture of Gaussians (GMM). It can also lead to overfitting. A nice feature of copulas is that it easily works with a mix of categorical, ordinal and continuous features.

Another issue with GAN, on this particular dataset, is the fact that the feature correlations in the synthetic data are exaggerated. This is true in the early epochs, and this phenomenon is attenuated in the last epochs, but it is still strongly noticeable, for instance on the left plot in Figure 10.2.

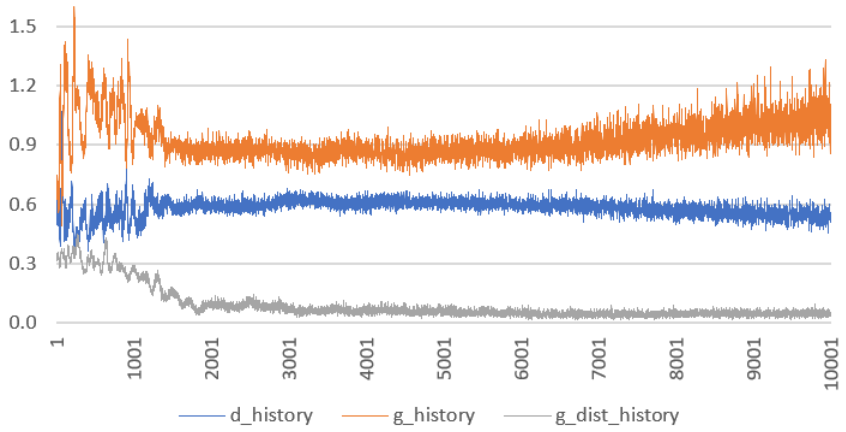

Figure 10.7: Loss function (orange) and distance (grey), circle dataset

The superiority of copulas, as seen in Figure 10.3 and 10.4, is due to the goal being achieved here: mimicking the correlation structure in the real data. Indeed, copulas are perfect at that. But what if the goal is different, or if the correlation matrix fails to capture the patterns in the real data? I tried with an artificial example, where most of the feature correlations are zero, but with strong non-linear dependencies instead. The dataset in question has 9 features; the last one is also a binary response for classification purposes, as in the medical dataset. The first two features represent points lying on two concentric circles: see Figure 10.6. It is trivial to synthesize the whole 9-D dataset with any method. However, I use it for illustration purposes as some real-life datasets have similar undetected or invisible patterns buried in very high dimensions.

In this case, it turns out that GAN does a better job. Both GAN and copula generate the correct correlation structure, though copula fails to recognize the circular patterns. Also, GAN iterations are very stable in this example, compared to the medical dataset. The copula method used in this example is based on two copulas, one for each group: the two concentric circles correspond to the two groups. This is not the case for GAN which is somewhat at a disadvantage, because of using the same model for both groups.

I computed the correlation between $X_1^2 + X_2^2$ (based on the first two features) and the binary response X_9. In the real data consisting of 400 observations, by design it is exactly 1 even though the correlation between X_1 and X_2 is zero. The copula method yields 0.014, and GAN yields a dramatic improvement with a value of 0.723, much closer to 1. Even when using a separate copula for each group, copula yields a much better correlation of 0.676 but still worse than GAN, even though GAN is based on a single model for both groups. Another interesting correlation is between X_1 and the response X_9. In the real dataset, the value is 0.067. The copula yields 0.128, and GAN yields 0.070. So GAN is slightly better. Given the way the real dataset was built, the true value would be zero if it had an infinite number of observations. More correlations are displayed in Table 10.2, and the full list is easy to obtain from the Excel spreadsheet.

Feature pair	Real data	Copula synth.	GAN synth.
$X_9, X_1^2 + X_2^2$	1.0000	0.0136	0.7235
X_1, X_9	0.0662	0.1281	0.0700
X_1, X_2	0.0641	0.1069	0.0660
X_1, X_3	1.0000	1.0000	0.9976
X_2, X_3	0.0641	0.1069	0.0495
$X_1, X_1^2 + X_2^2$	0.0662	0.1906	0.1186
X_1, X_5	−0.0278	−0.0278	−0.0047

Table 10.2: Correlations on 9D circle dataset: real vs copula and GAN

I stopped GAN at epoch 7727 which achieves the minimum overall correlation matrix distance of 0.017, a very good performance since the best possible value is zero, and the worst case is one. Epoch 10001 (the last one) yields 0.036 and epoch 9998 yields 0.057: it shows the benefit of using the enhanced version of GAN to capture the 0.017 minimum. The evolution of this GAN system is pictured in Figure 10.7. The labels `d_history`, `g_history`, `g_dist` are as in the Python code with "d" standing for the discriminator model, and "g" standing for the generator model in GAN (the one that creates the synthetization). The details are in my spreadsheet `circle8d.xlsx` on GitHub, here.

Note that even if GAN is not as good as copulas at replicating the correlation structure in the medical dataset, it is possible to first decorrelate the data, then apply GAN (or any method!) and then re-correlate, as explained in section 10.4.5. With this transformation, any synthetization algorithm that generates uncorrelated data will perfectly replicate the correlations found in the real data, after the re-correlation step.

10.5.1 Conclusion: getting the best out of copulas and GAN

I already discussed how to improve GANs in the context of tabular data, for instance by applying GAN to the decorrelated real data, or using your own distance metric or loss function, fine-tuning the learning rate, or using a faster version of the gradient descent such as LightGBM. Some improvements apply both to GANs and copulas: using a separate GAN model or copula for specific groups of observations, or for specific groups of features based on feature clustering. Or testing 10 different GANs (using different seeds) or 10 different copulas: the latter is a lot faster. Some implementations blend GAN and copulas. See for instance the CopulaGAN module in the SVD library.

To improve copulas methods specifically, you can replace the parameter-free empirical quantiles by quantiles from a parametric family of distributions, fit to the data, with parameters estimated on the real data. For instance, a Gaussian mixture model (GMM) for features with multimodal distribution. Then generate synthetic data using an iterative process based on the Hellinger distance. This distance measures the fit between the real data and the current synthesized version. And proceed iteratively as in GAN: successive iterations are obtained following the gradient path of the Hellinger distance, viewed as as multivariate function of the parameters of your model. In essence, this is very similar to the GAN approach, and can be done with or without neural networks.

In other words, you can improve GANs by integrating them with copulas and follow a gradient path that leads to an optimum of some discriminating function. And you can improve copulas by using a gradient descent algorithm (or stepwise procedure focusing on 2 parameters at a time) to navigate the parameter space until you optimize the Hellinger distance. In the end, the two techniques with the respective improvements may not be that different, especially when using multivariate parametric distributions spanning across multiple features, for the copula.

10.6 Data synthetization explained in one picture

Figure 10.8 summarizing many of the elements discussed in this book, 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.

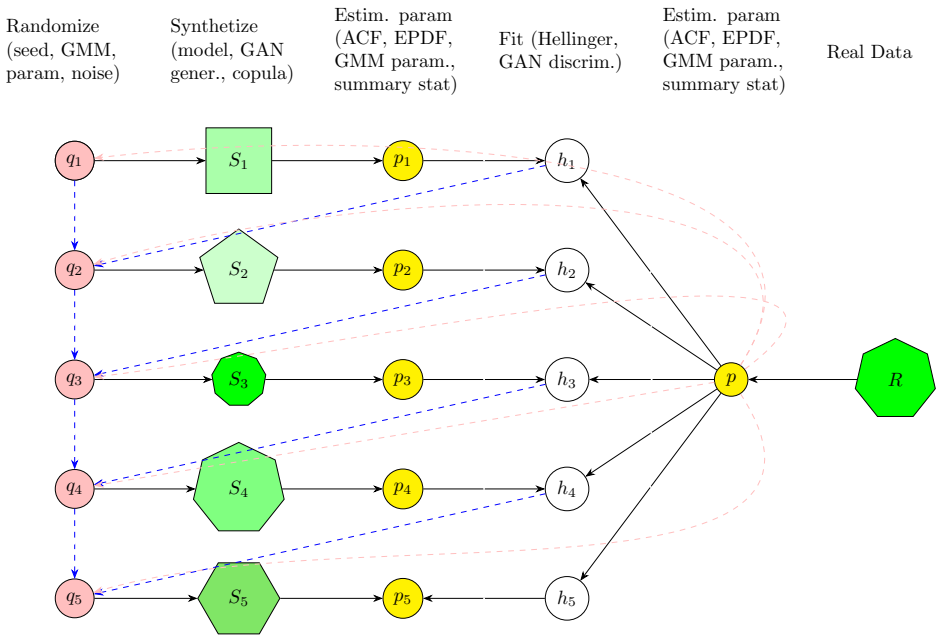

Figure 10.8: Data synthetization: general schema

10.7 Python code: GAN to synthesize medical data

I broke down the program into three pieces. First, reading the data and removing observations with missing values. During this step, I also run a classification algorithm (random forest) on the real data, as the goal is to discriminate between patients likely to get cancer, from the other ones. The rightmost column in the tabular data set, called `Outcome`, is the cancer indicator (1 = yes, 0 = no).

The second step is the core of the GAN procedure, including the production of synthetic data. Finally, the last part performs model evaluation – the fit between real and synthetic data – using the TableEvaluator library my matrix correlation distance defined in step 2. In the last part, I classify again the data with the random classifier, but this time the synthesized data, for comparison purposes with the classification on the real data obtained in the first step.

To run in enhanced mode, set `mode='Enhanced'`. The full program named `GAN_diabetes.py` is also on my GitHub repository, here. The real dataset `diabetes.csv` can be found here.

10.7.1 Classification problem

This step reads the data, removes observations with missing values, and performs a classification on the real data. It also imports all the libraries needed. and eliminates all sources of uncontrollable randomness by using a seed for all the random number generators involved (native Python, TensorFlow, Numpy). This leads to replicable results. The hyperparemeter `learning_rate` is also initialized here. You may need the most recent version of Numpy, TensorFlow and Pip.

```
import numpy as np
import pandas as pd
import os
import matplotlib.pyplot as plt
import random as python_random
from tensorflow import random
from keras.models import Sequential
from keras.layers import Dense
from keras.optimizers import Adam # type of gradient descent optimizer
from numpy.random import randn
from matplotlib import pyplot
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier
from sklearn import metrics

data = pd.read_csv('diabetes.csv')
```

```
# data located at https://github.com/VincentGranville/Main/blob/main/diabetes.csv

# rows with missing data must be treated separately: I remove them here
data.drop(data.index[(data["Insulin"] == 0)], axis=0, inplace=True)
data.drop(data.index[(data["Glucose"] == 0)], axis=0, inplace=True)
data.drop(data.index[(data["BMI"] == 0)], axis=0, inplace=True)
# no further data transformation used beyond this point
data.to_csv('diabetes_clean.csv')

print (data.shape)
print (data.tail())
print (data.columns)

seed = 102 # to make results replicable
np.random.seed(seed) # for numpy
random.set_seed(seed) # for tensorflow/keras
python_random.seed(seed) # for python

adam = Adam(learning_rate=0.001) # also try 0.01
latent_dim = 10
n_inputs = 9 # number of features
n_outputs = 9 # number of features


#--- STEP 1: Base Accuracy for Real Dataset

features = ['Pregnancies', 'Glucose', 'BloodPressure', 'SkinThickness', 'Insulin',
    'BMI', 'DiabetesPedigreeFunction', 'Age']
label = ['Outcome'] # OutCome column is the label (binary 0/1)
X = data[features]
y = data[label]

# Real data split into train/test dataset for classification with random forest

X_true_train, X_true_test, y_true_train, y_true_test = train_test_split(X, y,
    test_size=0.30, random_state=42)
clf_true = RandomForestClassifier(n_estimators=100)
clf_true.fit(X_true_train,y_true_train)
y_true_pred=clf_true.predict(X_true_test)
print("Base Accuracy: %5.3f" % (metrics.accuracy_score(y_true_test, y_true_pred)))
print("Base classification report:\n",metrics.classification_report(y_true_test,
    y_true_pred))
```

10.7.2 GAN method

The main function is `train`. Adding layers to the networks, combining the discriminator and generator models of GAN, selecting the loss functions and so on, and compiling the models, is done in the satellite functions defined here. In addition, my matrix correlation distance function is defined in this step. It is heavily used in the enhanced version, when `mode=='Enhanced'`. The last instruction saves the synthesized data `data_fake` to a CSV file.

```
#--- STEP 2: Generate Synthetic Data

def generate_latent_points(latent_dim, n_samples):
   x_input = randn(latent_dim * n_samples)
   x_input = x_input.reshape(n_samples, latent_dim)
   return x_input

def generate_fake_samples(generator, latent_dim, n_samples):
   x_input = generate_latent_points(latent_dim, n_samples) # random N(0,1) data
   X = generator.predict(x_input,verbose=0)
   y = np.zeros((n_samples, 1)) # class label = 0 for fake data
   return X, y
```

```
def generate_real_samples(n):
   X = data.sample(n) # sample from real data
   y = np.ones((n, 1)) # class label = 1 for real data
   return X, y

def define_generator(latent_dim, n_outputs):
   model = Sequential()
   model.add(Dense(15, activation='relu', kernel_initializer='he_uniform',
       input_dim=latent_dim))
   model.add(Dense(30, activation='relu'))
   model.add(Dense(n_outputs, activation='linear'))
   model.compile(loss='mean_absolute_error', optimizer=adam,
       metrics=['mean_absolute_error']) #
   return model

def define_discriminator(n_inputs):
   model = Sequential()
   model.add(Dense(25, activation='relu', kernel_initializer='he_uniform',
       input_dim=n_inputs))
   model.add(Dense(50, activation='relu'))
   model.add(Dense(1, activation='sigmoid'))
   model.compile(loss='binary_crossentropy', optimizer=adam, metrics=['accuracy'])
   return model

def define_gan(generator, discriminator):
   discriminator.trainable = False # weights must be set to not trainable
   model = Sequential()
   model.add(generator)
   model.add(discriminator)
   model.compile(loss='binary_crossentropy', optimizer=adam)
   return model

def gan_distance(data, model, latent_dim, nobs_synth):

   # generate nobs_synth synthetic rows as X, and return it as data_fake
   # also return correlation distance between data_fake and real data

   latent_points = generate_latent_points(latent_dim, nobs_synth)
   X = model.predict(latent_points, verbose=0)
   data_fake = pd.DataFrame(data=X, columns=['Pregnancies', 'Glucose', 'BloodPressure',
       'SkinThickness', 'Insulin', 'BMI', 'DiabetesPedigreeFunction', 'Age', 'Outcome'])

   # convert Outcome field to binary 0/1
   outcome_mean = data_fake.Outcome.mean()
   data_fake['Outcome'] = data_fake['Outcome'] > outcome_mean
   data_fake["Outcome"] = data_fake["Outcome"].astype(int)

   # compute correlation distance
   R_data   = np.corrcoef(data.T) # T for transpose
   R_data_fake = np.corrcoef(data_fake.T)
   g_dist = np.average(abs(R_data-R_data_fake))
   return(g_dist, data_fake)

def train(g_model, d_model, gan_model, latent_dim, mode, n_epochs=10000, n_batch=128,
    n_eval=200):

   # determine half the size of one batch, for updating the discriminator
   half_batch = int(n_batch / 2)
   d_history = []
   g_history = []
   g_dist_history = []
   if mode == 'Enhanced':
      g_dist_min = 999999999.0

   for epoch in range(0,n_epochs+1):
```

```
        # update discriminator
        x_real, y_real = generate_real_samples(half_batch) # sample from real data
        x_fake, y_fake = generate_fake_samples(g_model, latent_dim, half_batch)
        d_loss_real, d_real_acc = d_model.train_on_batch(x_real, y_real)
        d_loss_fake, d_fake_acc = d_model.train_on_batch(x_fake, y_fake)
        d_loss = 0.5 * np.add(d_loss_real, d_loss_fake)

        # update generator via the discriminator error
        x_gan = generate_latent_points(latent_dim, n_batch) # random input for generator
        y_gan = np.ones((n_batch, 1))           # label = 1 for fake samples
        g_loss_fake = gan_model.train_on_batch(x_gan, y_gan)
        d_history.append(d_loss)
        g_history.append(g_loss_fake)

        if mode == 'Enhanced':
           (g_dist, data_fake) = gan_distance(data, g_model, latent_dim, nobs_synth=400)
           if g_dist < g_dist_min and epoch > int(0.75*n_epochs):
             g_dist_min = g_dist
             best_data_fake = data_fake
             best_epoch = epoch
        else:
           g_dist = -1.0
        g_dist_history.append(g_dist)

        if epoch % n_eval == 0: # evaluate the model every n_eval epochs
           print('>%d, d1=%.3f, d2=%.3f d=%.3f g=%.3f g_dist=%.3f' % (epoch, d_loss_real,
               d_loss_fake, d_loss, g_loss_fake, g_dist))
           plt.subplot(1, 1, 1)
           plt.plot(d_history, label='d')
           plt.plot(g_history, label='gen')
           # plt.show() # un-comment to see the plots
           plt.close()

    OUT=open("history.txt","w")
    for k in range(len(d_history)):
       OUT.write("%6.4f\t%6.4f\t%6.4f\n" %(d_history[k],g_history[k],g_dist_history[k]))
    OUT.close()

    if mode == 'Standard':
       # best synth data is assumed to be the one produced at last epoch
       best_epoch = epoch
       (g_dist_min, best_data_fake) = gan_distance(data, g_model, latent_dim,
           nobs_synth=400)

    return(g_model, best_data_fake, g_dist_min, best_epoch)

#--- main part for building & training model

discriminator = define_discriminator(n_inputs)
discriminator.summary()
generator = define_generator(latent_dim, n_outputs)
generator.summary()
gan_model = define_gan(generator, discriminator)

mode = 'Enhanced' # options: 'Standard' or 'Enhanced'
model, data_fake, g_dist, best_epoch = train(generator, discriminator, gan_model,
    latent_dim, mode)
data_fake.to_csv('diabetes_synthetic.csv')
```

10.7.3 GAN Evaluation and post-classification

Evaluates the quality of the synthetic data with the TableEvaluator library and `g_dist`, the matrix correlation distance obtained in the previous step. Also, performs classification, but this time on the synthetic data, to compare with the results obtained on the real data in Step 1.

```
#--- STEP 3: Classify synthetic data based on Outcome field

features = ['Pregnancies', 'Glucose', 'BloodPressure', 'SkinThickness', 'Insulin',
    'BMI', 'DiabetesPedigreeFunction', 'Age']
label = ['Outcome']
X_fake_created = data_fake[features]
y_fake_created = data_fake[label]
X_fake_train, X_fake_test, y_fake_train, y_fake_test = train_test_split(X_fake_created,
    y_fake_created, test_size=0.30, random_state=42)
clf_fake = RandomForestClassifier(n_estimators=100)
clf_fake.fit(X_fake_train,y_fake_train)
y_fake_pred=clf_fake.predict(X_fake_test)
print("Accuracy of fake data model: %5.3f" % (metrics.accuracy_score(y_fake_test,
    y_fake_pred)))
print("Classification report of fake data
    model:\n",metrics.classification_report(y_fake_test, y_fake_pred))


#--- STEP 4: Evaluate the Quality of Generated Fake Data With g_dist and Table_evaluator

from table_evaluator import load_data, TableEvaluator

table_evaluator = TableEvaluator(data, data_fake)
table_evaluator.evaluate(target_col='Outcome')
# table_evaluator.visual_evaluation()

print("Avg correlation distance: %5.3f" % (g_dist))
print("Based on epoch number: %5d" % (best_epoch))
```

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, 172
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, 268
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, 277
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, 229, 277
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, 226, 227, 263, 266
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, 204, 268, 277
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, 277, 278
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, 278, 279
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, 150, 213, 216, 222, 228, 233, 235, 247
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, 277

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, 176, 192, 230

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, 259, 267, 277, 279

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, 143, 187, 188, 190, 197, 204, 279

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, 268, 277, 279

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, 205, 271, 272

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, 191, 278

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, 278

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, 277, 278

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, 277, 278

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, 270

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, 277, 279

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, 267, 269, 278

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, 278, 279

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, 149, 156, 273

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, 278, 279

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 279

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, 149, 162, 168, 176, 190, 197, 204, 264, 273, 277

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, 204, 268, 277, 279

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, 204, 268, 277, 278, 279

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