## Denoising Autoencoder to Fill Missing Values

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Harvard Extension School

## Introduction

- Denoising Autoencoder can be used to reconstruct damaged data.
- But...
  - Does it work with all kind of data?
  - Is it superior to other techniques?

- Performance comparison for 3 problems:
  - Only continuous variables;
  - Only categorical variables; and
  - Continuous and categorical variables.
- How to implement autoencoder for each of these situations.

Github: <a href="https://github.com/MaxWienandts/Denoising Autoencoder for Missing Data Imputation">https://github.com/MaxWienandts/Denoising Autoencoder for Missing Data Imputation</a>

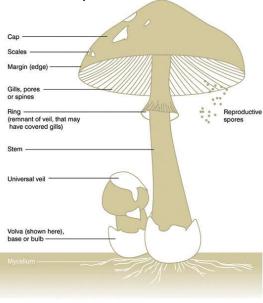
## The Data

- Wine Quality (<a href="https://archive.ics.uci.edu/dataset/186/wine+quality">https://archive.ics.uci.edu/dataset/186/wine+quality</a>)
  - Problem: Prediction of wine type (red or white);
  - Observations: 6,497;
  - Variables: 11 physicochemical continuous variables.
- Mushroom Dataset

(https://archive.ics.uci.edu/dataset/848/secondary+mushroom+dataset)

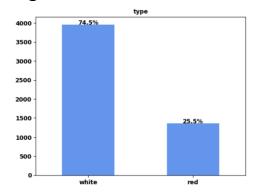
Problem: Prediction if a mushroom is edible or poisonous;

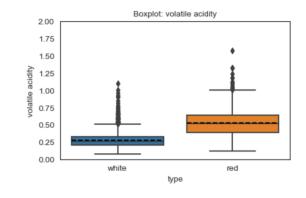
- Observations: 61,069;
- Variables: 20 physical characteristics:
  - 3 continuous;
  - 17 categorical.
- Two models:
  - Using only categorical variables;
  - Using all variables.



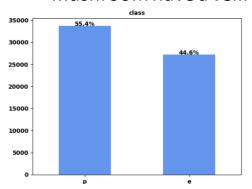
# **Exploratory Data Analysis**

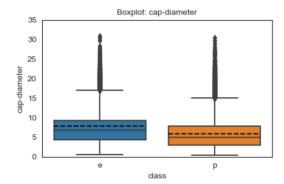
- Wine dataset:
  - Wine\1 EDA Denoising Autoencoder.ipynb;
  - No missing values.

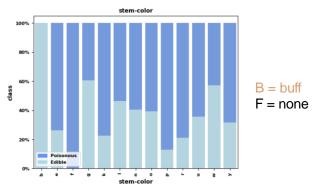




- Mushroom dataset:
  - Mushroom\1 EDA Denoising Autoencoder.ipynb;
  - There are missing values when a mushroom does not have a characteristic, i.e., not all mushroom have a veil.







4

## **Autoencoders**

- Wine dataset:
  - Wine\2 Denoising Autoencoder.ipynb
  - Coding: 8
  - Activation: SeLU
  - Loss function: Mean Squared Error

```
tf.keras.backend.clear_session()
model_encoder = models.Sequential([
   layers.Dense(8, activation = 'selu', input shape = [11])
1)
model decoder = models.Sequential([
   layers.Dense(11, activation = 'selu', input_shape = [8])
1)
model_autoencoder = models.Sequential([model_encoder, model_decoder])
model_autoencoder.compile(optimizer = keras.optimizers.SGD(learning_rate = 0.05),
                 loss = 'mse', metrics = ['mse'])
model autoencoder.summary()
Model: "sequential_2"
Layer (type)
                         Output Shape
                                               Param #
______
 sequential (Sequential)
                                               96
                         (None, 8)
 sequential_1 (Sequential)
                         (None, 11)
                                               99
_____
Total params: 195
Trainable params: 195
Non-trainable params: 0
```

## **Autoencoders**

- Mushroom dataset (only categorical variables):
  - Mushroom \2 Denoising Autoencoder only Category.ipynb
  - Coding: 90 (there are 92 dummies in total)
  - Activation: ReLU and sigmoid (It is a good idea to map results to 0 and 1)
  - Loss function: Binary Cross Entropy

```
input shape = X train aux.shape[1]
tf.keras.backend.clear session()
model encoder = models.Sequential([
    layers.Dense(90, activation = 'relu', input shape = [input shape]),
    layers.Dense(90, activation = 'sigmoid', input_shape = [90])
1)
model decoder = models.Sequential([
    layers.Dense(90, activation = 'relu', input_shape = [90]),
   layers.Dense(input shape, activation = 'sigmoid', input shape = [90])
])
model autoencoder = models.Sequential([model encoder, model decoder])
model autoencoder.compile(optimizer = keras.optimizers.SGD(learning rate = 0.05),
                   loss = 'binary crossentropy', metrics = ['binary accuracy'])
Model: "sequential_2"
                        Output Shape
 Layer (type)
                                              Param #
                             _____
 sequential (Sequential)
                        (None, 90)
                                              16560
 sequential_1 (Sequential)
                        (None, 92)
                                              16562
______
Total params: 33,122
Trainable params: 33,122
Non-trainable params: 0
```

## **Autoencoders**

- Mushroom dataset (categorical and continuous variables):
  - Mushroom \2 Denoising Autoencoder Continuous and category.ipynb
  - Coding: 93 (there are 92 dummies plus 3 continuous variables)
  - Activation: ReLU and sigmoid (It is a good idea to map results to 0 and 1)
  - Loss function: Mean Squared Error and Binary Cross Entropy

```
input shape = X train aux.shape[1]
                                                                                                                                             Model: "model"
output continuous shape = X train continuous original.shape[1]
output_category_shape = X_train_category_original.shape[1]
                                                                                                                                             Layer (type)
                                                                                                                                                                                Output Shape
tf.keras.backend.clear_session()
                                                                                                                                              input 1 (InputLayer)
                                                                                                                                                                                [(None, 95)]
inputs = tf.keras.layers.Input(shape=(input_shape,))
encoder_1 = layers.Dense(units = 93, activation = 'relu')(inputs)
                                                                                                                                              dense (Dense)
                                                                                                                                                                                (None, 93)
encoder_2_continuous = layers.Lambda(lambda x: x[:, 0: output_continuous_shape])(encoder_1)
encoder_2_category_aux = layers.Lambda(lambda x: x[:, output_continuous_shape: ])(encoder_1)
encoder_2_category = layers.Dense(units = 90, activation = 'sigmoid')(encoder_2_category_aux)
                                                                                                                                              lambda 1 (Lambda)
                                                                                                                                                                                (None, 90)
encoder_3 = layers.Concatenate(axis=1)([encoder_2_continuous, encoder_2_category])
                                                                                                                                              lambda (Lambda)
                                                                                                                                                                                (None, 3)
decoder 1 = layers.Dense(units = 93, activation = 'relu')(encoder 3)
decoder_2_continuous = layers.Lambda(lambda x: x[:, 0: output_continuous_shape], name = 'decoder_2_continuous')(decoder_1)
                                                                                                                                              dense 1 (Dense)
                                                                                                                                                                                 (None, 90)
decoder 2 category aux = layers.Lambda(lambda x: x[:, output continuous_shape: ])(decoder_1)
decoder_2_category = layers.Dense(units = output_category_shape, activation = 'sigmoid', name = 'decoder_2_category')(encoder_2_category_aux)
                                                                                                                                              concatenate (Concatenate)
                                                                                                                                                                                (None, 93)
model_autoencoder = models.Model(inputs = inputs, outputs = [decoder_2_continuous, decoder_2_category])
model_autoencoder.compile(optimizer = keras.optimizers.SGD(learning_rate = 0.05),
                                                                                                                                             dense 2 (Dense)
                                                                                                                                                                                (None, 93)
                          loss = {'decoder_2_continuous': 'mse',
                                  'decoder_2_category': 'binary_crossentropy'},
                                                                                                                                              decoder 2 continuous (Lambda)
                                                                                                                                                                                (None, 3)
                          metrics = {'decoder_2_continuous': 'mse',
                                     'decoder_2_category': 'binary_accuracy'}
                                                                                                                                              decoder_2_category (Dense)
                                                                                                                                                                                (None, 92)
model_1_history = model_autoencoder.fit(X_train_aux, (X_train_continuous_original, X_train_category_original)
                                       , validation_data = [X_val_aux, (X_val_continuous_original, X_val_category_original)]
                                                                                                                                             Total params: 34,232
                                       , verbose = 1
                                                                                                                                             Trainable params: 34,232
                                       , epochs = 100)
                                                                                                                                             Non-trainable params: 0
```

Layer (type)

Output Shape
Param # Connected to

input\_1 (InputLayer) [(None, 95)] 0 []

dense (Dense) (None, 93) 8928 ['input\_1[0][0]']

lambda\_1 (Lambda) (None, 90) 0 ['dense[0][0]']

lambda (Lambda) (None, 3) 0 ['dense[0][0]']

dense\_1 (Dense) (None, 90) 8190 ['lambda\_1[0][0]']

concatenate (Concatenate) (None, 93) 0 ['lambda[0][0]', 'dense\_1[0][0]']

dense\_2 (Dense) (None, 93) 8742 ['concatenate[0][0]']

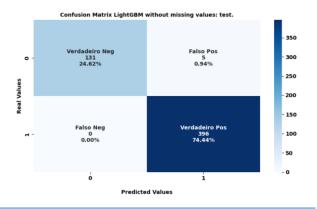
decoder\_2\_continuous (Lambda) (None, 3) 0 ['dense\_2[0][0]']

decoder\_2\_category (Dense) (None, 92) 8372 ['lambda\_1[0][0]']

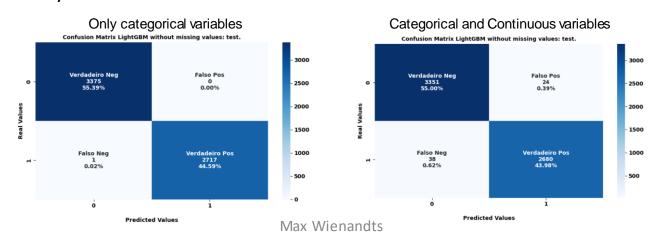
Total params: 34,232
Trainable params: 34,232
Non-trainable params: 0

# LightGBM without missing

- Wine:
  - Wine\2 Denoising Autoencoder.ipynb
  - Test set represent 10% of the data unseen by the model
  - Accuracy: 99%



- Mushroom (only categorical variables):
  - Mushroom \2 Denoising Autoencoder only Category.ipynb
  - Mushroom \2 Denoising Autoencoder Continuous and category.ipynb
  - Test set represent 10% of the data unseen by the model
  - Accuracy: 99%



# Missing Values Simulation

- 18 datasets for each problem were created
- Each dataset with a different proportion of randomly fabricated missing values. Proportions used: .05, .10, .15, .20, .25, .30, .35, .40, .45, .50, .55, .60, .65, .70, .75, .80, .85, .90
- For both mushroom studies, the missing values were only created in the categorical variables. First, the variables were one-hot encoded. After, each value was randomly set to zero.

## Results: Wine Dataset

LightGBM without denoising autoencoder: Missing values were filled with the median.

0.4

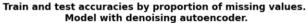
**Missing proportion** 

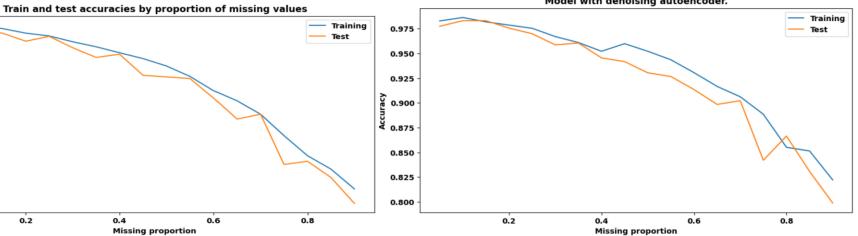
0.6

0.80

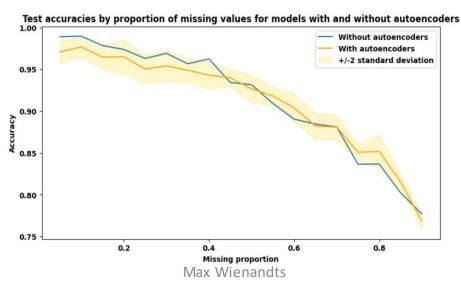
0.2

LightGBM with denoising autoencoder:





Comparison with and without autoencoder using bootstrap.



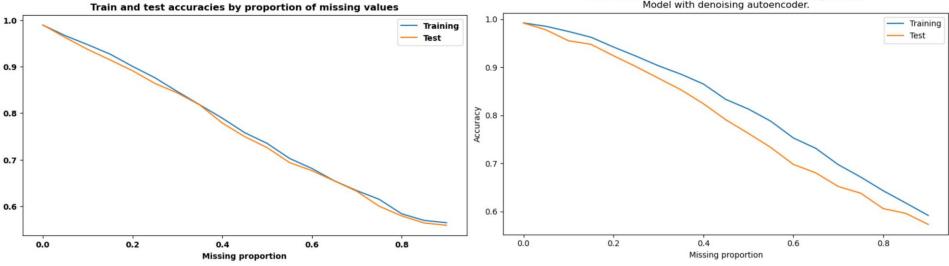
# Results: Mushroom Only Categoric

LightGBM without denoising autoencoder: Missing values were filled with the median.

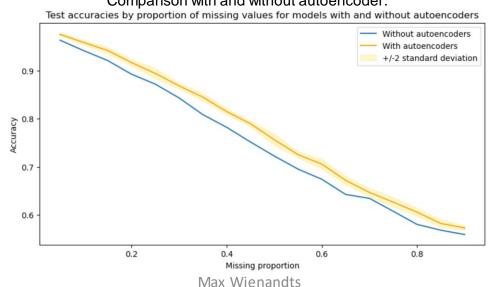
#### LightGBM with denoising autoencoder:

Train and test accuracies by proportion of missing values.

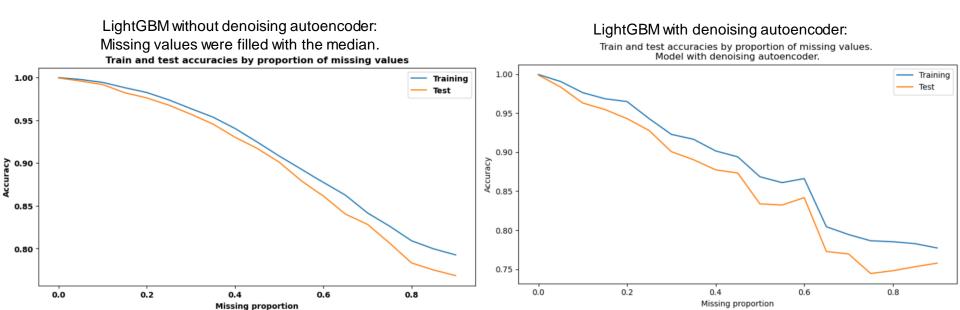
Model with denoising autoencoder.



#### Comparison with and without autoencoder.



## Results: Mushroom all variables



#### Comparison with and without autoencoder.

