Towards Ground Truth Explainability on Tabular Data

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Abstract

In data science, there is a long history of using synthetic data for method development, feature selection and feature engineering. Our current interest in synthetic data comes from recent work in explainability. Today's datasets are typically larger and more complex - requiring less interpretable models. In the setting of *post hoc* explainability, there is no ground truth for explanations. Inspired by recent work in explaining image classifiers that does provide ground truth, we propose a similar solution for tabular data. Using copulas, a concise specification of the desired statistical properties of a dataset, users can build intuition around explainability using controlled data sets and experimentation. The current capabilities are demonstrated on three use cases: one dimensional logistic regression, impact of correlation from informative features, impact of correlation from redundant variables.

1. Introduction

The combination of large public datasets and novel machine learning architectures has provided state of the art predictive power in many diverse fields, such as computer vision and machine translation. These models are largely regarded as opaque *black-box* models. With their prevalence and increasing adoption, an active field of research is eXplainable Artificial Intelligence (XAI), which has sought to provide explanations for their predictions.

One avenue of research is on building interpretability into the model architecture (Kim et al., 2015; Canini et al., 2016;

Lee et al., 2019). We focus on the area *post hoc* explanations – which occurs after model training. Currently there is no one size fits all solution. The method of explanation depends on model type (Chen et al., 2018; Krakovna & Doshi-Velez, 2016; Grath et al., 2018), desired granularity (Ribeiro et al., 2016; Ibrahim et al., 2019; Dhurandhar et al., 2018; Bhatt et al., 2020a; van der Linden et al., 2019), and audience (Wachter et al., 2017; Bhatt et al., 2020b).

In support of the methods, there are a growing number of packages that seek to provide an umbrella of methods such as AIX360 (Arya et al., 2019), ELI5 (TeamHG-Memex, 2019), and Alibi (Klaise et al., 2020).

Early methods were focused on explaining image classifiers. The use of sensitivities of the output class based on the input image pixels, provides a visual and immediately interpretable explanation for the classifier's prediction. For tabular data, the intuitive visual nature of sensitivities is not a natural metaphor. Additionally, where as computer vision typically relies on correlations between pixels as features, for tabular data that can be detrimental (Aas et al., 2019).

An ongoing challenge in XAI is the lack of ground truth. To add to the landscape of XAI, and move towards ground truth explainability for tabular data, we provide a flexible synthetic data generation method allowing generation of arbitrarily complex data. The current implementation is focused on the task of binary classification.

The paper is structured as follows: previous work is discussed in Section 2, Section 3 presents the method used to construct the synthetic tabular data, and Section 4 shows some results from three use cases: one dimensional logistic regression, impact of correlation from informative features, and impact of correlation from redundant variables.

2. Previous work

Early use cases of synthetic data focused on the tasks of feature and model selection (Guyon, 2003). This method is available in the scikit-learn (Pedregosa et al., 2011) module $make\_classification$. An alternative method of generating tabular data for classification is to generate clusters and apply class labels to them.

Another approach is to model joint probability $P(\boldsymbol{X}, y)$

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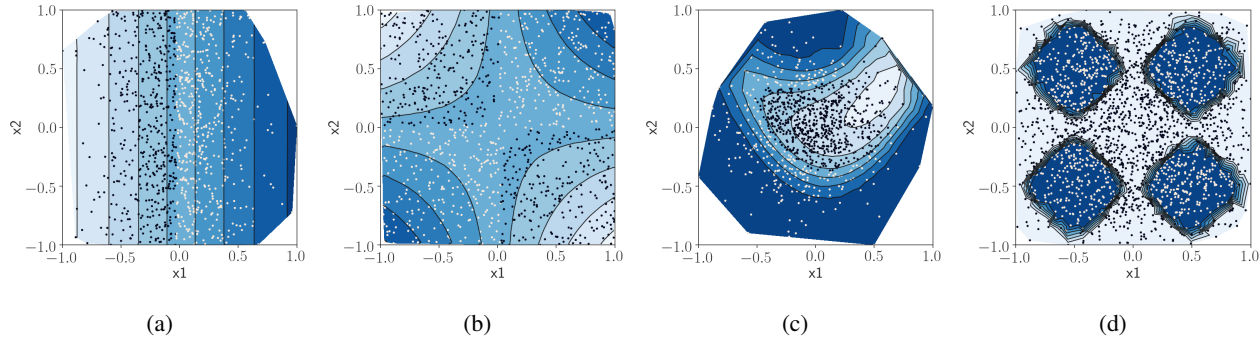
Figure 1. Sample datasets - (a) linear, (b) nonlinear, (c) rosenbrock function, and (d) rastrigin function. The background has contours of probability with a scatter plot of the sampled points, colored by class. The datasets in (a) and (b) will be used later for experiments in Section 4.

from an actual dataset. This can be helpful in dealing with sensitive data and as an aid in sharing data where there are privacy and regulatory restrictions on the use of actual data (Ping et al., 2017; Howe et al., 2017; Gonalves et al., 2020). Techniques used range from probabilistic models, to Bayesian networks, to generative adversarial neural networks (GANS). In finance, it is typical to use copulas. The theory of copulas has been developed considerably in mathematics, statistics, actuarial science, with significant interest in their application to finance (Genest et al., 2009), and their misuse may have led the financial crisis (Salmon, 2012). However, methods that mimic the statistics of other datasets are incapable of providing ground truth for explanations - since they lack the complete data generation process that imposes a functional dependence between X and y.

Our research is inspired from recent work in interpreting the image classifiers trained with a carefully crafted dataset that controls the relative feature importance (Yang & Kim, 2019). In this case, the model can be quantitatively evaluated in the form of known foreground and background images by providing ground truth of local feature importances.

We propose a similar method for tabular data. We use copulas to define the correlation structure and marginal distributions of the independent features. We specify the dependence of the underlying probability field as a symbolic expression. Binary class labels are assigned by setting a threshold probability. This method provides global explanations since we prescribe the coefficients of the terms in the symbolic expression. In some instances, where we build models only from informative features, we can provide ground truth local attributions.

Our contributions are providing a unique and flexible method for synthetic tabular data generation suitable for current model architectures and demonstration of its use in informative experiments highlighting that not all correlation in inputs change local attributions.

3. Synthetic data generation

The generation of synthetic data seeks a method to provide the joint probability $P(X, y)$ where X are the input features, and y is the output variable, and to draw samples from that joint distribution. From those samples, we will fit machine learned models that approximate the conditional probability $P(y|X)$ (via possibly black box models) and to provide explanations for those models.

We separate the input feature vectors, X, into three categories - informative, redundant, and nuisance features.

$$X = (X_I | X_r | X_n) \qquad (1)$$

Informative features, X_I, used to determine the binary labels, are specified by a copula. A multivariate distribution can be separated into a set of marginal distributions and the correlation structure between them. Copula theory is the mathematical framework of the separation of the correlation structure from the marginal distributions of the feature vectors. See (Jaworski et al., 2013; Nelsen, 1999) for further details. The current library supports any marginal distribution available in *scipy.stats*. The results for this paper use a multivariate Gaussian copula.

Redundant features, X_r, are a random linear combination of informative features. Nuisance features, X_n are random uncorrelated vectors drawn from the interval [-1, 1] which are useful as benchmarks to set the lower bound on explainability. Being purely random and not contributing to the specification of the labels, any feature found to have lower importance than a nuisance feature should be subjected to further scrutiny and possibly removed from the model.

The final step in the process is to generate binary labels for the inputs. First, a scalar regression value is created from the informative features via a symbolic expression using the
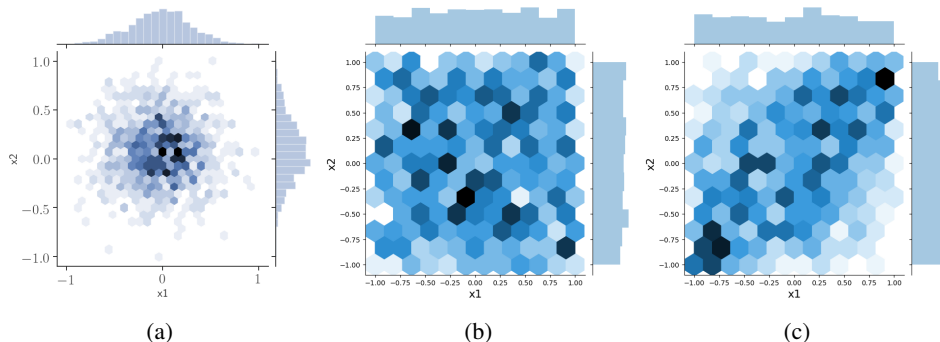
(a)   (b)   (c)

Figure 2. Joint probability plot for features x_1 and x_2 (a) with Gaussian marginals (b) with uniform marginals with no correlation and (c) uniform marginals with positive correlation.

sympy python module.

$$\vec{y}_{reg} = f(\mathbf{X}_I) \qquad (2)$$

$$h_k(y_{reg}) = \frac{1}{1 + e^{-k(y_{reg}-y_0)}} \qquad (3)$$

To generate binary classification probabilities, the regression value is squashed by a sigmoid to the range [0,1]. After setting a threshold probability, class labels are determined.

Additional post processing allows the addition of Gaussian noise to the informative features. A random seed can be specified so that repeated runs of a synthetic dataset yield the same values.

4. Experiments

This section demonstrates some of the capabilities of the synthetic tabular data through the process of modeling and providing local attributions via the SHAP library (Lundberg & Lee, 2017).

4.1. Logistic regression

The first synthetic data set is for two features, $x_1, x_2 \in [-1, 1]$, with no covariance and Gaussian marginal distributions for both. The joint probability plot is shown in Figure 2a.

The symbolic regression expression is $y = x_1$. The probability values and class labels are shown in Figure 1a. One thousand samples are generated.

The dataset is split 70/30 into a training and test set, with a logistic regression model fit to the training data. The AUC of the model is 99.8% and the coefficients of the model are $[11.98, 0.04]$. To provide local attributions, we fit a SHAP KernelExplainer to the training set with the results shown in Figure 3.
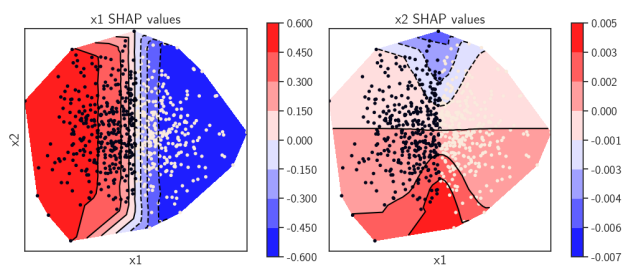

Figure 3. Contours of SHAP values for x_1 (left) and x_2 (right) for the simple 1-D logistic regression model.

The SHAP values for x_1 dominate by two orders of magnitude, roughly in keeping with the relative global importance found in the coefficients. Strong left to right symmetry is broken only in sparsely populated regions. Interesting to note that the SHAP values for x_2 also display symmetry from top to bottom - with the opposite sign of the coefficient.

4.2. Presence of correlation in informative features

We investigate the impact of correlation between the input features on model explanations. It is well known that the presence of correlation can alter a model's explanations, see for example (Breiman, 2001; Aas et al., 2019).

We again generate datasets for two features, $x_1, x_2 \in [-1, 1]$; the first with uniform marginal distributions, a baseline dataset with no correlation whose joint distribution can be seen in Figure 2b, and a second dataset, see Figure 2c with the covariance specified as:

$$cov = \begin{bmatrix} 1.0 & 0.5 \\ 0.5 & 1.0 \end{bmatrix}.$$

The symbolic regression expression for this experiment is:

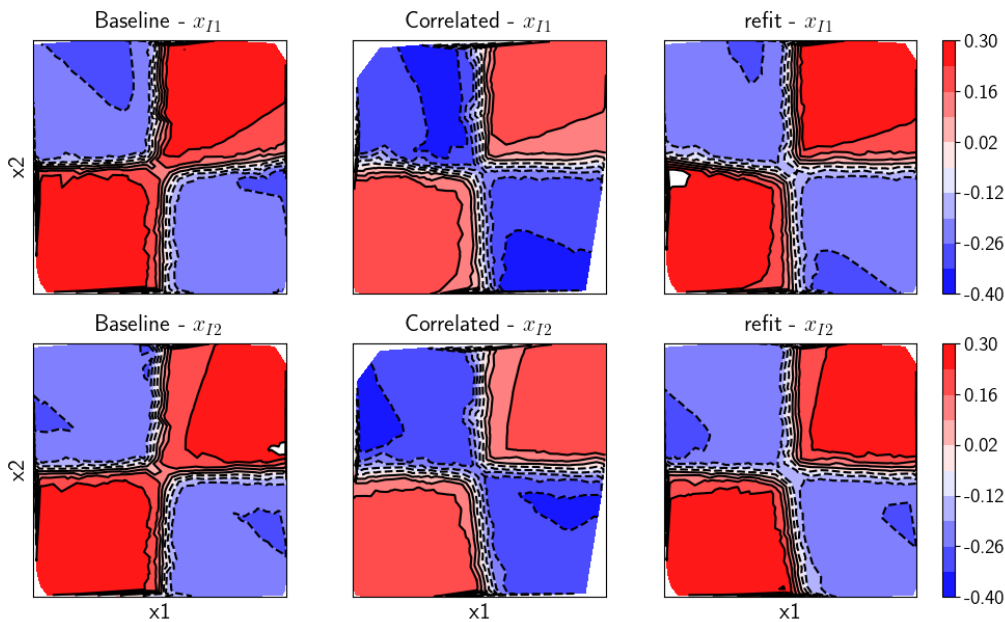$$y_{reg} = cos(x_1^2 \cdot \pi/180) - sin(x_2 \cdot \pi/180) + x_1 \cdot x_2$$

Figure 4. Contours of SHAP values for x_1 (top row) and x_2 (bottom row) for the baseline data and model (left), correlated model and data (center), and correlated model fit with baseline data (right).

We hold the probability field constant between the datasets. The probability values and class labels are shown in Figure 1b.

The dataset is split 70/30 into a training and test set, with a dense network with three hidden layers and a total of 255 weights in Tensorflow fit to the training data. The AUC of the resulting model is 100%. To provide local attributions, we fit a SHAP DeepExplainer to the training set with the results shown in Figure 4.

There is an apparent decrease in SHAP values in the presence of correlation in the input features. Recall that SHAP values are relative with respect to the expectation of the output. With correlation, their density is drawn out of quadrants 2 and 4, and placed in quadrants 1 and 3, leading to a higher expected predicted probability due to the imbalance of the class labels. If we account for that effect by refitting the explainer with the baseline data (which does not suffer the same level of imbalance), the SHAP values look essentially like those from the uncorrelated inputs (as shown in the last column of Figure 4)

In this context, the apparent effect of correlation is an artifact induced from the expectation of the correlated model predictions over the correlated training data – it is not a bias that the model has learned during training.

4.3. Presence of redundant variables

In contrast to the experiment in the previous section, this section considers the effect of correlation with unimportant features – since the redundant features are not explicitly used in the symbolic expression used to derive the binary labels. We reuse the baseline from the previous section. We create a second dataset by augmenting the baseline informative features with two redundant and two nuisance features.

The joint distribution of the informative features, the symbolic expression that maps the informative features to the binary labels all remain unchanged. We keep the same train/test split. The only change to the dense network is to increase the dimension of the input layer to accommodate the two redundant and two nuisance features.

Redundant features have a significant impact on SHAP's perception of feature importance. Summing the individual components of explanations for the redundant feature model does not recover the values obtained from the baseline model.

5. Conclusions

In this paper, we have described a method of generating synthetic tabular data utilizing copulas and symbolic expressions that provides users the ability to control the complexity of the resulting dataset. We have briefly demonstrated how the origin of correlation amongst inputs (informative vs redundant) influences model explainability. This method is a powerful investigative tool for data scientists, model developers, and explainable AI method developers.

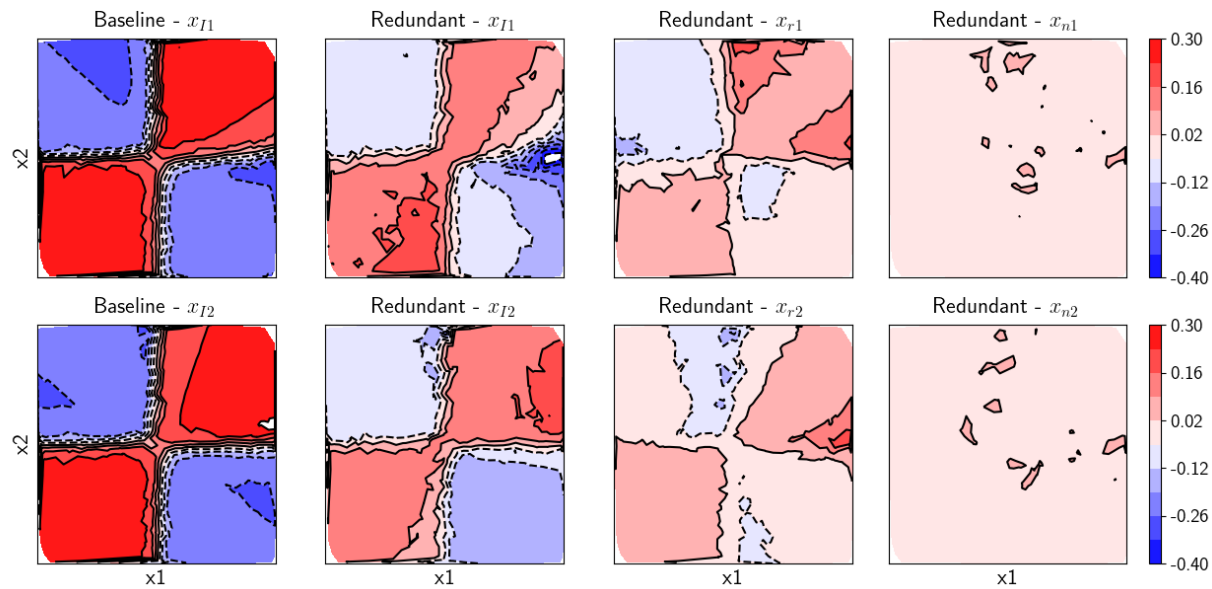Future work includes: further experimentation with more

Figure 5. Contours of SHAP values for x_1 (top row) and x_2 (bottom row) for the baseline data and model(left), redundant feature model for three components of explanation: informative, redundant, and nuisance.

complex data sets, bridging the gap between global explanations (provided by our symbolic expression) and local explanations, investigation of categorical and ordinal variables, as well as improving local attributions for tabular data.

At the time of publication, we were working on making the repository accessible. Please contact a corresponding author for further details.

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