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Stress Testing with GANs v2.4: Generating FHL based data

The current notebook implements our revised GAN model (WGAN-GP-Mixed) to generate data based on the FHL public dataset. The improved Generative Adversarial Network is able to work with highly structured multivariate distributions containing both continuous and discrete marginal distributions. The new model is able to overcome any gradient vanishing problems we encountered before and is based on the set of papers described below. The Federal Home Loan Bank Purchased Mortgage dataset is obtained through the Federal Housing Finance Agency and contains granular loan-level information of US-based mortgages. The dataset contains 82 variables, both continuous and discrete, and has some variables that exhibit a mixed distribution with a Dirac zero delta point. The dataset contains about 65.000 instances making it easily to digest in test settings. The high degree of variability in the data makes it especially challenging to learn the underlying manifold for our GAN model.

c

Setup:

Section 1.1 Setup working environment
 Section 2 The FHL dataset

- Section 3 Preprocessing of data

- Section 4 Implement a composite GAN NN

- Section 5 Training of the compiled GAN model

- Section 6 Evaluating the performance of our trained model

- Section 7 Evaluate the *similarity* between real and artificial distributions

- Section 8 Save the calibrated Generator and the synthetic dataset

Main papers utilized:

- Overview of GANs: GAN Google
- Seminal GAN paper of Goodfellow et al.: GAN Seminal paper
- Instability problems with GANs: Stabilizing GANs
- Wasserstein GAN to deal with vanishing gradients: WGAN
- Improved WGAN with Gradient Penalty: WGAN-GP
- How to add custom gradient penalty in Keras: WGAN and Keras and Change model.fit()
- Multi-categorical variables and GAN: Multi-categorical GAN
- Alternative to WGAN: DRAGAN
- Conditional DRAGAN on American Express dataset: DRAGAN & American Express
- Mulitvariate KL-divergence by KNN: KL by KNN
- Multivariate KL-divergence by KNN p2: KL by KNN

1.1 Environment variables

Connect to Google Colab Directory containing our repository (only executed on GColab)

```
[1]: # Initiate notebook (only to be ran once, or when kernel restarts)
activated_reload= False
activated_chdir= False
GCOLAB= False
```

```
[2]: if GCOLAB:
    from google.colab import drive
    import sys
    drive.mount('/content/gdrive/')
    sys.path.append('/content/gdrive/My Drive/Stress Testing with GANs/notebooks')
```

1.2 Settings & environment setup

```
[3]: # Settings for auto-completion: In case greedy is turned off and jedi blocks auto-completion
%config IPCompleter.greedy=True
%config Completer.use_jedi = False

# Autoreload modules: in case in-house libraries aren't finalised
if not activated_reload:
    activated_reload= True
    %load_ext autoreload
    %autoreload 2

# Set working directory for user to main project directory
import os
if not activated_chdir:
    activated_chdir= True
    os.chdir('...')
    print('Working directory: ', os.getcwd())
```

Working directory: C:\Users\ilias\Desktop\Stress Testing with GANs-Gdrive\Stress Testing with GANs

1.3 Import libraries (including in-house build modules)

```
[25]: # Standard libs
from datetime import datetime
from IPython.display import Latex, Markdown
import os
import functools
import operator

# External libs
from sklearn.preprocessing import LabelEncoder
from sklearn.preprocessing import OneHotEncoder
from sklearn.feature_selection import mutual_info_classif
from sklearn.feature_selection import mutual_info_regression
```

```
import plotly.express as px
from plotly.subplots import make_subplots
import plotly.graph_objects as go
import plotly.io as pio

# In-house libs
from src.GAN_functions import * # TODO: modularize source code
```

```
[5]: ## Global settings
     # Matplotlib
     import matplotlib.font_manager
     from matplotlib_inline.backend_inline import set_matplotlib_formats
    %config InlineBackend.figure_format = 'png'
    %matplotlib inline
     set_matplotlib_formats('pdf', 'png')
    plt.rcParams['savefig.dpi'] = 75
    plt.rcParams['figure.autolayout'] = False
    plt.rcParams['figure.figsize'] = 10, 6
     plt.rcParams['axes.labelsize'] = 18
    plt.rcParams['axes.titlesize'] = 20
     plt.rcParams['font.size'] = 16
    plt.rcParams['lines.linewidth'] = 2.0
     plt.rcParams['lines.markersize'] = 8
    plt.rcParams['legend.fontsize'] = 14
     plt.rcParams['text.usetex'] = False
     plt.rcParams['font.family'] = "serif"
     #plt.rcParams['font.serif'] = "cm"
    plt.rcParams['text.latex.preamble'] = r"\usepackage{subdepth}, \usepackage{type1cm}"
     # plotly
    pio.renderers.default = "notebook+pdf"
     # numpy
    np.set_printoptions(precision=2)
```

```
# Pandas thousand separator + 2 decimal rounding
pd.set_option('display.float_format', '{:,.2f}'.format)

# pandas latex
pd.set_option('display.notebook_repr_html', True)
def _repr_latex_(self):
    return "\begin{center} \n %s \n \\end{center}" % self.to_latex()
pd.DataFrame._repr_latex_ = _repr_latex_ # monkey patch pandas DataFrame to latex

# Surpress warnings
os.environ['TF_CPP_MIN_LOG_LEVEL'] = '2' #no info and warnings printed
import warnings
warnings.filterwarnings('ignore')
```

The Federal Housing Finance Agency dataset

2.1 Importing the FHL dataset

We have three general ways of importing the data:

- 1. Use a local environment and extract the data from the same environment
- 2. Use a cloud environment and extract data from the local environment
- 3. Use a cloud environment and extract data from the same cloud environment

2.1.1 Jupyter notebook on local environment

```
[6]: if not GCOLAB:
    filename= 'FHLbank.csv'
    path= os.path.join('data/raw', filename)
    FHL_bank = pd.read_csv(path)
```

2.1.2 Google Colab when importing dataset from local environment

```
[7]: if GCOLAB:
    # Import files module
    from google.colab import files
    # Upload FHL_bank dataset into GColab
```

```
FHL_bank = files.upload()
# Read the file
import io
FHL_bank = pd.read_csv(io.BytesIO(ppnr['FHLbank.csv']))
# Convert to the right data type
FHL_bank = FHL_bank.astype(dtype = 'float64')
```

2.1.3 Google Colab when importing dataset directly from Google Drive

```
[8]: if GCOLAB:
         # Read csv file into Colaboratory
         !pip install -U -q PyDrive
        from pydrive.auth import GoogleAuth
        from pydrive.drive import GoogleDrive
        from google.colab import auth
        from oauth2client.client import GoogleCredentials
         # Authenticate and create the PyDrive client
         auth.authenticate_user()
        gauth = GoogleAuth()
        gauth.credentials = GoogleCredentials.get_application_default()
        drive = GoogleDrive(gauth)
[9]: if GCOLAB:
         # Shareable link from the dataset in Google drive
        link= 'https://drive.google.com/file/d/11qeFxTx3MEZKhwowRWzUKTdYPpwvWDUd/view?usp=sharing'
         #we only need the id-key portion of the link
        id= '1lqeFxTx3MEZKhwowRWzUKTdYPpwvWDUd'
         # Import dataset
         downloaded = drive.CreateFile({'id':id})
        downloaded.GetContentFile('FHLbank.csv')
        FHL_bank = pd.read_csv('FHLbank.csv')
```

2.2 Brief overview of the dataset

The FHL dataset contains 65,703 mortgages granted within the US in 2018, with no missing values. The median borrower(s) total annual income is equal to \$95,000 USD, whereas the median family income of the immediate area where the house is purchased is only \$73,600 USD. The median interest rate is set to 4.63% whereas the average rate is slightly lower (4.55%) indicating that the interest rate is slightly left-skewed. When looking at the amount borrowed, we see that the median amount is equal to \$211,000 USD while the average amount is \$237,000 USD, indicating a right-skewed distribution. Moving on to the loan-to-value, we see that the interquartile ranges from 72% to 85%, with a mean value of 77%. The LTV value exceeds the 100% mark for a substantial amount of mortgages (about 2% of all mortgages).

```
[7]: # Missing values
print('Missing values:', FHL_bank.isnull().values.any())
# Quick overview of random set of variables within the dataset
display(FHL_bank.sample(n=12,axis='columns').head())
```

Missing values: False

	Race5	FedGuar	PrepayP	HOEPA	Bed2	Rent1	Corace4	BoEth	FeatureID	AssignedID	Product	Self
0	6	2	12/31/9999	2	98	999999999	6	3	999999999	2131406	1	2
1	6	2	12/31/9999	2	98	999999999	6	2	999999999	2131407	1	2
2	6	2	12/31/9999	2	98	999999999	6	2	999999999	2131408	1	2
3	6	2	12/31/9999	2	98	999999999	8	2	999999999	2131409	1	2
4	6	1	12/31/9999	2	98	999999999	8	2	999999999	2131410	1	2

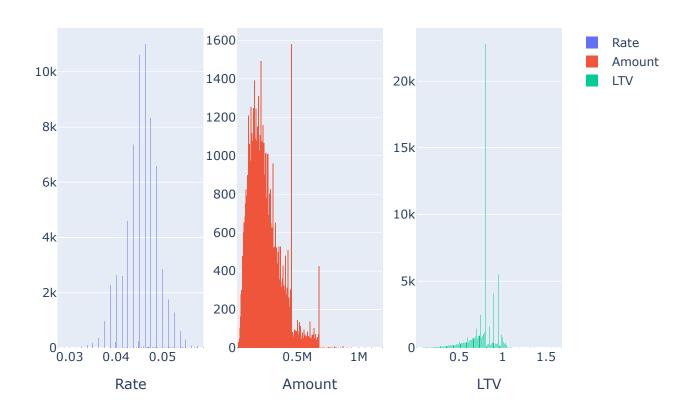
```
[8]: # Zoom into specific variables

cols= ['Income', 'CurAreY', 'LTV', 'Rate', 'Amount']

display(FHL_bank[cols].describe())
```

	Income	CurAreY	LTV	Rate	Amount
count	65,703.00	65,703.00	65,703.00	65,703.00	65,703.00
mean	112,688.93	75,020.09	0.77	0.05	237,562.64
std	102,115.05	13,510.58	0.15	0.00	132,077.09
min	11,004.00	18,600.00	0.01	0.03	10,400.00
25%	63,492.00	65,800.00	0.72	0.04	139,920.00
50%	95,000.00	73,600.00	0.80	0.05	211,000.00
75%	137,035.00	80,600.00	0.85	0.05	307,000.00
max	9,614,088.00	134,800.00	1.68	0.06	1,190,000.00

Histogram of Interest rate, Amount Borrowed and the LTV



2.3 Brief overview of the dataset: discrete distributions

When looking at discrete distributions, we see that multiple marginal distributions are highly imbalanced. The *purpose of the borrower* is in more than 99% of the cases either to purchase a new home or to refinance a current home, only .02% of borrowers enter a mortgage for a new construction. An imbalance is also seen when looking at the *number of borrower's for one mortgage*, with more than 99% of mortgages having either one or two underlying borrowers, and only a small percentile of mortgages (less than 1%) consist of three or four borrowers. The majorities of borrowers are identified as white (83%), about 10% of borrower's didn't provide their race information, and the remaining 7% is either Native, Asian, African American or Hawaiian.

```
[10]: # Compute relative frequencies
cols= ['Purpose', 'NumBor', 'BoRace', 'BoGender']
rel_freq= FHL_bank[cols].apply(pd.Series.value_counts, args=(True,))
rel_freq.index= [f'class {i}' for i in range(len(rel_freq))]
display(rel_freq)
```

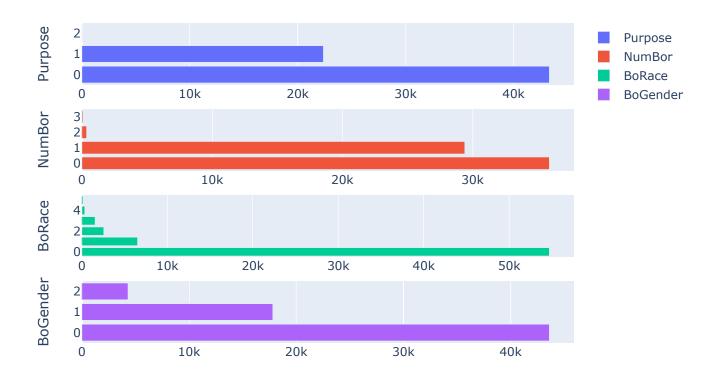
	Purpose	NumBor	BoRace	BoGender
class 0	0.66	0.45	0.00	0.66
class 1	0.34	0.55	0.04	0.27
class 2	NaN	0.01	0.02	0.07
class 3	0.00	0.00	0.00	NaN
class 4	NaN	NaN	0.83	NaN
class 5	NaN	NaN	0.10	NaN

```
[11]: cols= ['Purpose', 'NumBor', 'BoRace', 'BoGender', ]

fig = make_subplots(rows= len(cols), cols=1, )
for i, eachCol in enumerate(cols):
    fig.add_trace( go.Bar( x= FHL_bank[eachCol].value_counts(), name= eachCol), row= i+1, col=1)
    fig['layout'][f'yaxis{i+1}']['title']= eachCol

fig.update_layout(title_text= 'Discrete sample distributions')
config = {'staticPlot': True}
fig.show(config= config)
```

Discrete sample distributions



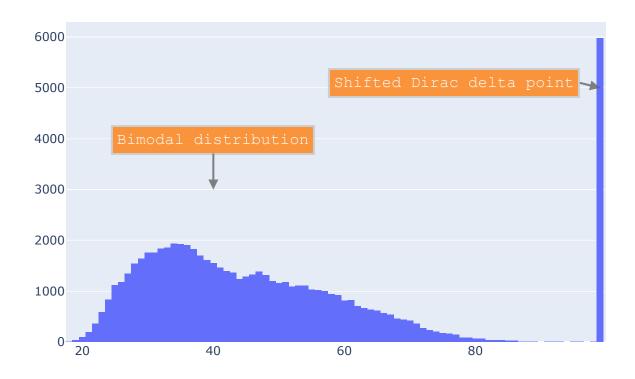
Two interesting characteristics can be noted when looking at the *age distribution* of the data. First note the slightly bimodality of the distribution, with the first being located around the 35 year age and the second one at the 55 year mark. Secondly, note the large amount of mass concentrated at the right side of the distribution. These borrower's haven't included their age in the application form resulting in the value 99 being entered in the dataset. We can thus see the age distribution as a mixed distribution containing on the one hand a bimodal Gaussian mixture distribution and

the other hand a Dirac delta point with all mass concentrated at 99. The last point is highly relevant, as there might a consistent reasoning as to why applicants choose not to disclose their age and their performance on the repayment of the mortgage. When estimating a Gaussian mixture model we do see indeed a decomposition in three unimodel Gaussians with means of respectively 54.9 years, 34 years and 99 "years". It is interesting to see how and if our GAN model is going to be able to capture these intricities and generate them successfully.

```
[12]: cols= ['BoAge']
      fig= go.Figure(data=[go.Histogram(x= FHL_bank['BoAge'])])
      fig.update_layout(title_text= "Histogram of borrower's age (in years)")
      fig.add_annotation(
              x = 99,
              y = 5000,
              xanchor= 'right',
              xref="x",
              yref="y",
              text="Shifted Dirac delta point",
              showarrow=True,
              font=dict(
                  family="Courier New, monospace",
                  size=16,
                  color="#fffff"
                  ),
              align="left",
              arrowhead=2,
              arrowsize=1,
              arrowwidth=2,
              arrowcolor="#636363",
              ax=-20,
              ay=-5,
              bordercolor="#c7c7c7",
              borderwidth=2,
              borderpad=4,
              bgcolor="#ff7f0e",
              opacity=0.8
      fig.add_annotation(
              x=40,
              y=3000,
              xanchor= 'center',
```

```
xref="x",
       yref="y",
        text="Bimodal distribution",
        showarrow=True,
        font=dict(
            family="Courier New, monospace",
            size=16,
            color="#ffffff"
            ),
        #align="left",
        arrowhead=2,
        arrowsize=1,
        arrowwidth=2,
        arrowcolor="#636363",
        ax=0,
        ay = -50,
        bordercolor="#c7c7c7",
        borderwidth=2,
        borderpad=4,
        bgcolor="#ff7f0e",
        opacity=0.8
config = {'staticPlot': True}
fig.show(config= config)
```

Histogram of borrower's age (in years)



```
[13]: # Estimate a Gaussian mixture model on the Age distribution
from sklearn.mixture import GaussianMixture
gm = GaussianMixture(3).fit(FHL_bank[cols])
# Get the estimated parameters
```

```
gm_params = pd.DataFrame(
    np.concatenate(
        (gm.means_, gm.covariances_.reshape(gm.means_.shape)), axis=1),
    columns=['Means', 'Variance'],
    index=['firstDecomposition', 'secondDecomposition', 'thirdDecomposition'])
display(Markdown("The estimated _Gaussian mixture model_ has the following parameters:"))
gm_params
```

The estimated *Gaussian mixture model* has the following parameters:

[13]:

	Means	Variance
firstDecomposition	34.38	45.95
${\tt secondDecomposition}$	99.00	0.00
thirdDecomposition	55.47	103.67

Preprocessing of data

Now that we have an idea of the peculiarities of the dataset we can move on to the preprocessing of the dataset. We first need to separate the data into continous variables and discrete variables as our neural network digest these type of variables in a distinct different way. We also remove variables that don't contain any real statistical information like IDs, these can easily be later on added and anonymized.

```
datasetNominal= FHL_bank[nominalColumns]

# Continuous data (including ordinal data)
datasetContinuous= FHL_bank[continuousColumns]

# Get number of categorical values of each nominal variable
nominalColumnsValues= datasetNominal.nunique().values
```

3.1 Preprocessing of nominal data

Nominal (discrete) data creates the additional problem that we end up with a non-differentiable bottleneck in our neural network leading to problems down the road. To deal with this issue, we follow the solutions implemented in NLP based networks in asimplified manner as the number of categories of our nominal is much smaller compared to NLP vocabularies.

We use the following setup:

1. we transform discrete marginals into a onehot encoding as:

$$\mathbf{n}_{i,j} \leftarrow n_{i,j} \tag{3.1}$$

with $n_{i,j}$ the i-th sample with the jth discrete variable and $\mathbf{n}_{i,j}$ its one-hot encoded vector representation

2. We add a small amount of noise to the one-hot vector:

$$\mathbf{n_{i,j}^{noise}} \leftarrow n_{i,j} + \sqrt{\sigma}\epsilon$$
 (3.2)

with ϵ either a standard Gaussian distribution or uniform distribution and σ either the variance of the Gaussian distribution or a scaling constant of the uniform distribution

3. Normalize the noisy one-hot vector in order to have a coherent probability measure:

$$\mathbf{n}_{i,j}^{\text{noise}} \leftarrow \mathbf{n}_{i,j}^{\text{noise}} / \sum_{k=1}^{J} \mathbf{n}_{i,j}^{\text{noise},k}$$
(3.3)

```
[15]: nameFeatures = nominalColumns
    ohe = OneHotEncoder(sparse= False) #create encoder object
    datasetEncoded = ohe.fit_transform(datasetNominal) #transform nominal data
    datasetEncoded = pd.DataFrame(datasetEncoded) #transform output to df
```

```
datasetEncoded.columns = ohe.get_feature_names(nameFeatures) #name columns appropriately
```

```
[16]: # Transforms ohe dataset to list of individual ohe variables
      def variableSeparator(nominalColumnValues, nominalDataset):
          # nominalColumnValues: A list containing the number of unique values of each variable
          # nominalDataset: a dataset containing one-hot encoded nominal variables
          Separates all of the individual variables into a list, so it's easy to perform computations on individual variables
          dim= len(nominalColumnsValues)
          variablesSeparated= []
          for eachVariable in range(dim):
              if eachVariable == 0:
                  tmp= nominalDataset[:, eachVariable:eachVariable+nominalColumnsValues[eachVariable]]
                  variablesSeparated.append(tmp)
                  idx= eachVariable+nominalColumnsValues[eachVariable]
              else:
                  tmp= nominalDataset[:, idx:idx+nominalColumnsValues[eachVariable]]
                  variablesSeparated.append(tmp)
                  idx+= nominalColumnsValues[eachVariable]
          return variablesSeparated
```

```
[17]: # Create noise
noise = np.random.uniform(0, 0.2, datasetEncoded.shape) #noise level of 0.2 is the standard
# Add noise to dataset
dataset_with_noise = datasetEncoded.values + noise

# Normalize each variable separately (from ohe to probabilities)
datasetNominalNormalized = np.array([]).reshape(len(dataset_with_noise), -1) #initialize
variablesSeparated= variableSeparator(nominalColumnValues = nominalColumnsValues, nominalDataset= dataset_with_noise)
for eachVariable in variablesSeparated:
    tmp= ( eachVariable / np.sum(eachVariable, axis= 1)[:, None] )
    datasetNominalNormalized= np.concatenate( (datasetNominalNormalized, tmp), axis= 1)
```

3.2 Preprocessing of continous data

Most papers recommend using a bounded activation function to train a GAN model as it leads to more stable results. As mentioned in Radford et al., Unsupervised representation learning with DCGAN: "The ReLU activation (Nair & Hinton, 2010) is used in the generator with the exception of the output layer which uses the Tanh function. We observed that using a bounded activation allowed the model to learn more quickly to saturate and cover the color space of the training distribution." Thus we use the Tanh activation function when generating continuous data with the Generator. To make the output of the Generator match with the input dataset to the Discriminator we preprocess the continuous data to [-1,1]. However, it might be the case that other bounded activation functions yield better results and thus this should be regarded as a hyperparameter that can be calibrated.

```
[18]: maximum = np.max(datasetContinuous)
minimum = np.min(datasetContinuous)
datasetContinuousNormalized= ( 2 * (datasetContinuous - minimum) / (maximum - minimum) - 1 )
```

3.3 Create final processed dataset

```
[19]: dataset= np.concatenate((datasetContinuousNormalized, datasetNominalNormalized), axis=1)
```

Setting up our GAN model

We can either generate our data from the modified Vanilla GAN or our newest version of the WGAN-GP-MIXED model.

```
[20]: # Turn the desired model on:
VGAN= False
WGAN_GP_MIXED= True
```

4.1 Modified Vanilla GAN model

```
[21]: if VGAN:
    ## DISCRIMINATOR

# Shape of the dataset
    input_shape= dataset.shape[1]
    # Create the discriminator
    discriminator = discriminator_setup_CTGAN(input_shape)

## GENERATOR

# Shape of the latent space of the generator
latent_dim= 100 #used in many papers
    # create the generator
```

```
generator = generator_setup_CTGAN(input_shape, latent_dim,)

## GAN

# create the gan
gan_model = gan_setup(generator, discriminator)
```

4.2 WGAN-GP-Mixed

• TODO: Modify to easier compile the model (WIP)

The basic GAN suffers from a vanishing gradient of the Discriminator which results in the Discriminator failing to provide useful gradient information (during backpropagation) to the Generator as soon as the Discriminator is well-trained. In contrast, the WGAN-GP Discriminator does not saturate and converges to a linear function with clean gradients. An easy way to see this is to run both the basic GAN and WGAN-GP on the FHL dataset and evaluate the training process. A more detailed discussion can be found in Arjovsky et al., Wasserstein GAN.

```
# Define the loss functions to be used for generator
def generator_loss(Xfake):
    return -tf.reduce_mean(Xfake)
# Epochs to train
epochs = 10
noise_dim= 512
batch_size= 512
# MODEL
d_model = discriminator_setup_WGANGP(dataset.shape[1])
g_model = generator_setup_WGANGP_GENERIC(dataset.shape[1],noise_dim, 256, 2,
                                         nominalColumnsValues, nominalColumns, datasetContinuousNormalized.shape[1])
# Get the wgan model
wgan = WGAN(
    discriminator=d_model,
    generator=g_model,
    latent_dim=noise_dim,
    discriminator_extra_steps=5,
# Compile the wgan model
wgan.compile(
    d_optimizer=discriminator_optimizer,
    g_optimizer=generator_optimizer,
    g_loss_fn=generator_loss,
    d_loss_fn=discriminator_loss,
)
# Custom callback to get KL-divergence
cbk= GANMonitor(dataset, 1000, noise_dim, 10)
```

Training of the compiled GAN model

We can either train one of our compiled models (VGAN or WGAN-GP-Mixed) or load in a previously trained model

```
[22]: # Choose to train a model or load a previous trained model (locally or from the cloud)

TRAIN_NEW= False

SAVE_LCL= False

LOAD_LCL= True

LOAD_CL= False
```

5.1 Vanilla GAN

5.2 WGAN-GP-Mixed

5.3 Loading of a previous trained model

5.3.1 Load model saved in local or cloud environment

```
[50]: mdl_name = 'fhl_generator_29-11-2021_151623.h5'
if LOAD_LCL:
    mdl= f'mdl/{mdl_name}'
    g_model = tf.keras.models.load_model(mdl, compile=False)
if LOAD_CL:
    mdl= f'/content/gdrive/My Drive/Stress Testing with GANs/mdl/{mdl_name}'
    g_model = tf.keras.models.load_model(mdl)
```

Evaluating the performance of our trained model

6.1 Loss functions for WGAN-GP

• Still a work-in-progress

We have the following minimax problem with the WGAN-GP model (ignoring the GP for now):

$$\min_{G} \max_{D} \mathbb{E}_{\mathbf{x} \sim \mathbf{p}(\mathbf{X})} \{ D(x) \} - \mathbb{E}_{\mathbf{z} \sim \mathbf{p}(\mathbf{Z})} \{ D(G(z)) \}$$
(6.1)

with p(X) the true distribution, p(Z) the latent distribution, G(z) the Generator and D(x) the Discriminator.

Which results in the following loss functions:

Discriminator:

$$\min_{D} \mathbb{E}_{\mathbf{z} \sim \mathbf{p}(\mathbf{Z})} \{ D(G(z)) \} - \mathbb{E}_{\mathbf{x} \sim \mathbf{p}(\mathbf{X})} \{ D(x) \}$$
(6.2)

Generator:

$$\min_{G} -\mathbb{E}_{\mathbf{z} \sim \mathbf{p}(\mathbf{Z})} \{ D(G(z)) \} \tag{6.3}$$

We approximate the Expected values by taking the arithmetic means.

Since the Discriminator has an output space of $[-\infty, +\infty]$ we can expect quite erratic behaviour which would result in problems during the backpropagation phase. To ensure a well-behaved function we constrain the Discriminator to

be 1-Lipschitz continuous. We can do this by either weightclipping (WGAN) or adding a gradient penalty (WGAN-GP). Weightclipping is suboptimal so we use the Gradient Penalty.

The Gradient Penalty ensures that the norm of the gradient of the Discriminator (with the input being an interpolation of the real and fake distribution) is at most one, which ensures that the Discriminator is 1-Lipschitz continuous (see Proof of Proposition 1, page 12, Improved WGANs). The Discriminator loss function then becomes:

$$\min_{D} \mathbb{E}_{\mathbf{z} \sim \mathbf{p}(\mathbf{Z})} \{ D(G(z)) \} - \mathbb{E}_{\mathbf{x} \sim \mathbf{p}(\mathbf{X})} \{ D(x) \} + \lambda \mathbb{E}_{\mathbf{w} \sim \mathbf{p}(\mathbf{W})} \{ (\|\nabla D(w)\|_2 - 1)^2 \}$$

$$(6.4)$$

with λ a Langrage multiplier and p(W) an interpolated distribution.

During backpropagation the weights of the Discriminator will be adjusted to minimize the added Gradient Penalty, ensuring that the weights and Discriminator conform to the 1-Lipschitz requirement in a more natural way than directly clipping the weights.

Within the current notebooks (07/09) the two loss functions are simply defined within the notebook (see above), whereas the Gradient Penalty is defined within the in-house library within the custom made WGAN class by utilizing Tensorflow to create interpolated distributions. The loss function of the Discriminator and the Gradient Penalty are then added together during the training (when calling the fit() function).

6.2 How should I interpret the loss functions of WGAN-GP?

The loss function of the discriminator is an approximation of the Earth-Mover distance (i.e. the minimum transportation cost when transporting mass of probability Q in order to approximate probability P) up to a constant scaling factor dependent on the Discriminator's architecture and the Gradient Penalty. The constant scaling factor makes it hard to compare the loss functions between different model specifications. Note also, that the loss function is simply an approximation of the true EM-distance, so it's hard to know how closely the loss function is to the true EM-distance.

However, we can use the loss function as an indication of how well the training relatively improves the performance of our model. A lower loss would indicate an improvement in the generated distribution. In our case the loss function is inverted so an increase in the loss would indicate an improvement in the generated distribution. Examples of plots of the loss function can be found back in the Wasserstein GAN and Improved Training of WGANs papers.

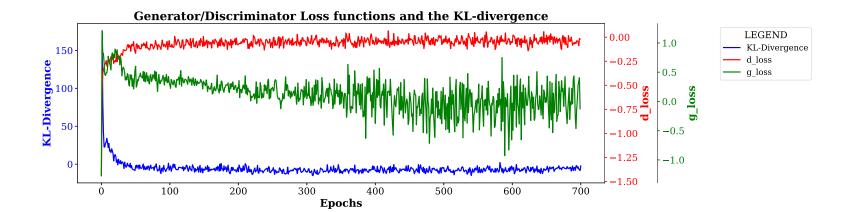
The Generator is dependent on the Discriminator during the backpropagation phase and thus the loss function of the Generator does not provide a meaningful absolute metric. However, we should expect the generator to oscillate between a certain range during convergence or to gradually increase/decrease, without any erratic behaviour.

The KL-divergence quantifies how much one probability distribution differs from another probability distribution. The range of the KL-divergence is $[0,+\infty]$ with a value of zero indicating that the two distributions are identical. Thus we should expect the KL-divergence to decrease during the training phase and converge towards zero.

```
[30]: # Plots the loss functions of Discriminator and Generator and the KL-divergence obtained during training
     from mpl_toolkits.axes_grid1.inset_locator import zoomed_inset_axes
      from mpl_toolkits.axes_grid1.inset_locator import mark_inset
      ## Main function
      def plot_metric(history= None, cbk= None, _list= None):
          if not _list:
             g_loss= history.history['g_loss']
             d_loss= history.history['d_loss']
             kl= np.array(cbk.kl_tracker)
         elif list:
             g_loss= _list[0]
             d_loss= _list[1]
             kl= _list[2]
          #function to set our spines invisible
         def make_patch_spines_invisible(ax):
             ax.set_frame_on(True)
             ax.patch.set_visible(False)
             for sp in ax.spines.values():
                  sp.set_visible(False)
          # _____
          ## Main Graph
          # -----
          #setup figure
         fig, host = plt.subplots(figsize=[20, 5])
         fig.subplots_adjust(right=0.75)
         par1 = host.twinx()
         par2 = host.twinx()
          # Offset the right spine of par2. The ticks and label have already been
          # placed on the right by twinx above.
         par2.spines["right"].set_position(("axes", 1.1))
```

```
# Having been created by twinx, par2 has its frame off, so the line of its
# detached spine is invisible. First, activate the frame but make the patch
# and spines invisible.
make_patch_spines_invisible(par2)
# Second, show the right spine.
par2.spines["right"].set_visible(True)
# Ready to plot our graphs
epochs = range(1, len(g_loss) + 1)
p1, = host.plot(epochs, kl, 'b', label="KL-Divergence")
p2, = par1.plot(d_loss, 'r', label="d_loss")
p3, = par2.plot(g_loss, 'g', label="g_loss")
# Name labels appropriately
host.set_xlabel("Epochs", fontweight='bold')
host.set_ylabel("KL-Divergence", fontweight='bold')
par1.set_ylabel("d_loss", fontweight='bold')
par2.set_ylabel("g_loss", fontweight='bold')
# Keep coloring uniform across the entire figure
host.yaxis.label.set_color(p1.get_color())
par1.yaxis.label.set_color(p2.get_color())
par2.yaxis.label.set_color(p3.get_color())
# Clean up ticks
tkw = dict(size=4, width=1.5)
host.tick_params(axis='y', colors=p1.get_color(), **tkw)
par1.tick_params(axis='y', colors=p2.get_color(), **tkw)
par2.tick_params(axis='y', colors=p3.get_color(), **tkw)
host.tick_params(axis='x', **tkw)
# Add outside legend and give title
lines = [p1, p2, p3]
host.legend(lines, [l.get_label() for l in lines], title= 'LEGEND', bbox_to_anchor=(1.40, 1),)
plt.title('Generator/Discriminator Loss functions and the KL-divergence', fontweight='bold')
# ______
## Zoom-ins to get more detail
# -----
# Zoom into a part of KL-divergence graph
  axins = zoomed_inset_axes(host, 2, loc= 5) # (graph, zoom-in factor, location on graph to display the zoom)
```

```
#What to zoom in on
     axins.plot(epochs, kl, '--')
      x1, x2, y1, y2 = len(kl) - 100, len(kl), -20, 20 # specify the limits
     axins.set_xlim(x1, x2) # apply the x-limits
     axins.set_ylim(y1, y2) # apply the y-limits
     #Add connecting lines to original plot
      mark_inset(host, axins, loc1=3, loc2=4, fc="none", ec="0", )
      #Zoom into a part of the graph
      axins = zoomed_inset_axes(par1, 2, loc= 10) # (graph, zoom-in factor, location on graph to display the zoom)
     #What to zoom in on
     axins.plot(epochs, d_loss, 'r')
     x1, x2, y1, y2 = len(d_loss) - 100, len(d_loss), -0.1, 0 # specify the limits
     axins.set_xlim(x1, x2) # apply the x-limits
     axins.set_ylim(y1, y2) # apply the y-limits
     #Add connecting lines to original plot
     mark_inset(par1, axins, loc1=2, loc2=4, fc="None", ec="0", )
## Load in data if mdl was trained on GColab
# -----
_dir= os.listdir('data/interim')
g_loss = []
d_{loss} = []
kl= []
for eachFolder in _dir:
   g_loss.append(list(np.load(f'data/interim/{eachFolder}/g_loss.npy')))
   d_loss.append(list(np.load(f'data/interim/{eachFolder}/d_loss.npy')))
   kl.append(list(np.load(f'data/interim/{eachFolder}/kl.npy')))
g_loss = functools.reduce(operator.iconcat, g_loss, [])
d_loss = functools.reduce(operator.iconcat, d_loss, [])
kl = kl[-1]
plot_metric(_list= [g_loss, d_loss, kl])
```



6.3 Postprocess datasets back to original shape

Let's first generate some samples from the real data, Xreal, as well as some samples from our trained Generator, Xfake. Note that that we sample Xreal from the pre-processed dataset and not the raw dataset.

```
[51]: n_samples= 20000

Xfake, _= generate_artificial_samples(g_model, noise_dim, n_samples)

Xreal, _= generate_real_samples(dataset, n_samples)
```

Now, let's estimate the KLdivergence between Xreal and Xfake:

```
[133]: #Latex(print('Estimated KL-divergence:', KLdivergence(Kreal, Kfake, k=5)));
# Get results from cloud
display(Latex("Estimated KL-divergence: 4.190287702424854"))
```

Estimated KL-divergence: 4.190287702424854

Let's start post-processing both Xreal and Xfake. The goal is to reverse engineer the pre-processing steps we took initially in order to convert Xreal back to it's raw state. In the meantime we apply the exact same set of transformations for Xfake to have the generated data in the same format as the original raw data.

We first decompose the datasets in their conntinous and discrete variables:

```
[52]: # Dimensions
    dimContinuous= len(continuousColumns)
    dimNominal= len(nominalColumns)

# Artificial Dataset
    Xfake_continuous= Xfake[:,0:dimContinuous]
    Xfake_nominal= Xfake[:, dimContinuous:]

# Real Dataset
    Xreal_continuous= Xreal[:, 0:dimContinuous]
    Xreal_nominal= Xreal[:, dimContinuous:]
```

Then we start to post-process the nominal data by going from noisy marginal distributions to a clean one-hot encoded format:

```
[53]: | # Divide datasets into separated columns for each nominal variable
      XrealSeparated= variableSeparator(nominalColumnsValues = nominalColumnsValues, nominalDataset= Xreal_nominal)
      XfakeSeparated= variableSeparator(nominalColumnsValues = nominalColumnsValues, nominalDataset= Xfake_nominal)
      # Function to transform from p() to ohe
      def retransformer(nominalVariable):
        idx = nominalVariable.argmax(axis=1)
        out = np.zeros_like(nominalVariable,dtype=float)
        out[np.arange(nominalVariable.shape[0]), idx] = 1
        return out
      # Transform columns into one-hot encoding format
      Xreal_transformed= []
     Xfake_transformed= []
      for eachVariable in XrealSeparated:
          tmp= retransformer(eachVariable)
         Xreal_transformed.append(tmp)
      for eachVariable in XfakeSeparated:
          tmp= retransformer(eachVariable)
          Xfake_transformed.append(tmp)
      # Concatenate back into one dataset
```

```
Xreal_nominal = np.concatenate((Xreal_transformed), axis=1)
Xfake_nominal = np.concatenate((Xfake_transformed), axis=1)
```

Next, we post-process the continous data from the range [-1,1] back to their original domain:

6.3.1 Real dataset

```
[54]: Xreal_continuous_renormalized= ( ((Xreal_continuous + 1) / 2) * (maximum[:, None].T - minimum[:, None].T) + minimum[:, None].T)
```

6.3.2 Artificial dataset

```
[55]: Xfake_continuous_renormalized= ( ((Xfake_continuous + 1) / 2) * (maximum[:, None].T - minimum[:, None].T) + minimum[:, None].T)
```

Finally, we merge all post-processed data into final matrix/dataFrame:

```
[56]: # Real dataset
Xreal= np.concatenate( (Xreal_continuous_renormalized, Xreal_nominal), axis= 1)
# Artificial dataset
Xfake= np.concatenate( (Xfake_continuous_renormalized, Xfake_nominal), axis= 1)
```

Chapter 7

Evaluate the *similarity* between real and artificial distributions

Let's recompute the KL-divergence but now for the postprocessed datasets. We see that the divergence is much larger than before. Two possible reasons:

- 1. Our implementation of the KL-divergence estimator doesn't work properly with mixed distributions (see the KL-divergence notebook for more information)
- 2. Postprocessing setup contains errors.

```
[128]: #Latex(print('Estimated KL-divergence:', KLdivergence(Xreal, Xfake, k=10)));
# Get results from cloud
display(Latex("Estimated KL-divergence: 66.49804921560046"))
```

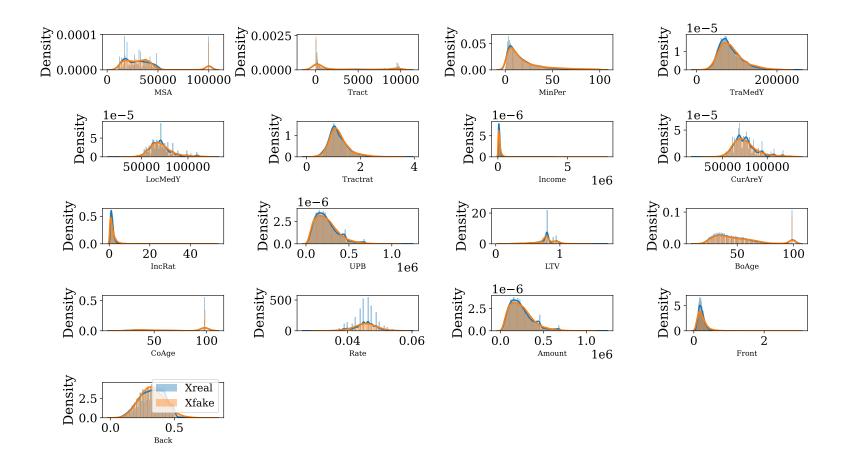
Estimated KL-divergence: 66.49804921560046

7.1 Visualisation of real and artificial distributions

Let us plot the continuous marginal distributions of the real dataset (blue) and overlay them with the continuous marginals of the generated dataset (orange). We observe quite satisfactory visual results with the artificial dataset being able to capture most marginals quite closely. Note especially, on the zoomed in plots, how the improved model is able to capture a wider range of multimodal distributions, which is in great contrast with the earlier versions we implemented.

```
[57]: dim= Xreal_continuous_renormalized.shape[1]
    fig= plt.figure(figsize=[15, 30])
    for eachDimension in range(dim):
        plt.subplot(dim, 4, eachDimension+1)
        sns.distplot(Xreal_continuous_renormalized[:,eachDimension], bins= 100, label= 'Xreal')
        sns.distplot(Xfake_continuous_renormalized[:,eachDimension], bins= 100, label= 'Xfake')
        plt.xlabel(continuousColumns[eachDimension], fontsize = 10)
    plt.legend()
    plt.suptitle('Real vs. Generated Continous Marginal Distributions', fontweight= 'bold')
    fig.tight_layout(rect=[0, 0.03, 1, 0.97])
```

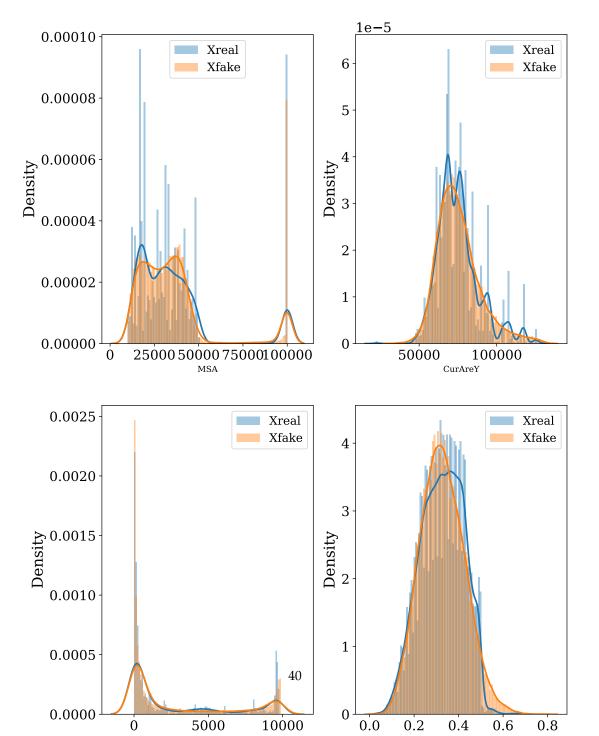
Real vs. Generated Continous Marginal Distributions



```
[58]: # Close up of some marginal distributions

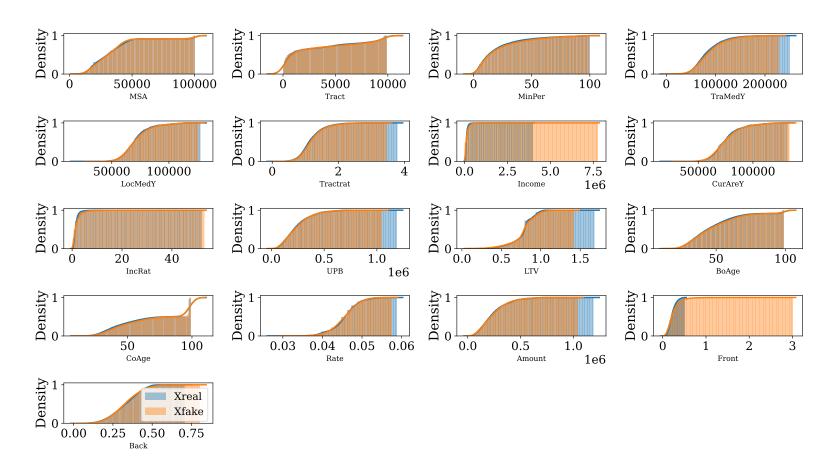
fig= plt.figure(figsize=[10,15])
plt.subplot(2,2,1)
```

```
sns.distplot(Xreal_continuous_renormalized[:,0], bins= 100, label= 'Xreal')
sns.distplot(Xfake_continuous_renormalized[:,0], bins= 100, label= 'Xfake')
plt.xlabel(continuousColumns[0], fontsize = 10)
plt.legend();
plt.subplot(2,2,2)
sns.distplot(Xreal_continuous_renormalized[:, 7], bins= 100, label= 'Xreal')
sns.distplot(Xfake_continuous_renormalized[:, 7], bins= 100, label= 'Xfake')
plt.xlabel(continuousColumns[7], fontsize = 10)
plt.legend();
plt.subplot(2,2,3)
sns.distplot(Xreal_continuous_renormalized[:,1], bins= 100, label= 'Xreal')
sns.distplot(Xfake_continuous_renormalized[:,1], bins= 100, label= 'Xfake')
plt.xlabel(continuousColumns[11], fontsize = 10)
plt.legend();
plt.subplot(2,2,4)
sns.distplot(Xreal_continuous_renormalized[:,-1], bins= 100, label= 'Xreal')
sns.distplot(Xfake_continuous_renormalized[:,-1], bins= 100, label= 'Xfake')
plt.xlabel(continuousColumns[-1], fontsize = 10)
plt.legend();
```



```
[59]: dim= Xreal_continuous_renormalized.shape[1]
    fig= plt.figure(figsize=[15, 30])
    for eachDimension in range(dim):
        plt.subplot(dim, 4, eachDimension+1)
        kwargs = {'cumulative': True}
        sns.distplot(Xreal_continuous_renormalized[:,eachDimension], bins= 100, label= 'Xreal', hist_kws=kwargs,u=kde_kws=kwargs)
        sns.distplot(Xfake_continuous_renormalized[:,eachDimension], bins= 100, label= 'Xfake', hist_kws=kwargs,u=kde_kws=kwargs)
        plt.xlabel(continuousColumns[eachDimension], fontsize = 10)
    plt.legend()
    plt.suptitle('Real vs. Generated Continuous Cumulative Marginal Distributions', fontweight= 'bold')
    fig.tight_layout(rect=[0, 0.03, 1, 0.97])
```

Real vs. Generated Continous Cumulative Marginal Distributions



It is of interest to see whether we are able to capture the Dirac delta point embedded within the Age variable distribution. If we look at the number of 99 values within the original dataset we see a frequency of 1721. However, the synthetic dataset contains only 420 observations with 99 values. If we instead look at the number of observations with an age value of *around* 99 we see a frequency of 1536. Thus, it seems as if MIXED-WGAN-GP tries to approximate the delta point through a local Gaussian like distribution with high excess kurtosis.

7.2 Correlations between continuous variables

Xfake - number of values around 99: 1536

Next, we evaluate the pairwise correlation matrix of the generated with that of the original dataset. After computing the (Pearson) correlation matrices for both datasets, we compute the elementwise difference. The absolute difference matrix contains elements $|D_{i,j}| \in [0,2]$ with $D_{i,j} = 0$ indicating that the Pearson correlation between variables i and j is the exact same whether we compute the correlation with the original or the generated dataset. On the other hand, when $D_{i,j} = 2$ we witness a maximum divergence between the computed correlations across the true and generated dataset. Looking at the results we see that the generated data is mostly aligned with the original one, except for some outliers that need to be further investigated.

A sample of the difference correlation matrix:

	UPB	TraMedY	BoAge	MinPer	Back	Tract	Tractrat	IncRat	LocMedY	CoAge
UPB	0.00	0.03	0.00	0.01	0.05	0.03	0.00	0.04	0.03	0.06
TraMedY	0.03	0.00	0.07	0.02	0.07	0.02	0.01	0.05	0.03	0.07
BoAge	0.00	0.07	0.00	0.09	0.03	0.05	0.11	0.13	0.07	0.07
MinPer	0.01	0.02	0.09	0.00	0.08	0.02	0.01	0.01	0.07	0.12
Back	0.05	0.07	0.03	0.08	0.00	0.08	0.03	0.08	0.08	0.18
Tract	0.03	0.02	0.05	0.02	0.08	0.00	0.01	0.08	0.01	0.00
Tractrat	0.00	0.01	0.11	0.01	0.03	0.01	0.00	0.07	0.01	0.03
IncRat	0.04	0.05	0.13	0.01	0.08	0.08	0.07	0.00	0.04	0.10
LocMedY	0.03	0.03	0.07	0.07	0.08	0.01	0.01	0.04	0.00	0.21
CoAge	0.06	0.07	0.07	0.12	0.18	0.00	0.03	0.10	0.21	0.00

7.3 Plot nominal marginal distributions

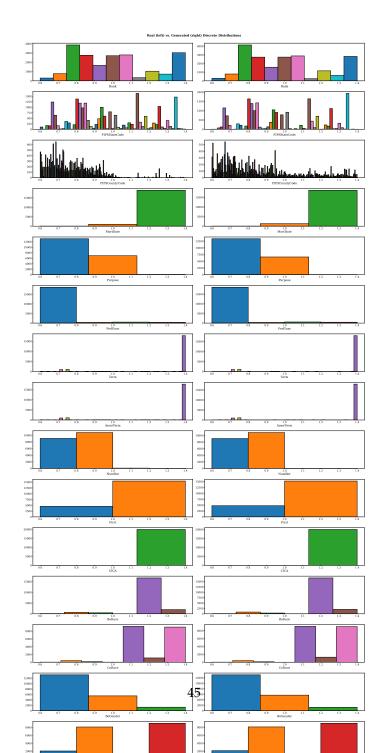
Next, we take a look at the nominal marginal distributions of the real and generated datasets. We see that the generated data is closely aligned with the original dataset. Note especially how MIXED-WGAN-GP is able to capture highly imbalanced distributions. When the number of potential categories increases (see Country Codes) we see that the model has trouble replicating the data.

```
[110]: #fig= plt.figure(figsize=[10, 45])
dim= len(nominalColumnsValues)
idx_Xreal=np.arange(1,dim*2,2)
idx_Xfake=np.arange(2,dim*2+2,2)
plt.figure(figsize=(30, 150))
for eachVariable in range(dim-20):

    plt.subplot(dim, 2, idx_Xreal[eachVariable], )
    plt.hist(retransformer(XrealSeparated[eachVariable]), bins=[.5,.5,1.5], ec= 'k')
    plt.xlabel(nominalColumns[eachVariable])

    plt.subplot(dim, 2, idx_Xfake[eachVariable])
    plt.hist(retransformer(XfakeSeparated[eachVariable]), bins=[.5,.5,1.5], ec= 'k')
    plt.xlabel(nominalColumns[eachVariable])

plt.suptitle('Real (left) vs. Generated (right) Discrete Distributions', fontweight= 'bold');
plt.tight_layout(rect=[0, 0, 1, 0.98])
```



To analyse how well the model is able to capture the relationship between nominal distributions we rely on the pairwise mutual information matrix. The *mutual information* between two random discrete variables X and Y measures the amount of information that is being shared by the two variables. In case the two variables are independent from each other, they won't share any mutual information with each other and I(X;Y)=0. On the other hand, if knowing something about X gives us additional information about the (expected) behaviour of Y then we do have mutual information across both variables and I(X;Y)>0. Similar to the correlation matrix of continuous variables, we compute the *difference* matrix between the pairwise mutual information matrix of the true and generated datasets.

The absolute difference matrix contains elements $|D_{i,j}| \in [0,\infty]$ with $D_{i,j}=0$ indicating that the mutual information between variables i and j is the exact same whether we compute the measure with the original or the generated dataset. On the other hand, when $D_{i,j}>0$ we witness a divergence between the computed mutual information measure across the true and generated dataset. Looking at the results ...

```
[114]: ## Convert nominal synthetic data to condensed df
       #get all of the nominal variables (in one-hot encoded format)
       nominalVariablesList = variableSeparator(nominalColumnsValues = nominalColumnsValues, nominalDataset= Xreal_nominal)
       #initialize dataframe before loop
       df_Xfake_nominal= pd.DataFrame()
       #Tranform from one-hot encoding to original shape for each nominal variable
       for eachColumn in range(len(nominalVariablesList)):
           #create dataFrame object
           tmp= pd.DataFrame(nominalVariablesList[eachColumn])
           #equate column names to unique values of the variable
           uniqueValues= datasetNominal.iloc[:,eachColumn].unique()
           uniqueValues.sort() #sort values (just like ohe of sklearn does)
           tmp.columns= uniqueValues
           #condense one-hot encoding back to original shape
           tmp2= tmp.idxmax(axis='columns')
           #concatenate into one dataFrame containing all of the nominal columns
           df_Xfake_nominal= pd.concat([df_Xfake_nominal, tmp2], axis= 1)
       #name the columns appropriately
       df_Xfake_nominal.columns= nominalColumns
       # Convert categories to int
       df_Xfake_nominal = df_Xfake_nominal.apply(lambda col:pd.Categorical(col).codes)
```

```
## Convert nominal real data to condensed df
#get all of the nominal variables (in one-hot encoded format)
nominalVariablesList = variableSeparator(nominalColumnsValues = nominalColumnsValues, nominalDataset= Xfake_nominal)
#initialize dataframe before loop
df_Xreal_nominal= pd.DataFrame()
#Tranform from one-hot encoding to original shape for each nominal variable
for eachColumn in range(len(nominalVariablesList)):
    #create dataFrame object
    tmp= pd.DataFrame(nominalVariablesList[eachColumn])
    #equate column names to unique values of the variable
    uniqueValues= datasetNominal.iloc[:,eachColumn].unique()
    uniqueValues.sort() #sort values (just like ohe of sklearn does)
   tmp.columns= uniqueValues
    #condense one-hot encoding back to original shape
   tmp2= tmp.idxmax(axis='columns')
    #concatenate into one dataFrame containing all of the nominal columns
    df_Xreal_nominal= pd.concat([df_Xreal_nominal, tmp2], axis= 1)
#name the columns appropriately
df_Xreal_nominal.columns= nominalColumns
# Convert categories to int
df_Xreal_nominal = df_Xreal_nominal.apply(lambda col:pd.Categorical(col).codes)
```

```
#Compute PMI for every column of the real dataset
for eachColumn in range(0, df_Xfake_nominal.shape[1]):
    PMI_fake[:, eachColumn]= mutual_info_classif(df_Xfake_nominal.values, df_Xfake_nominal.iloc[:, eachColumn],
    discrete_features= True)
#convert to DataFrame
PMI_fake= pd.DataFrame(data= PMI_fake, columns=nominalColumns, index= nominalColumns)

## Difference between PMI of Real and Fake dataset
PMI_diff= PMI_real - PMI_fake
display(Latex('A sample of the difference Pairwise Mutual Information matrix:'))
    _sample= PMI_diff.sample(n=10, axis=1)
display(_sample.loc[_sample.columns].abs())
```

A sample of the difference Pairwise Mutual Information matrix:

	PropType	BoRace	Race4	NumUnits	MortDate	Corace2	SpcHsgGoals	Bank	FIPSStateCode	FedGuar
PropType	0.03	0.00	0.00	0.03	0.00	0.00	0.00	0.03	0.05	0.00
BoRace	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.03	0.00
Race4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NumUnits	0.03	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00
MortDate	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00	0.00	0.00
Corace2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00
SpcHsgGoals	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00
Bank	0.03	0.01	0.00	0.00	0.00	0.00	0.01	0.02	0.49	0.02
FIPSStateCode	0.05	0.03	0.00	0.00	0.00	0.02	0.01	0.49	0.24	0.02
FedGuar	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.02	0.02

Lastly, we can try to get a summary measure of the overall similarity between the dependence strutucture found in the true data and the generated data. To do so we first compute the pairwise mutual information matrix across all variables (both continous and discrete variables) for both the true and generated data, $I(\mathbf{X}_{true})$ and $I(\mathbf{X}_{generated})$. Note how I(X) also captures non-linear dependencies across variables (in contrast with the Pearson correlation matrix). Next we compute the *Frobenius norm* of the resulting matrices,

$$|I(.)|_F := \sqrt{\sum_{i=1}^m \sum_{j=1}^n |I_{ij}|^2}$$

The Frobenius norm can be seen as the extension of the Euclidian distance from the vector space to the matrix space. Next, we take the absolute difference of the Frobenius norm of the true and generated data, $D = I(\mathbf{X}_{true}) - I(\mathbf{X}_{generated})$. the closer |D| is to 0, the more aligned the dependence structures found in the true and generated data are.

```
[116]: ## Pairwise Mutual Information of all variables
       # -----
       from sklearn.feature_selection import mutual_info_regression
       ## Real dataset
       #Initialize Pairwise Mutual Information Matrix
       PMI_real= np.empty([Xreal_continuous_renormalized.shape[1] + df_Xreal_nominal.shape[1],
                           Xreal_continuous_renormalized.shape[1] + df_Xreal_nominal.shape[1]])
       idx = 0
       #Compute PMI for every column of the real dataset
       for eachColumn in range(0, Xreal_continuous_renormalized.shape[1] + df_Xreal_nominal.shape[1]):
           if eachColumn < Xreal_continuous_renormalized.shape[1]:</pre>
               PMI_real[:, eachColumn] = mutual_info_regression(np.concatenate( (Xreal_continuous_renormalized,__

→df_Xreal_nominal), axis= 1),
                                                               Xreal_continuous_renormalized[:, eachColumn])
           else:
               PMI_real[:, eachColumn] = mutual_info_classif(np.concatenate( (Xreal_continuous_renormalized, df_Xreal_nominal),,
        \rightarrowaxis= 1),
                                                            df_Xreal_nominal.iloc[:, idx])
               idx += 1
       #convert to DataFrame
       PMI_real= pd.DataFrame(data= PMI_real, columns= continuousColumns + nominalColumns, index= continuousColumns + 1
        →nominalColumns)
       ## Fake dataset
       #Initialize Pairwise Mutual Information Matrix
       PMI_fake= np.empty([Xfake_continuous_renormalized.shape[1] + df_Xfake_nominal.shape[1],
                           Xfake_continuous_renormalized.shape[1] + df_Xfake_nominal.shape[1]])
       idx = 0
       #Compute PMI for every column of the real dataset
       for eachColumn in range(0, Xfake_continuous_renormalized.shape[1] + df_Xfake_nominal.shape[1]):
           if eachColumn < Xfake_continuous_renormalized.shape[1]:</pre>
```

```
PMI_fake[:, eachColumn] = mutual_info_regression(np.concatenate( (Xfake_continuous_renormalized,,,

df_Xfake_nominal), axis= 1),
                                                      Xfake_continuous_renormalized[:, eachColumn])
    else:
        PMI_fake[:, eachColumn] = mutual_info_classif(np.concatenate( (Xfake_continuous_renormalized, df_Xfake_nominal),_
 \rightarrowaxis= 1),
                                                   df_Xfake_nominal.iloc[:, idx])
        idx += 1
#convert to DataFrame
PMI_fake= pd.DataFrame(data= PMI_fake, columns= continuousColumns + nominalColumns, index= continuousColumns + nominalColumns.
 →nominalColumns)
## Difference between PMI of Real and Fake dataset
PMI_diff= PMI_real - PMI_fake
display(Latex('A sample of the difference Pairwise Mutual Information matrix (including continuous variables):'))
_sample= PMI_diff.sample(n=10, axis=1)
display(_sample.loc[_sample.columns].abs())
```

A sample of the difference Pairwise Mutual Information matrix (including continuous variables):

	PMI	CoGender	MSA	FIPSStateCode	CoRace	Race4	${\tt BoCreditScore}$	CoEth	Corace2	Race5
PMI	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CoGender	0.00	0.00	0.01	0.03	0.02	0.00	0.00	0.02	0.02	0.00
MSA	0.00	0.00	3.40	0.00	0.00	0.00	0.01	0.00	0.00	0.00
FIPSStateCode	0.01	0.02	0.00	0.24	0.00	0.00	0.00	0.01	0.02	0.00
CoRace	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.00
Race4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
${\tt BoCreditScore}$	0.00	0.00	0.01	0.01	0.01	0.00	0.04	0.00	0.01	0.00
CoEth	0.00	0.02	0.01	0.02	0.01	0.00	0.01	0.02	0.02	0.00
Corace2	0.01	0.02	0.00	0.02	0.02	0.00	0.00	0.01	0.00	0.00
Race5	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00

```
[119]: # Frobenius norm of real dataset PMI matrix
Xreal_fro= np.linalg.norm(PMI_real, ord= 'fro')
# Frobenius norm of synthetic dataset PMI matrix
Xfake_fro= np.linalg.norm(PMI_fake, ord= 'fro')
# Difference in norms
```

```
X_fro_diff= np.abs(Xreal_fro - Xfake_fro)
display(Latex(f"""The absolute difference between the Frobenius norm
of the Real and Synthetic dataset PMI matrices is equal to ${np.round(X_fro_diff,2)}$."""))
```

The absolute difference between the Frobenius norm of the Real and Synthetic dataset PMI matrices is equal to 3.04.

7.4 We can train the model further if we believe convergence isn't reached yet:

Go back to Section 6 to re-evaluate the new model:

```
[47]: | #wgan.fit(dataset, batch_size= batch_size, epochs= epochs, callbacks= [cbk])
   Epoch 1/10
   g_loss: 0.7462
   Epoch 2/10
   g_loss: 0.7029
   Epoch 3/10
   129/129 [============= ] - 53s 410ms/step - d_loss: -0.2383 -
   g_loss: 0.7551
   Epoch 4/10
   g_loss: 0.8087
   Epoch 5/10
   129/129 [============= ] - 53s 411ms/step - d_loss: -0.2354 -
   g_loss: 0.8221
   Epoch 6/10
   129/129 [=============== ] - 56s 432ms/step - d_loss: -0.2383 -
   g_loss: 0.8330
   Epoch 7/10
   g_loss: 0.8447
   Epoch 8/10
   129/129 [=============== ] - 53s 408ms/step - d_loss: -0.2289 -
   g_loss: 0.8164
   Epoch 9/10
   129/129 [============= ] - 55s 427ms/step - d_loss: -0.2328 -
   g_loss: 0.8085
```

[47]: <tensorflow.python.keras.callbacks.History at 0x1a4117e3790>

Chapter 8

Save the calibrated Generator and the synthetic dataset

If model performance is satisfactory we can go ahead and save our trained Generator together with the synthetic dataset.

8.1 Create a Pandas DataFrame of synthetic generated data

Now that we have evaluated the performance of the model and similarity of the generated data with the original dataset, we can go ahead and create a finalized dataframe. The continuous data part is already fully post-processed to the same form as the raw dataset. For the nominal (discrete) part we still need to decode the one-hot encondings into the original variables (including the original set of possible categories of every variable and their associated data types (!). Afterwards, we simply concatenate the two parts and make sure that metaschema is aligned with the original dataset. Below you see an example set of the finalized dataframe. This dataset can then either be ingested into a database or saved locally in your desired format (csv, xlsx, pickle, etc.) to be shared intrainstitutional. In case of transferring data across entities, one can simply transfer the calibrated *Generator* which can then generate the data at the target entity.

```
[121]: ## Convert continuous synthetic data to df

df_Xfake_continuous= pd.DataFrame(data= Xfake_continuous_renormalized, columns= continuousColumns)

## Convert nominal synthetic data to df

#get all of the nominal variables (in one-hot encoded format)
nominalVariablesList = variableSeparator(nominalColumnsValues = nominalColumnsValues, nominalDataset= Xreal_nominal)

#initialize dataframe before loop
```

```
df_Xfake_nominal= pd.DataFrame()
#Tranform from one-hot encoding to original shape for each nominal variable
for eachColumn in range(len(nominalVariablesList)):
    #create dataFrame object
    tmp= pd.DataFrame(nominalVariablesList[eachColumn])
    #equate column names to unique values of the variable
   uniqueValues= datasetNominal.iloc[:,eachColumn].unique()
   uniqueValues.sort() #sort values (just like ohe of sklearn does)
   tmp.columns= uniqueValues
    #condense one-hot encoding back to original shape
   tmp2= tmp.idxmax(axis='columns')
    #concatenate into one dataFrame containing all of the nominal columns
    df_Xfake_nominal= pd.concat([df_Xfake_nominal, tmp2], axis= 1)
#name the columns appropriately
df_Xfake_nominal.columns= nominalColumns
## Merge the continuous and nominal synthetic data to one df
df_Xfake= pd.concat([df_Xfake_continuous, df_Xfake_nominal], axis= 1)
#match the same layout of the original dataset
df_Xfake= df_Xfake[ [i for i in list(FHL_bank.columns) + redudantColumns if i not in list(FHL_bank.columns) or i not in___
 →redudantColumns] ]
```

[122]: display(df_Xfake.head()[df_Xfake.columns[:11]])

	Bank	FIPSStateCode	FIPSCountyCode	MSA	Tract	MinPer	TraMedY	LocMedY	Tractrat	Income	CurAreY
0	Cincinnati	39	61	15,782.47	168.61	0.93	66,082.29	57,131.52	1.14	18,225.54	61,375.05
1	Pittsburgh	42	119	20,414.34	49.24	48.79	75,290.76	85,041.13	0.77	80,696.87	90,718.98
2	Topeka	20	65	99,998.99	7,899.64	24.09	57,703.41	58,268.30	0.92	15,749.39	56,595.93
3	Cincinnati	13	121	16,844.86	8,401.20	53.23	78,219.19	77,038.09	0.97	257,826.18	77,046.98
4	Chicago	17	119	25,068.78	695.42	15.85	109,221.54	68,532.93	1.60	44,106.94	73,211.93

8.2 Save Generator and synthetic dataset either locally or on the cloud:

[123]: LCL= True

Chapter 9

Experimental

We add one more robustness check to validate the performance of generative models. The idea is to utilize a machine learning classifier to try and learn the difference between the true data and the synthetic data generated by a calibrated *Generator*. In case the ML model fails to find a hyperplane that separates the real and synthetic data, and allocates a 50% probability of a sample coming from either the real or synthetic dataset, we can conclude that the synthetic data is highly similar to the original dataset. We choose the XGBoost classifier for the exercise, as it has the best performance on Kaggle for binary classification problems.

9.1 Import libs to setup XGBoost model

```
[125]: ## XGBoost libs
from xgboost import XGBClassifier
from sklearn.model_selection import train_test_split
from sklearn.metrics import (accuracy_score, confusion_matrix,
    classification_report, recall_score, precision_score)
```

9.2 Create one randomly mixed dataset containing both real world and synthetic samples

The mixed dataset contains random samples drawn from both the real world dataset as well as from data directly generated by our calibrated *Generator*. We add a boolean target variable to the mixed dataset, with 1 representing the fact that the observation is drawn from the *Generator* and 0 indicating that the observation is a real world sample. We further make the distinction between a mixed dataset that is not yet post-processed, and one that is fully post-processed and is identicial

(in terms of meta schema) to the original dataset. We also make a further distinction between continous and discrete data, such that we can further pinpoint where the *Generator* potentially fails to produce high quality data.

```
[129]: ## Create one dataset consisting of real and fake data
      # -----
      ## Entire dataset (not post-processed)
      # ______
      #Generate mixed dataset
      n_samples= 10 #len(FHL_bank)
      Xfake, _= generate_artificial_samples(g_model, noise_dim, n_samples)
      Xreal, _= generate_real_samples(dataset, n_samples)
      #synthetic data gets labeled with 1
      Xfake_new= np.ones((n_samples, Xfake.shape[1]+1))
      Xfake_new[:,:-1] = Xfake
      #real data gets labeled with 0
      Xreal_new= np.zeros((n_samples, Xfake.shape[1]+1))
      Xreal_new[:,:-1] = Xreal
      #combine synthetic and real data
      df_XGBOOST_Entire= np.concatenate( (Xfake_new, Xreal_new), axis=0)
      ## Entire dataset (post-processed)
      # -----
      #synthetic data gets labeled with 1
      Xfake_new= np.ones((n_samples, df_Xfake.shape[1]+1))
      df_Xfake = df_Xfake.apply(lambda col:pd.Categorical(col).codes) # Convert categories of dataset to type int
      Xfake_new[:,:-1] = df_Xfake.iloc[:n_samples, :]
      #real data gets labeled with 0
      Xreal_new= np.zeros((n_samples,df_Xfake.shape[1]+1))
      FHL_bank = FHL_bank.apply(lambda col:pd.Categorical(col).codes) # Convert categories of dataset to type int
      Xreal_new[:,:-1] = FHL_bank[ continuousColumns + nominalColumns].sample(n = n_samples)
      #combine synthetic and real data
      df_XGBOOST_Entire_processed= np.concatenate( (Xfake_new, Xreal_new), axis=0)
```

```
## Nominal dataset (not post-processed)
#generate data
Xfake, _= generate_artificial_samples(g_model, noise_dim, n_samples)
Xreal, _= generate_real_samples(dataset, n_samples)
Xfake_nominal= Xfake[:, dimContinuous:]
Xreal_nominal= Xreal[:, dimContinuous:]
#synthetic data gets labeled with 1
Xfake_new= np.ones((n_samples, Xfake_nominal.shape[1]+1))
Xfake_new[:,:-1] = Xfake_nominal
#real data gets labeled with 0
Xreal_new= np.zeros((n_samples, Xreal_nominal.shape[1]+1))
Xreal_new[:,:-1] = Xreal_nominal
#combine synthetic and real data
df_XGBOOST_Nominal= np.concatenate( (Xfake_new, Xreal_new), axis=0)
## Nominal dataset (post-processed)
# -----
#synthetic data gets labeled with 1
Xfake_new= np.ones((n_samples, df_Xfake_nominal.shape[1]+1))
df_Xfake_nominal = df_Xfake_nominal.apply(lambda col:pd.Categorical(col).codes) # Convert categories of dataset to type__
 \rightarrow int
Xfake_new[:,:-1] = df_Xfake_nominal.iloc[:n_samples, :]
#real data gets labeled with 0
Xreal_new= np.zeros((n_samples,df_Xfake_nominal.shape[1]+1))
datasetNominal = datasetNominal.apply(lambda col:pd.Categorical(col).codes) # Convert categories of dataset to type int
Xreal_new[:,:-1] = datasetNominal.sample(n= n_samples)
#combine synthetic and real data
df_XGBOOST_Nominal_processed= np.concatenate( (Xfake_new, Xreal_new), axis=0)
## Continuous dataset (not post-processed)
```

```
#generate data
      Xfake, _= generate_artificial_samples(g_model, noise_dim, n_samples)
      Xreal, _= generate_real_samples(dataset, n_samples)
      Xfake_continuous= Xfake[:,0:dimContinuous]
      Xreal_continuous= Xreal[:, 0:dimContinuous]
       #synthetic data gets labeled with 1
      Xfake_new= np.ones((n_samples, Xfake_continuous.shape[1]+1))
      Xfake_new[:,:-1] = Xfake_continuous
       #real data gets labeled with 0
      Xreal_new= np.zeros((n_samples, Xreal_continuous.shape[1]+1))
       Xreal_new[:,:-1] = Xreal_continuous
       #combine synthetic and real data
       df_XGBOOST_Continuous= np.concatenate( (Xfake_new, Xreal_new), axis=0)
       ## Continuous dataset (post-processed)
       #synthetic data gets labeled with 1
      Xfake_new= np.ones((n_samples, df_Xfake_continuous.shape[1]+1))
      Xfake_new[:,:-1] = df_Xfake_continuous.iloc[:n_samples, :]
       #real data gets labeled with 0
       Xreal_new= np.zeros((n_samples,df_Xfake_continuous.shape[1]+1))
       Xreal_new[:,:-1] = datasetContinuous.sample(n= n_samples)
       #combine synthetic and real data
       df_XGBOOST_Continuous_processed= np.concatenate( (Xfake_new, Xreal_new), axis=0)
[130]: ## Train and evaluate XGBOOST using different datasets
       # Initialize loop
       datasets_XGBOOST= [df_XGBOOST_Entire, df_XGBOOST_Entire_processed,
                          df_XGBOOST_Nominal, df_XGBOOST_Nominal_processed,
                          df_XGBOOST_Continuous, df_XGBOOST_Continuous_processed]
       names= ['Entire dataset', 'Entire dataset + processed',
               'Nominal dataset', 'Nominal dataset + processed',
```

```
'Continuous dataset', 'Continuous dataset + processed']
j= 0
# Main loop
for everyDataset in datasets_XGBOOST:
  ## Create train and training set
 #qet labels
 X= everyDataset[:,0:-1]
 y= everyDataset[:,-1]
 #setup train en test sets
 seed = 1
 test size = 0.33
 X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=test_size, random_state=seed)
  ## Train model and get accuracy on test set
 model = XGBClassifier(use_label_encoder=False, eval_metric= 'error')
 model fit(X_train, y_train);
 y_pred = model.predict(X_test)
 predictions = [round(value) for value in y_pred]
 accuracy = accuracy_score(y_test, predictions)
 \rightarrow 100.0)))
# if j % 2 != 0:
  print('----')
 j += 1
```

The accuracy of the trained XGBoost model on the Entire dataset is equal to: 57.14%

The accuracy of the trained XGBoost model on the Entire dataset + processed is equal to: 100.00%

The accuracy of the trained XGBoost model on the Nominal dataset is equal to: 57.14%

The accuracy of the trained XGBoost model on the Nominal dataset + processed is equal to: 100.00%

The accuracy of the trained XGBoost model on the Continuous dataset is equal to: 71.43%

The accuracy of the trained XGBoost model on the Continuous dataset + processed is equal to: 71.43%

The results of the robustness check are quite interesting. When looking at the accuracy of the classifier for the unprocessed dataset, we see a performance close to 50%. This indicated that indeed the *Generator* is able to create synthetic data that is statistically almost indistinguishable from the real data. However, as soon as the synthetic data is post-processed, the classifier is able to perfectly distinguish the data from the original dataset.

We can try to pinpoint the reason of this behaviour by splitting the data into two subsets: continuous and discrete variables. Looking at the subset of continuous variables, we see consistent performance across unprocessed and post-processed data with the classifier achieving an accuracy of about 70%. Looking at the subset of discrete data however, we see inconsistencies across unprocessed and post-processed data. Although the performance of the classifier is only 57% with unprocessed data, it achieved a perfect score when it comes to post-processed discrete data. This indicates that the processing of discrete data needs to be further investigated. Although the model trained has probably not yet achieved convergence (indicating the possibility of better performance with continuous data), this won't matter too much with the performance of post-processed discrete data.