

UNIVERSITY OF CATANIA DEPARTMENT OF ECONOMICS & BUSINESS MASTER'S DEGREE IN DATA SCIENCE FOR MANAGEMENT

Neural Computing Project Sephora Sales Data

Ylenia Messina – 1000008815

Index

1. Introduction	1
1.1. Dataset: Sephora Sales	1
1.2. Data Cleaning	3
2. Exploratory Analysis	8
2.1. Numerical variables	9
2.2. Categorical variables	14
2.3. Binary variables	14
3. Problem designing	17
3.1. Data pre-processing	17
4. Architecture setting	20
5. Hyperparameters optimization	27
6. Training & Testing	32

1 Introduction

The work in this project is aimed at building a neural network infrastructure in the context of a classification problem.

```
[]: # Import libraries & modules
     import io
     import requests
     import warnings
     warnings.filterwarnings('ignore')
     import pandas as pd
     import numpy as np
     import matplotlib.pyplot as plt
     import seaborn as sns
     from sklearn.model_selection import train_test_split
     from sklearn.preprocessing import RobustScaler
     from sklearn.metrics import confusion_matrix
     import torch
     from torch import nn
     import torch.utils.data as dt
     # Set seed for results reproducibility
     random_seed = 42
     torch.manual_seed(random_seed)
     np.random.seed(random_seed)
```

1.1 Dataset: Sephora Sales

```
[]: # Import dataset from Github
github_session = requests.Session()
github_session.auth = ('yleniamess', 'e5285f9bd63591528490fa3ae9053e8cff4dde61')

url = "https://raw.githubusercontent.com/yleniamess/neural-computing-project/

→main/sephora_sales.csv?token=ASJN3JDYGQQQTU5GUI7NOP3ABSAOK"
```

Number of observations: 9168; Number of features: 20

```
[]: id brand ... limited_edition limited_time_offer 0 2218774 Acqua Di Parma ... 0 0 0 1 2044816 Acqua Di Parma ... 0 0 0 2 1417567 Acqua Di Parma ... 0 0 0 3 1417617 Acqua Di Parma ... 0 0 0 4 2218766 Acqua Di Parma ... 0 0 0
```

[5 rows x 20 columns]

The dataset used includes information about *Sephora sales*, the French multinational retailer of personal care and beauty products.

It consists of **9168 observations** (products) and **20 features** with mixed datatypes:

- 1. **id** (*integer*): id of the product;
- 2. **brand** (*object*): brand of the product at Sephora's website;
- 3. **category** (*object*): category of the product at Sephora's website;
- 4. **name** (*object*): name of the product at Sephora's website;
- 5. **size** (*object*): size of the product;
- 6. **rating** (*float*): customers can rate a product on a scale of 1 to 5 stars, so a product rating represents the average number of stars;
- 7. **number_of_reviews** (*integer*): number of reviews of the product;
- 8. **love** (*integer*): number of people loving the product, that is number of people who flagged the "heart" icon on the product sheet;
- 9. **price** (*float*): price of the product;
- 10. **value_price** (*float*): value price of the product (for discounted products) that is the perceived or estimated value of the product for the customer;
- 11. **MarketingFlags** (boolean): marketing flags of the product from the website if they were exclusive or sold online only etc.;
- 12. MarketingFlags_content (object): kinds of marketing flags of the product;
- 13. **options** (object): options available on the website for the product such as colors and sizes;
- 14. **details** (*object*): details of the product available on the website;
- 15. **how_to_use** (*object*): instructions on how to use the product (if available);
- 16. **ingredients** (*object*): ingredients of the product (if available);
- 17. **online_only** (*integer*): whether the product is sold online only;
- 18. **exclusive** (*integer*): whether the product is sold exclusively on Sephora's website;
- 19. **limited_edition** (*integer*): whether the product is limited edition;
- 20. **limited_time_offer** (integer): whether the product has a limited time offer.

```
[]: # View the type of each feature data.dtypes
```

```
[]: id
                                   int64
     brand
                                  object
     category
                                  object
                                  object
     name
     size
                                  object
     rating
                                 object
     number_of_reviews
                                 float64
     love
                                 float64
     price
                                float64
     value_price
                                 float64
     MarketingFlags
                                  object
     MarketingFlags_content
                                  object
     options
                                  object
     details
                                  object
     how_to_use
                                  object
     ingredients
                                  object
     online_only
                                  object
     exclusive
                                  object
     limited_edition
                                  object
     limited_time_offer
                                  object
     dtype: object
```

1.2 Data cleaning

This first section is dedicated to the preliminary phase of data cleaning, which resulted in a resetting of the general shape of the dataset.

In particular:

- The number of features was reduced to 10, dropping those features considered not so useful for the purpose of the analysis, such as the *id* feature, as well as the ones with textual content (brand, size, options, details etc.), and also MarketingFlags and MarketingFlags_content since they were basically a repetition of the binary variables online_only, exclusive, limited_edition and limited_time_offer.
- The number of observations was reduced as well, as a consequence of the removal of all the rows containing missing values and/or wrong records (whose presence was due to an incorrect configuration of the csv format file used to store the data). Furthermore, as it will be seen in the exploratory analysis section, a large portion of *outliers* was removed too.

```
'options',
                        'details'.
                        'how_to_use',
                        'ingredients'], axis=1)
     # Check if there are any duplicates
     data.duplicated().any()
[]: False
[]: # Set 'name' column as dataframe index
     data = data.set_index('name')
     print('Number of observations: ', data.shape[0],'; Number of features: ', data.
     \hookrightarrowshape[1])
     data.head()
    Number of observations: 9168; Number of features: 10
[]:
                                       category ... limited_time_offer
    name
                                                                     0
     Blu Mediterraneo MINIATURE Set Fragrance
     Colonia
                                        Cologne ...
                                                                     0
                                        Perfume ...
     Arancia di Capri
                                                                     0
     Mirto di Panarea
                                        Perfume ...
                                                                     0
     Colonia Miniature Set
                                                                     0
                                      Fragrance ...
     [5 rows x 10 columns]
[]: # Check for missing values
     data.isnull().sum()
                            0
[]: category
                            5
     rating
    number_of_reviews
                            5
     love
                            5
                            3
    price
    value_price
                            3
     online_only
                            43
     exclusive
                           29
     limited edition
                            27
     limited_time_offer
                            21
     dtype: int64
[]: # Remove observations with missing values (nan values)
     initial_n_obs = data.shape[0]
     data = data.dropna(0)
```

```
print("Removed", (initial_n_obs - data.shape[0]), "observations that contained \_ \_ missing values.")
```

Removed 52 observations that contained missing values.

Despite having apparently removed all the missing values reported as "nan", a more accurate exploration of the features taken one by one brought to light the presence of further missing values, however, labeled by strings such as "unknown", "no category". Even "0" is to be considered as missing value as regards the **rating** feature for which the minimum value is 1, inasmuch 0 would indicate that no rating has been left to the product by the customer who purchased it. Consequently, such observations were removed.

Furthermore, in some features there are wrong values pertaining to other features. This circumstance is due to the fact that the initial features with textual content such as *ingredients*, *details* etc. contain commas, and since the dataset is a comma-delimited csv file, it resulted in an incorrect import of the latter. Therefore, further observations were obviously removed.

```
[]: ## Remove missing values and wrong records
     initial_n_obs = data.shape[0]
     # category
     data = data[data.category != "no category"]
     # rating
     data = data.drop(data[(data.rating == "0")].index)
     data = data.drop(data[data.rating == " gel: 0.0253 oz/ 0.75 mL"].index)
     data = data.drop(data[data.rating == " 0.33 oz/ 10 mL each"].index)
     data = data.drop(data[data.rating == " 0.08 oz/2.5 g Catch The Light_
     →Highlighter"].index)
     data = data.drop(data[data.rating == " 0.08 oz/2.5 g Catch The Light_
     →Highlighter"].index)
     data['rating'] = data['rating'].astype('float64')
     # online_only
     data = data[(data.online_only == "0") | (data.online_only == "1")]
     data['online_only'] = data['online_only'].astype('uint8')
     # exclusive
     data = data[(data.exclusive == "0") | (data.exclusive == "1")]
     data['exclusive'] = data['exclusive'].astype('uint8')
     # limited edition
     data = data[(data.limited_edition == "0") | (data.limited_edition == "1")]
     data['limited_edition'] = data['limited_edition'].astype('uint8')
     # limited_time_offer
     data = data[(data.limited_time_offer == "0") | (data.limited_time_offer == "1")]
     data['limited_time_offer'] = data['limited_time_offer'].astype('uint8')
```

Removed 711 observations that contained missing values or wrong records.

The **category** feature - as the name itself suggests - lent itself well to be used as a *categorical* variable. So, all its values were grouped among 6 categories, each one identifying a different type of beauty/personal care product (*skincare*, *makeup*, *bath_body*, *hair*, *fragrance*, *other*).

```
[]: # Transform 'category' feature into a categorical one
     skincare = ["Anti-Aging", "Blemish & Acne Treatments", "Decollete & Neck Creams", u
      "Eye Masks", "Face Masks", "Face Oils", "Face Serums", "Face

Sets", "Face Wash",

                 "Face Wash & Cleansers", "Face Wipes", "Facial Cleansing
      →Brushes", "Facial Peels",
                 "Facial Rollers", "For Face", "Face Brushes", "Moisturizer &
      \hookrightarrowTreatments", "Moisturizers",
                 "Night Creams", "Sheet Masks", "Skincare", "Skincare Sets", "Toners"]
     makeup = ["BB & CC Cream", "BB & CC Creams", "Blotting,
      →Papers", "Blush", "Bronzer", "Brush Sets",
               "Cheek Palettes", "Eye Palettes", "Color__
      →Correct", "Concealer", "Contour", "Eye Brushes",
               "Eye Sets", "Eyelash Curlers", "Eye Cream", "Eye Creams & ...
      →Treatments", "Eye Primer", "Eyebrow",
               "Eyeliner", "Eyeshadow", "Face Primer", "False
      →Eyelashes", "Foundation", "Highlighter", "Lid Shadow Brush",
               "Lip Balm & Treatment", "Lip Balms & Treatments", "Lip Brushes", "Lip_
      →Gloss", "Lip Liner", "Lip Plumper",
               "Lip Sets", "Lip Stain", "Lip Sunscreen", "Lip___
      →Treatments", "Lipstick", "Liquid Lipstick", "Makeup",
               "Makeup & Travel Cases", "Makeup Bags & Travel Cases", "Makeup
      →Palettes", "Makeup Removers", "Mascara",
               "Powder Brush", "Setting Spray & Powder", "Tinted Moisturizer"]
     bath_body = ["Bath & Body", "Bath & Shower", "Bath Soaks & Bubble Bath", "Body_
      "Body Moisturizers", "Body Products", "Body Sprays &∟
      →Deodorant", "Body Wash & Shower Gel",
                  "Cellulite & Stretch Marks", "Deodorant &
      →Antiperspirant", "Deodorant for Men", "Hand Cream & Foot Cream",
                  "Scrub & Exfoliants", "Lotions & Oils", "For Body"]
     hair = ["Color Care", "Conditioner", "Curling Irons", "Curls & Coils", "Hair"
     →, "Hair Accessories", "Hair Brushes & Combs",
```

```
"Hair Dryers", "Hair Masks", "Hair Oil", "Hair Primers", "Hair
 →Products", "Hair Spray", "Hair Straighteners & Flat Irons",
        "Hair Styling & Treatments", "Hair Styling Products", "Hair Thinning &
→Hair Loss", "Scalp & Hair Treatments", "Shampoo",
        "Dry Shampoo", "Leave-In Conditioner", "Shampoo & Conditioner"]
fragrance = ["Body Mist & Hair Mist", "Mists & Essences", "Cologne",
             "Cologne Gift Sets", "Fragrance", "Perfume",
             "Perfume Gift Sets", "Rollerballs & Travel Size"]
other = ["Accessories", "After Sun Care", "Aftershave", "Beauty Supplements",
         "Body Sunscreen", "Brush Cleaners", "Candles", "Candles & Home,
 →Scents", "Cleansing Brushes",
         "Diffusers", "Face Sunscreen", "Hair Removal", "Hair Removal &
 →Shaving", "High Tech Tools",
         "Holistic Wellness", "Mini Size", "Mirrors & Sharpeners", "Nail", "Self (

¬Tanners", "Shaving",

         "Spa Tools", "Sponges & Applicators", "Sunscreen", "Teeth
 →Whitening", "Tweezers & Eyebrow Tools",
         "Value & Gift Sets", "Wellness"]
for x in data['category']:
    if x in skincare:
        data.category[data.category == x] = "skincare"
    elif x in makeup:
        data.category[data.category == x] = "makeup"
    elif x in bath_body:
        data.category[data.category == x] = "bath_body"
    elif x in hair:
        data.category[data.category == x] = "hair"
    elif x in fragrance:
        data.category[data.category == x] = "fragrance"
    elif x in other:
        data.category[data.category == x] = "other"
data['category'] = data['category'].astype('category')
data['category'].cat.categories
```

```
[]: Index(['bath_body', 'fragrance', 'hair', 'makeup', 'other', 'skincare'], dtype='object')
```

Even the **rating** feature, as it will be better explained in the exploratory analysis section, was converted into a categorical one with **5** categories.

```
[]: # Convert 'rating' into categorical
for x in data['rating']:
    if 1 <= x < 2:</pre>
```

```
data.rating[data.rating == x] = "1 Star"
elif 2 <= x < 3:
    data.rating[data.rating == x] = "2 Stars"
elif 3 <= x < 4:
    data.rating[data.rating == x] = "3 Stars"
elif 4 <= x < 5:
    data.rating[data.rating == x] = "4 Stars"
elif x == 5:
    data.rating[data.rating == x] = "5 Stars"
data['rating'] = data['rating'].astype('category')
data['rating'].cat.categories</pre>
```

```
[]: Index(['1 Star', '2 Stars', '3 Stars', '4 Stars', '5 Stars'], dtype='object')
```

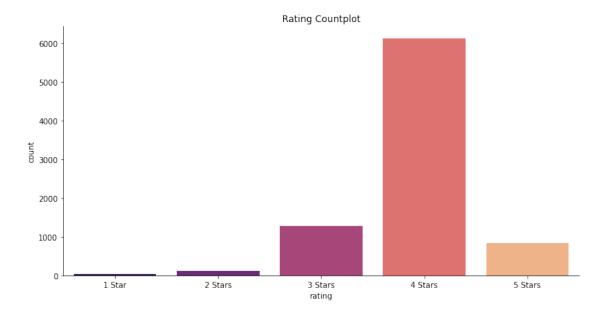
2 Exploratory Analysis

Firstly, let's focus on the **rating** feature, which is going to be considered as the response variable to predict in the classification problem. Customers can rate a product on a scale of 1 to 5 stars, so the overall product rating is computed as the sum of all the ratings made for that product divided by the number of people who rated. Obviously it is a continuous variable, as it can take any value in the range from 1 to 5 (0 if no one rated that product). However, the available dataset collected only products with a rating of 1, 1.5, 2, 2.5, 3, 3.5, 4, 4.5 or 5. Consequently, it seems to make more sense to treat this feature as a multi-class categorical variable rather than a continuous one: this is why it was transformed as such in data-cleaning process.

The countplot shows how the dataset is very *unbalanced*, containing a lot of observations (products) rated mostly with 4 Stars, and very few with a rating of 1 Star or 2 Stars.

```
[]: # Countplot
sns.catplot(x="rating", kind="count", palette="magma", data=data, aspect=2).

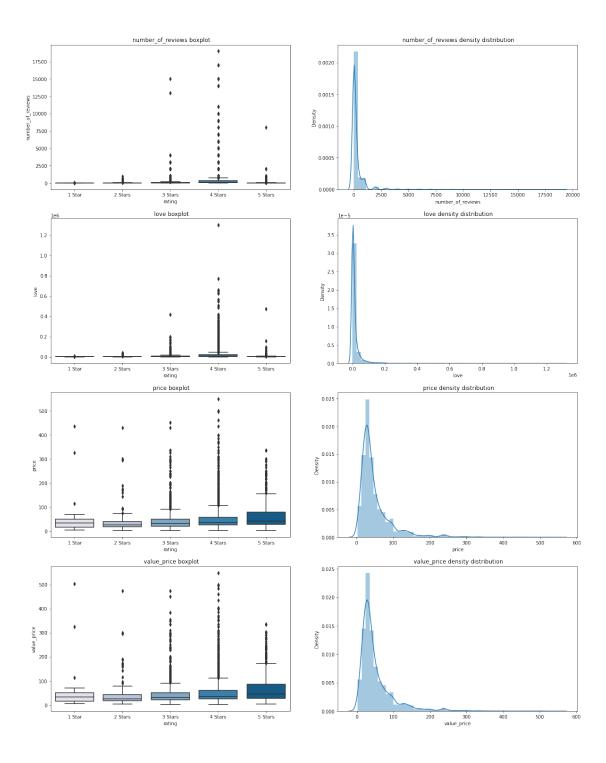
→set(title="Rating Countplot");
```



2.1 Numerical variables

Here, the *numerical* features **number_of_reviews**, **love**, **price** and **value_price** are analyzed, by visualizing their distribution as well as their boxplot with respect to the **rating** feature.

At first sight, we can only say how noisy the data are: the plots obtained are not so easy to interpret due to the presence of a significant number of outliers for all four variables.



Therefore, observations representing outliers were removed, in order to avoid as much as possible not to invalidate the analysis with any anomalies.

```
[]: # Remove outliers
initial_n_obs = data.shape[0]
```

Removed 4232 outliers.

Number of observations: 4173; Number of features: 10

However, not all outliers were removed: in particular the number of outliers for *number_of_reviews* is still large. But otherwise there was the risk of excessively reducing the dataset and lose those few observations with a rating of "1 Star". In fact, after the data cleaning process and the removal of the outliers, the dataset now counts 4173 observations out of the initial 9168.

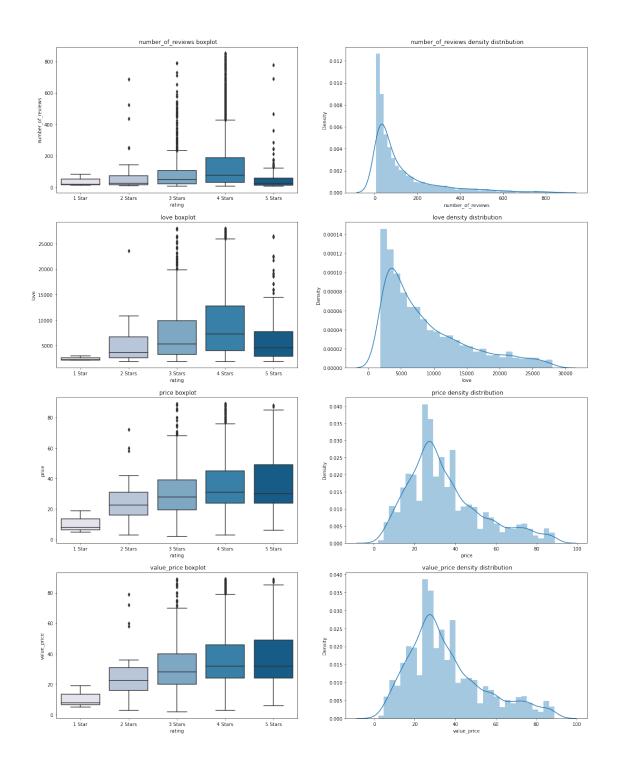
At least, we can now observe more clearly how <code>number_of_reviews</code> and <code>love</code> don't follow a gaussian distribution, being positively skewed instead. In fact, in the density distribution plots there are long right-tails. Also, in the boxplots the medians are closer to the bottom of the box, and the whiskers are shorter on the lower end of the box. Both plot characteristics indicate the asymmetrical natural of the features distribution (positive-skewness).

On the other hand, *price* and *value_price* boxplots suggest a more symmetric distribution. The density distribution plots are closer to a gaussian distribution, with some skewness on the right presumably due to the presence of outliers. However the presence of these observations with values further away from the median makes sense considering that the products with higher prices (and value prices) are a minority.

As regards number_of_reviews and love, it is assumed that the longer a product has been on the market, the more reviews it will have received and the more consent (love) it will have garnered from customers. In this sense, outliers are presumably those observations representing the "older" products.

```
[]: # Boxplot & density distribution after outliers removal
num_cols = data[['number_of_reviews','love','price','value_price']]
numerical = list(num_cols.columns.values)

fig, ax = plt.subplots(4, 2, figsize=(20,26))
ax = ax.ravel()
```



[]: round(num_cols.describe(), 2)

[]: number_of_reviews love price value_price count 4173.00 4173.00 4173.00 4173.00 mean 132.03 8804.22 35.03 35.61

std	159.77	6377.70	18.39	18.77
min	7.00	1900.00	2.00	2.00
25%	26.00	3800.00	22.50	23.00
50%	65.00	6700.00	30.00	30.00
75%	169.00	12200.00	45.00	45.00
max	852.00	28000.00	89.00	89.00

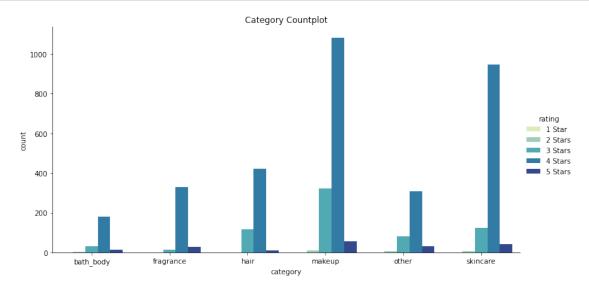
2.2 Categorical variables

The **category** feature is analyzed by visualizing its countplot, put in relationship with the **rating** feature.

We can observe that most of the products in the dataset belong to the "makeup" and "skincare" categories. The minority category is "bath_body". However, for each category, the countplot "shape" is almost the same, suggesting there is likely no difference between the groups of products in terms of rating behavior: as it was quite predictable, most of the products within each category are rated as "4 Stars".

```
[]: # Countplot
sns.catplot(x="category", hue='rating', kind="count", palette="YlGnBu",

data=data, aspect=2).set(title="Category Countplot");
```



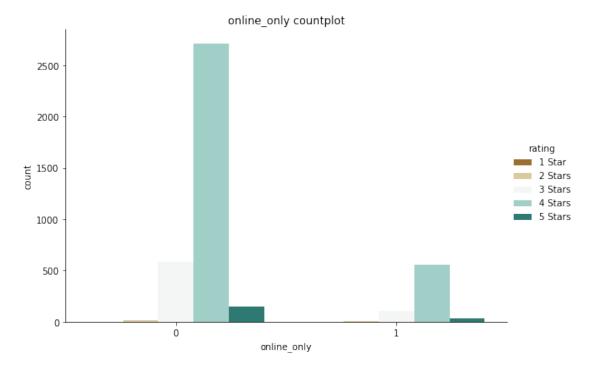
2.3 Binary variables

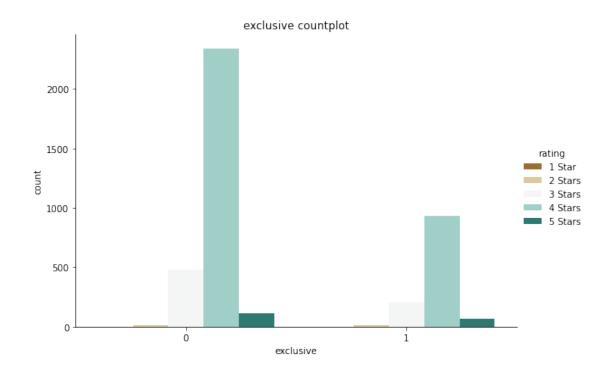
The binary features online_only, exclusive, limited_edition and limited_time_offer are analyzed by visualizing their countplot, put in relationship with the rating feature.

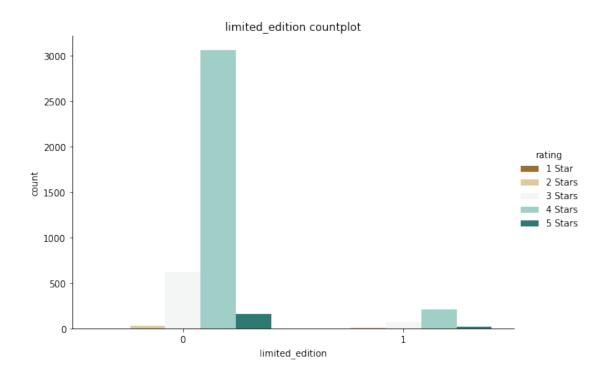
We can observe that only a minority of products is exclusive, sold online only, limited edition and/or offered in a limited time, which makes sense.

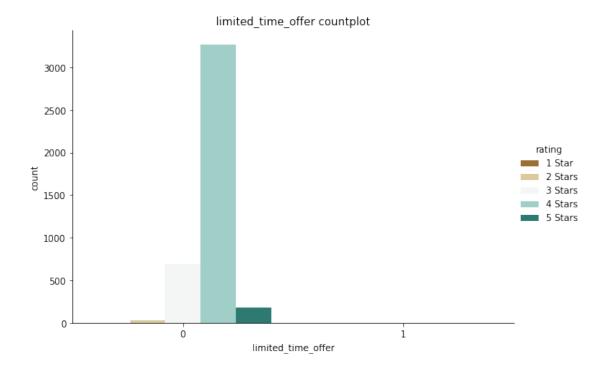
For each binary feature the proportional distribution of the counts among the rating classes is

almost the same, suggesting that whether the product has some marketing flags (online_only, exclusive, limited_edition, limited_time_offer) or not, it doesn't really affect in terms of rating behavior: most of the products are always rated with "4 Stars".









3 Problem designing

The problem outlined in this project is a **classification** problem: predict the **rating** - from 1 to 5 stars - of any product in the Sephora online catalog, starting from some of the quantitative and non-quantitative information that can be found on the Sephora webpage.

In this sense, the "rating" feature represents the *response* variable, while the *predictors* are the number of reviews for a product, the number of people loving the product, the price, the value-price as perceived by the customers, the category, and the information whether the product is sold online only, is exclusive, limited edition and/or offered for a limited time.

Before the neural network can be defined and built, data requires some pre-processing.

3.1 Data pre-processing

Firstly, both "rating" and "category" features need to be encoded due to their categorical datatype. Two different approaches are used to encode the variables.

Rating is label encoded, that is each label is simply converted to a number (starting from 0).

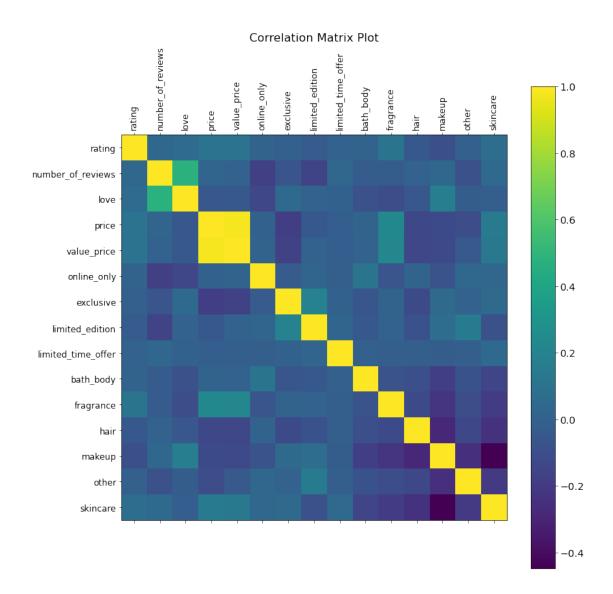
On the other hand, for *category* using an ordinal scale will not make sense as it conveys purely qualitative information. "One-hot encoding" is the most appropriate option. It consists in replacing the categorical feature with the creation of new so-called "dummy" variables – which are binary variables – one for each possible label of the original variable. For each observation, one-hot encoding assigns 1 to the dummy variable that represents the original label and 0 to all the others.

```
[]: # One-hot encoding 'category'
data = pd.concat([data, pd.get_dummies(data['category'])],axis=1).

→drop('category',axis=1)
```

From the analysis of the correlation matrix, we can observe that all predictors have approximately the same level of correlation - which is not particularly high, neither in positive nor in negative - with the *target* variable **rating**. We can instead notice, some stronger correlations between the predictor variables that were quite predictable, in particular:

- number_of_reviews and love are highly and positively correlated;
- price and value_price are even more positively correlated;
- dummy variables corresponding to the labels of the original 'category' variable, are negatively correlated between each other, especially *skincare* and *makeup*.



The dataset is then split in training and test set such that training test contains the 65% of the original observations while test set contains the remaining 35%.

Also, both training and test set are scaled, exploiting the "robust scaler" provided by scikit-learn library. This Scaler removes the median and scales the data according to the default IQR (Interquartile Range), which is the range between the 1st quartile (25th quantile) and the 3rd quartile (75th quantile). For that, such scaler is more robust to outliers than usual standardization done by removing the mean and scaling to unit variance (since outliers can often influence the sample mean / variance in a negative way).

```
[]: # Split into training and test set

target = data['rating']

data = data.drop('rating', axis=1)

train_features, test_features, train_labels, test_labels = 
→ train_test_split(data, target,
```

```
test_size = 0.35,

random_state = random_seed)

# Normalization
train_features = RobustScaler().fit_transform(train_features)
test_features = RobustScaler().fit_transform(test_features)

# Save dataframe with products names in test set (for later)
products = test_labels.index.to_frame()
products.index = range(len(products.index))
```

As emerged in the exploratory analysis, the dataset used is *unbalanced*. Therefore, also training and test sets obtained from the split are inevitably unbalanced in the same way.

Note that test set does not contain observations with a rating of "1 Star" (coded as class 0).

```
train_labels.value_counts(normalize=True)*100
[]: 3
          77.802360
     2
          16.887906
           4.719764
     4
     1
           0.516224
     0
           0.073746
     Name: rating, dtype: float64
[]: test_labels.value_counts(normalize=True)*100
[]: 3
          79.534565
     2
          15.742642
           3.696099
     4
     1
           0.958248
           0.068446
     0
     Name: rating, dtype: float64
```

At this point, data only need to be converted into tensors to serve as inputs for the neural network.

```
[]: # Convert data into tensor
train_features = torch.tensor(train_features, dtype=torch.float)
test_features = torch.tensor(test_features, dtype=torch.float)
train_labels = torch.tensor(train_labels, dtype=torch.long)
test_labels = torch.tensor(test_labels, dtype=torch.long)
```

4 Architecture setting

The most appropriate solution in terms of deep learning model is a basic feed-forward neural network. A feed-forward neural network is an artificial neural network where the information

moves in only one direction from the input nodes, through the hidden nodes (if any) and to the output nodes.

In this case, the information will move from the initial **14 input nodes** (the *predictor features*), and then eventually converge to a layer with **5 output nodes** (*rating classes*). Before **output layer**, information pass through a *ReLU* (*rectified linear activation function*) layer. The *ReLU* activation function basically will output the input directly if it is positive, otherwise it will output zero.

In order to define the number of *hidden layers* as well as the number of nodes that each of them should have, multiple alternatives with different configurations of the neural network were tested, using the resampling method of **k-fold cross validation**. Then, the architecture setting of the neural network that performed best was chosen.

The loss measure used is the **Cross-Entropy Loss**, also called "logarithmic loss" which measures the cross-entropy between the predicted and the actual value. This criterion combines the *Softmax activation function* principle and the *negative log likelihood loss*, but unlike negative log loss, cross-entropy also penalizes wrong but confident predictions and correct but less confident predictions, while negative log loss does not penalize according to the confidence of predictions. Also, Since the training set is unbalanced, the *nn.CrossEntropyLoss()* function was provided of the optional argument "weight", taking a 1D Tensor assigning weight to each of the 5 classes.

All nodes of each layer are initialized with values from a normal distribution using the "Xavier initialization" method in order to avoid stability issues while training (such as vanishing or exploding gradients). Each bias is instead initialized with the scalar value 0.

```
[]: # Construct a PyTorch data iterator
     def load_array(data_arrays, batch_size, is_train=True):
         dataset = dt.TensorDataset(*data_arrays)
         return dt.DataLoader(dataset, batch_size, shuffle=is_train)
     # Loss measure
     weights = torch.tensor([0.07, 0.51, 16.89, 77.80, 4.72])
     loss = nn.CrossEntropyLoss(weight=weights)
     # Define net with 1 or 2 hidden layers
     in features = train features.shape[1]
     out_labels = 5
     def get net(num nodes1, num nodes2):
         if num_nodes2 is not None:
           net = nn.Sequential(nn.Linear(in_features,num_nodes1),
                               nn.Linear(num_nodes1,num_nodes2),
                               nn.ReLU(),
                               nn.Linear(num_nodes2,out_labels))
         else:
           net = nn.Sequential(nn.Linear(in_features,num_nodes1),
                               nn.ReLU(),
                               nn.Linear(num nodes1,out labels))
         return net
```

```
# Initialize model parameters
def init_weights(m):
   if type(m) == nn.Linear:
        nn.init.xavier_normal_(m.weight)
        nn.init.zeros_(m.bias)
```

```
[]: # Train function
     def train(net, train features, train labels, test features, test labels,
               num_epochs, learning_rate, weight_decay, batch_size):
         train_ls, test_ls, acc_train_ls, acc_test_ls = [], [], [], []
         train_iter = load_array((train_features, train_labels), batch_size)
         # Adam optimizer
         optimizer = torch.optim.Adam(net.parameters(),
                                      lr = learning rate,
                                      weight decay = weight decay)
         for epoch in range(num_epochs):
             for X, y in train_iter:
                 optimizer.zero_grad()
                 l = loss(net(X), y)
                 1.backward()
                 optimizer.step()
             train_ls.append(loss(net(train_features), train_labels))
             # train accuracy
             out = net(train_features).detach()
             _, predicted = torch.max(out.data, 1)
             total_train = train_labels.size(0)
             correct_train = (predicted == train_labels).sum().item()
             acc train = correct train / total train
             acc train ls.append(acc train)
             if test_labels is not None:
               test_ls.append(loss(net(test_features), test_labels))
               # test accuracy
               out = net(test_features).detach()
               _, predicted = torch.max(out.data, 1)
               total_test = test_labels.size(0)
               correct_test = (predicted == test_labels).sum().item()
               acc_test = correct_test / total_test
               acc_test_ls.append(acc_test)
         return train_ls, test_ls, acc_train_ls, acc_test_ls
```

```
[]: # K-fold Cross validation
def get_k_fold_data(k, i, X, y):
    assert k > 1
    fold_size = X.shape[0] // k
```

```
X_train, y_train = None, None
    for j in range(k):
        idx = slice(j * fold_size, (j + 1) * fold_size)
        X_part, y_part = X[idx, :], y[idx]
        if j == i:
            X_valid, y_valid = X_part, y_part
        elif X train is None:
            X_train, y_train = X_part, y_part
        else:
            X_train = torch.cat([X_train, X_part], 0)
            y_train = torch.cat([y_train, y_part], 0)
    return X_train, y_train, X_valid, y_valid
def k_fold(k, X_train, y_train, num_nodes1, num_nodes2, num_epochs, u
 →learning_rate, weight_decay, batch_size):
    train_l_sum, valid_l_sum = 0, 0
    net = get_net(num_nodes1, num_nodes2)
    net.apply(init_weights)
    for i in range(k):
      data = get_k_fold_data(k, i, X_train, y_train)
      train_ls, valid_ls, _, _ = train(net, *data, num_epochs, learning_rate,
                                 weight_decay, batch_size)
      train_l_sum += train_ls[-1]
      valid_l_sum += valid_ls[-1]
    return train_l_sum / k, valid_l_sum / k
```

In particular, 54 neural network models with different configurations in terms of number of hidden layers (from 1 to 2) and number of nodes in each of them, were tried out exploiting 5-fold cross validation.

Here, an untuned set of hyperparameters - learning rate, weight decay etc. - is picked, but they will be optimized in next section.

So for now, the network's weights are updated using **adam optimizer** on batches with a **batch** size of **128**: meaning weights are updated after every 128 samples have been evaluated. The entire training set is trained for **50 epochs**. The network learns with a **learning rate** of 0.1, while the **weight decay** is instead set as 0.

```
learning_rate = 0.1
weight_decay = 0
batch_size = 128
k = 5
i = 0
# Nets with 1 hidden layer
for num_nodes1 in net_components['num_nodes1']:
  i = i + 1
 num nodes2 = None
 train_1, valid_1 = k_fold(k, train_features, train_labels, num_nodes1,_
 →num_nodes2, num_epochs,
                            learning_rate, weight_decay, batch_size)
 print(f'({i}) 1 hidden layer - nodes: {num_nodes1}')
 print(f'{k}-fold validation | avg train loss: {float(train_l):f}, '
        f'avg valid loss: {float(valid_l):f}')
 nets = nets.append({'num_nodes layer 1': num_nodes1, #'num_nodes layer 2':u
\rightarrow None,
                      'avg train loss': train_l.item(), 'avg valid loss':
→valid_l.item()}, ignore_index=True)
# Nets with 2 hidden layers
for num_nodes1 in net_components['num_nodes1']:
 for num_nodes2 in net_components['num_nodes2']:
   i = i + 1
   train_1, valid_1 = k_fold(k, train_features, train_labels, num_nodes1,__
→num_nodes2, num_epochs,
                              learning_rate, weight_decay, batch_size)
   print(f'({i}) 2 hidden layers - layer 1 nodes: {num_nodes2},'
          f' layer 2 nodes: {num_nodes2}')
   print(f'{k}-fold validation | avg train loss: {float(train_l):f}, '
          f'avg valid loss: {float(valid_l):f}')
   nets = nets.append({'num_nodes layer 1': num_nodes1, 'num_nodes layer 2':u
→num_nodes2,
                        'avg train loss': train_l.item(), 'avg valid loss':
→valid_l.item()}, ignore_index=True)
bestnet = nets.loc[[(nets["avg valid loss"]).idxmin()]]
layer2 = bestnet['num_nodes layer 2'].notnull().values[0]
if layer2 != False:
 num_nodes1, num_nodes2 = int(bestnet['num_nodes layer 1'].values[0]), u
→int(bestnet['num_nodes layer 2'].values[0])
else:
 num_nodes1, num_nodes2 = int(bestnet['num_nodes layer 1'].values[0]), None
```

(1) 1 hidden layer - nodes: 4
5-fold validation | avg train loss: 0.197169, avg valid loss: 0.202632

```
(2) 1 hidden layer - nodes: 6
5-fold validation | avg train loss: 0.195746, avg valid loss: 0.203608
(3) 1 hidden layer - nodes: 8
5-fold validation | avg train loss: 0.193651, avg valid loss: 0.212758
(4) 1 hidden layer - nodes: 10
5-fold validation | avg train loss: 0.195669, avg valid loss: 0.204873
(5) 1 hidden layer - nodes: 12
5-fold validation | avg train loss: 0.193164, avg valid loss: 0.208906
(6) 1 hidden layer - nodes: 14
5-fold validation | avg train loss: 0.191238, avg valid loss: 0.206913
(7) 1 hidden layer - nodes: 16
5-fold validation | avg train loss: 0.195453, avg valid loss: 0.203084
(8) 1 hidden layer - nodes: 18
5-fold validation | avg train loss: 0.191862, avg valid loss: 0.207186
(9) 1 hidden layer - nodes: 20
5-fold validation | avg train loss: 0.189435, avg valid loss: 0.211882
(10) 2 hidden layers - layer 1 nodes: 4, layer 2 nodes: 4
5-fold validation | avg train loss: 0.198189, avg valid loss: 0.200809
(11) 2 hidden layers - layer 1 nodes: 8, layer 2 nodes: 8
5-fold validation | avg train loss: 0.199526, avg valid loss: 0.202167
(12) 2 hidden layers - layer 1 nodes: 12, layer 2 nodes: 12
5-fold validation | avg train loss: 0.198595, avg valid loss: 0.201599
(13) 2 hidden layers - layer 1 nodes: 16, layer 2 nodes: 16
5-fold validation | avg train loss: 0.204007, avg valid loss: 0.205748
(14) 2 hidden layers - layer 1 nodes: 20, layer 2 nodes: 20
5-fold validation | avg train loss: 0.204736, avg valid loss: 0.205816
(15) 2 hidden layers - layer 1 nodes: 4, layer 2 nodes: 4
5-fold validation | avg train loss: 0.203226, avg valid loss: 0.203935
(16) 2 hidden layers - layer 1 nodes: 8, layer 2 nodes: 8
5-fold validation | avg train loss: 0.199744, avg valid loss: 0.201888
(17) 2 hidden layers - layer 1 nodes: 12, layer 2 nodes: 12
5-fold validation | avg train loss: 0.203626, avg valid loss: 0.204269
(18) 2 hidden layers - layer 1 nodes: 16, layer 2 nodes: 16
5-fold validation | avg train loss: 0.204673, avg valid loss: 0.205530
(19) 2 hidden layers - layer 1 nodes: 20, layer 2 nodes: 20
5-fold validation | avg train loss: 0.205331, avg valid loss: 0.207088
(20) 2 hidden layers - layer 1 nodes: 4, layer 2 nodes: 4
5-fold validation | avg train loss: 0.205353, avg valid loss: 0.205810
(21) 2 hidden layers - layer 1 nodes: 8, layer 2 nodes: 8
5-fold validation | avg train loss: 0.205353, avg valid loss: 0.207374
(22) 2 hidden layers - layer 1 nodes: 12, layer 2 nodes: 12
5-fold validation | avg train loss: 0.203810, avg valid loss: 0.204306
(23) 2 hidden layers - layer 1 nodes: 16, layer 2 nodes: 16
5-fold validation | avg train loss: 0.204667, avg valid loss: 0.205840
(24) 2 hidden layers - layer 1 nodes: 20, layer 2 nodes: 20
5-fold validation | avg train loss: 0.204940, avg valid loss: 0.206718
(25) 2 hidden layers - layer 1 nodes: 4, layer 2 nodes: 4
5-fold validation | avg train loss: 0.204156, avg valid loss: 0.205919
```

```
(26) 2 hidden layers - layer 1 nodes: 8, layer 2 nodes: 8
5-fold validation | avg train loss: 0.205103, avg valid loss: 0.205613
(27) 2 hidden layers - layer 1 nodes: 12, layer 2 nodes: 12
5-fold validation | avg train loss: 0.204708, avg valid loss: 0.205714
(28) 2 hidden layers - layer 1 nodes: 16, layer 2 nodes: 16
5-fold validation | avg train loss: 0.202836, avg valid loss: 0.203494
(29) 2 hidden layers - layer 1 nodes: 20, layer 2 nodes: 20
5-fold validation | avg train loss: 0.203285, avg valid loss: 0.204841
(30) 2 hidden layers - layer 1 nodes: 4, layer 2 nodes: 4
5-fold validation | avg train loss: 0.205119, avg valid loss: 0.206249
(31) 2 hidden layers - layer 1 nodes: 8, layer 2 nodes: 8
5-fold validation | avg train loss: 0.204749, avg valid loss: 0.206246
(32) 2 hidden layers - layer 1 nodes: 12, layer 2 nodes: 12
5-fold validation | avg train loss: 0.204904, avg valid loss: 0.205894
(33) 2 hidden layers - layer 1 nodes: 16, layer 2 nodes: 16
5-fold validation | avg train loss: 0.205479, avg valid loss: 0.204527
(34) 2 hidden layers - layer 1 nodes: 20, layer 2 nodes: 20
5-fold validation | avg train loss: 0.205741, avg valid loss: 0.207611
(35) 2 hidden layers - layer 1 nodes: 4, layer 2 nodes: 4
5-fold validation | avg train loss: 0.205262, avg valid loss: 0.206109
(36) 2 hidden layers - layer 1 nodes: 8, layer 2 nodes: 8
5-fold validation | avg train loss: 0.205410, avg valid loss: 0.207369
(37) 2 hidden layers - layer 1 nodes: 12, layer 2 nodes: 12
5-fold validation | avg train loss: 0.205650, avg valid loss: 0.207346
(38) 2 hidden layers - layer 1 nodes: 16, layer 2 nodes: 16
5-fold validation | avg train loss: 0.205326, avg valid loss: 0.206269
(39) 2 hidden layers - layer 1 nodes: 20, layer 2 nodes: 20
5-fold validation | avg train loss: 0.205241, avg valid loss: 0.206645
(40) 2 hidden layers - layer 1 nodes: 4, layer 2 nodes: 4
5-fold validation | avg train loss: 0.204791, avg valid loss: 0.204674
(41) 2 hidden layers - layer 1 nodes: 8, layer 2 nodes: 8
5-fold validation | avg train loss: 0.205025, avg valid loss: 0.206121
(42) 2 hidden layers - layer 1 nodes: 12, layer 2 nodes: 12
5-fold validation | avg train loss: 0.205156, avg valid loss: 0.206322
(43) 2 hidden layers - layer 1 nodes: 16, layer 2 nodes: 16
5-fold validation | avg train loss: 0.205222, avg valid loss: 0.207436
(44) 2 hidden layers - layer 1 nodes: 20, layer 2 nodes: 20
5-fold validation | avg train loss: 0.204876, avg valid loss: 0.205561
(45) 2 hidden layers - layer 1 nodes: 4, layer 2 nodes: 4
5-fold validation | avg train loss: 0.205126, avg valid loss: 0.205160
(46) 2 hidden layers - layer 1 nodes: 8, layer 2 nodes: 8
5-fold validation | avg train loss: 0.204537, avg valid loss: 0.204995
(47) 2 hidden layers - layer 1 nodes: 12, layer 2 nodes: 12
5-fold validation | avg train loss: 0.205372, avg valid loss: 0.206491
(48) 2 hidden layers - layer 1 nodes: 16, layer 2 nodes: 16
5-fold validation | avg train loss: 0.205301, avg valid loss: 0.206352
(49) 2 hidden layers - layer 1 nodes: 20, layer 2 nodes: 20
5-fold validation | avg train loss: 0.205685, avg valid loss: 0.206474
```

```
(50) 2 hidden layers - layer 1 nodes: 4, layer 2 nodes: 4
5-fold validation | avg train loss: 0.205457, avg valid loss: 0.206752
(51) 2 hidden layers - layer 1 nodes: 8, layer 2 nodes: 8
5-fold validation | avg train loss: 0.203762, avg valid loss: 0.204743
(52) 2 hidden layers - layer 1 nodes: 12, layer 2 nodes: 12
5-fold validation | avg train loss: 0.205091, avg valid loss: 0.206318
(53) 2 hidden layers - layer 1 nodes: 16, layer 2 nodes: 16
5-fold validation | avg train loss: 0.206193, avg valid loss: 0.207357
(54) 2 hidden layers - layer 1 nodes: 20, layer 2 nodes: 20
5-fold validation | avg train loss: 0.205520, avg valid loss: 0.206294
```

The neural network that performs better, in terms of **avg cross-entropy loss** on validation set, is the one with:

```
[]: bestnet.head()
[]: num_nodes layer 1 num_nodes layer 2 avg train loss avg valid loss
9     4.0     4.0     0.198189     0.200809
```

5 Hyperparameters optimization

In this section 5-fold cross validation is again exploited: this time to tune the **hyperparameters** for training, in order to select the combination of values that would make the neural network perform as accurate as possible. In particular, **90** different combinations of learning rate, weight decay and batch size, were tried out overall.

```
[]: # Hyperparameters setting via k-fold cross validation
     k = 5
     num_epochs = 50
     param_grid = {'lr': [0.001, 0.005, 0.01, 0.05, 0.1, 0.9]},
                   'weight_decay': np.insert((np.logspace(-4, -1, num=4, base=10)),__
      \rightarrow 0, 0).tolist(),
                   'batch_size': [128, 256, 512]}
     hyperparams = pd.DataFrame(columns=["learning rate", "weight decay", "batch_
      ⇔size",
                                          "avg train loss", "avg valid loss"])
     def hyperparams_optim(param_grid, k, train_features, train_labels, num_nodes1,_
      →num_nodes2, num_epochs):
         i = 0
         for learning_rate in param_grid['lr']:
             for weight_decay in param_grid['weight_decay']:
                 for batch_size in param_grid['batch_size']:
                     i = i + 1
```

```
train_l, valid_l = k_fold(k, train_features, train_labels,__
 →num_nodes1, num_nodes2, num_epochs,
                                          learning_rate, weight_decay,_
 →batch size)
                print(f'({i}) parameters: [lr: {learning_rate},'
                       f' weight_decay: {weight_decay},'
                       f' batch_size: {batch_size}')
                print(f'{k}-fold validation | avg train loss: {float(train_l):
 \hookrightarrowf}, '
                       f'avg valid loss: {float(valid_l):f}')
                 global hyperparams
                hyperparams = hyperparams.append({'learning rate':__
 →learning_rate, 'weight decay': weight_decay, 'batch size': batch_size,
                                                   'avg train loss': train_1.
 →item(), 'avg valid loss': valid_l.item()}, ignore_index=True)
    best_nn = hyperparams.loc[[(hyperparams["avg valid loss"]).idxmin()]]
    return best_nn['learning rate'].values[0], best_nn['weight decay'].
 →values[0], int(best_nn['batch size'].values[0])
# Perform hyperparameter optimization
learning_rate, weight_decay, batch_size = hyperparams_optim(param_grid, k,__
 →train_features, train_labels,
                                                             num_nodes1,
 →num_nodes2, num_epochs)
(1) parameters: [lr: 0.001, weight_decay: 0.0, batch_size: 128
5-fold validation | avg train loss: 0.199198, avg valid loss: 0.202379
(2) parameters: [lr: 0.001, weight_decay: 0.0, batch_size: 256
5-fold validation | avg train loss: 0.212446, avg valid loss: 0.215709
(3) parameters: [lr: 0.001, weight_decay: 0.0, batch_size: 512
5-fold validation | avg train loss: 0.263483, avg valid loss: 0.268750
(4) parameters: [lr: 0.001, weight_decay: 0.0001, batch_size: 128
5-fold validation | avg train loss: 0.199570, avg valid loss: 0.201753
(5) parameters: [lr: 0.001, weight_decay: 0.0001, batch_size: 256
5-fold validation | avg train loss: 0.205088, avg valid loss: 0.207412
(6) parameters: [lr: 0.001, weight_decay: 0.0001, batch_size: 512
5-fold validation | avg train loss: 0.237143, avg valid loss: 0.239522
(7) parameters: [lr: 0.001, weight_decay: 0.001, batch_size: 128
5-fold validation | avg train loss: 0.203155, avg valid loss: 0.205719
(8) parameters: [lr: 0.001, weight_decay: 0.001, batch_size: 256
5-fold validation | avg train loss: 0.206623, avg valid loss: 0.208165
(9) parameters: [lr: 0.001, weight_decay: 0.001, batch_size: 512
5-fold validation | avg train loss: 0.238525, avg valid loss: 0.241135
```

(10) parameters: [lr: 0.001, weight_decay: 0.01, batch_size: 128

(11) parameters: [lr: 0.001, weight decay: 0.01, batch size: 256

5-fold validation | avg train loss: 0.205130, avg valid loss: 0.206679

```
5-fold validation | avg train loss: 0.211632, avg valid loss: 0.213192
(12) parameters: [lr: 0.001, weight_decay: 0.01, batch_size: 512
5-fold validation | avg train loss: 0.433716, avg valid loss: 0.435609
(13) parameters: [lr: 0.001, weight_decay: 0.1, batch_size: 128
5-fold validation | avg train loss: 0.258681, avg valid loss: 0.259549
(14) parameters: [lr: 0.001, weight_decay: 0.1, batch_size: 256
5-fold validation | avg train loss: 0.259699, avg valid loss: 0.261337
(15) parameters: [lr: 0.001, weight_decay: 0.1, batch_size: 512
5-fold validation | avg train loss: 0.304065, avg valid loss: 0.305401
(16) parameters: [lr: 0.005, weight_decay: 0.0, batch_size: 128
5-fold validation | avg train loss: 0.196740, avg valid loss: 0.199216
(17) parameters: [lr: 0.005, weight_decay: 0.0, batch_size: 256
5-fold validation | avg train loss: 0.196067, avg valid loss: 0.199384
(18) parameters: [lr: 0.005, weight_decay: 0.0, batch_size: 512
5-fold validation | avg train loss: 0.197383, avg valid loss: 0.200346
(19) parameters: [lr: 0.005, weight decay: 0.0001, batch size: 128
5-fold validation | avg train loss: 0.196122, avg valid loss: 0.201048
(20) parameters: [lr: 0.005, weight decay: 0.0001, batch_size: 256
5-fold validation | avg train loss: 0.196933, avg valid loss: 0.199953
(21) parameters: [lr: 0.005, weight decay: 0.0001, batch size: 512
5-fold validation | avg train loss: 0.197344, avg valid loss: 0.200054
(22) parameters: [lr: 0.005, weight decay: 0.001, batch size: 128
5-fold validation | avg train loss: 0.197688, avg valid loss: 0.199841
(23) parameters: [lr: 0.005, weight_decay: 0.001, batch_size: 256
5-fold validation | avg train loss: 0.198308, avg valid loss: 0.200472
(24) parameters: [lr: 0.005, weight_decay: 0.001, batch_size: 512
5-fold validation | avg train loss: 0.199422, avg valid loss: 0.201943
(25) parameters: [lr: 0.005, weight_decay: 0.01, batch_size: 128
5-fold validation | avg train loss: 0.204954, avg valid loss: 0.206932
(26) parameters: [lr: 0.005, weight_decay: 0.01, batch_size: 256
5-fold validation | avg train loss: 0.204823, avg valid loss: 0.206349
(27) parameters: [lr: 0.005, weight_decay: 0.01, batch_size: 512
5-fold validation | avg train loss: 0.205587, avg valid loss: 0.207190
(28) parameters: [lr: 0.005, weight_decay: 0.1, batch_size: 128
5-fold validation | avg train loss: 0.254465, avg valid loss: 0.255235
(29) parameters: [lr: 0.005, weight_decay: 0.1, batch_size: 256
5-fold validation | avg train loss: 0.253273, avg valid loss: 0.253931
(30) parameters: [lr: 0.005, weight_decay: 0.1, batch_size: 512
5-fold validation | avg train loss: 0.253524, avg valid loss: 0.254447
(31) parameters: [lr: 0.01, weight_decay: 0.0, batch_size: 128
5-fold validation | avg train loss: 0.194717, avg valid loss: 0.198043
(32) parameters: [lr: 0.01, weight_decay: 0.0, batch_size: 256
5-fold validation | avg train loss: 0.195617, avg valid loss: 0.199258
(33) parameters: [lr: 0.01, weight_decay: 0.0, batch_size: 512
5-fold validation | avg train loss: 0.198589, avg valid loss: 0.201027
(34) parameters: [lr: 0.01, weight_decay: 0.0001, batch_size: 128
5-fold validation | avg train loss: 0.195554, avg valid loss: 0.201447
(35) parameters: [lr: 0.01, weight_decay: 0.0001, batch_size: 256
```

```
5-fold validation | avg train loss: 0.194748, avg valid loss: 0.198595
(36) parameters: [lr: 0.01, weight_decay: 0.0001, batch_size: 512
5-fold validation | avg train loss: 0.196223, avg valid loss: 0.199060
(37) parameters: [lr: 0.01, weight_decay: 0.001, batch_size: 128
5-fold validation | avg train loss: 0.196660, avg valid loss: 0.199709
(38) parameters: [lr: 0.01, weight_decay: 0.001, batch_size: 256
5-fold validation | avg train loss: 0.199001, avg valid loss: 0.200966
(39) parameters: [lr: 0.01, weight_decay: 0.001, batch_size: 512
5-fold validation | avg train loss: 0.198108, avg valid loss: 0.201002
(40) parameters: [lr: 0.01, weight_decay: 0.01, batch_size: 128
5-fold validation | avg train loss: 0.204935, avg valid loss: 0.206179
(41) parameters: [lr: 0.01, weight_decay: 0.01, batch_size: 256
5-fold validation | avg train loss: 0.204509, avg valid loss: 0.205552
(42) parameters: [lr: 0.01, weight_decay: 0.01, batch_size: 512
5-fold validation | avg train loss: 0.204718, avg valid loss: 0.206207
(43) parameters: [lr: 0.01, weight_decay: 0.1, batch_size: 128
5-fold validation | avg train loss: 0.249993, avg valid loss: 0.250813
(44) parameters: [lr: 0.01, weight_decay: 0.1, batch_size: 256
5-fold validation | avg train loss: 0.255393, avg valid loss: 0.255999
(45) parameters: [lr: 0.01, weight decay: 0.1, batch size: 512
5-fold validation | avg train loss: 0.253847, avg valid loss: 0.254598
(46) parameters: [lr: 0.05, weight decay: 0.0, batch size: 128
5-fold validation | avg train loss: 0.197339, avg valid loss: 0.200659
(47) parameters: [lr: 0.05, weight decay: 0.0, batch size: 256
5-fold validation | avg train loss: 0.194856, avg valid loss: 0.201189
(48) parameters: [lr: 0.05, weight_decay: 0.0, batch_size: 512
5-fold validation | avg train loss: 0.195322, avg valid loss: 0.200411
(49) parameters: [lr: 0.05, weight_decay: 0.0001, batch_size: 128
5-fold validation | avg train loss: 0.197002, avg valid loss: 0.200996
(50) parameters: [lr: 0.05, weight_decay: 0.0001, batch_size: 256
5-fold validation | avg train loss: 0.194973, avg valid loss: 0.199974
(51) parameters: [lr: 0.05, weight_decay: 0.0001, batch_size: 512
5-fold validation | avg train loss: 0.195445, avg valid loss: 0.200020
(52) parameters: [lr: 0.05, weight_decay: 0.001, batch_size: 128
5-fold validation | avg train loss: 0.198834, avg valid loss: 0.200212
(53) parameters: [lr: 0.05, weight_decay: 0.001, batch_size: 256
5-fold validation | avg train loss: 0.197227, avg valid loss: 0.199738
(54) parameters: [lr: 0.05, weight_decay: 0.001, batch_size: 512
5-fold validation | avg train loss: 0.198187, avg valid loss: 0.200346
(55) parameters: [lr: 0.05, weight_decay: 0.01, batch_size: 128
5-fold validation | avg train loss: 0.205334, avg valid loss: 0.206714
(56) parameters: [lr: 0.05, weight_decay: 0.01, batch_size: 256
5-fold validation | avg train loss: 0.205019, avg valid loss: 0.206635
(57) parameters: [lr: 0.05, weight_decay: 0.01, batch_size: 512
5-fold validation | avg train loss: 0.205223, avg valid loss: 0.206490
(58) parameters: [lr: 0.05, weight_decay: 0.1, batch_size: 128
5-fold validation | avg train loss: 0.249431, avg valid loss: 0.250445
(59) parameters: [lr: 0.05, weight_decay: 0.1, batch_size: 256
```

```
5-fold validation | avg train loss: 0.256479, avg valid loss: 0.257750
(60) parameters: [lr: 0.05, weight_decay: 0.1, batch_size: 512
5-fold validation | avg train loss: 0.255512, avg valid loss: 0.256193
(61) parameters: [lr: 0.1, weight_decay: 0.0, batch_size: 128
5-fold validation | avg train loss: 0.203676, avg valid loss: 0.204015
(62) parameters: [lr: 0.1, weight_decay: 0.0, batch_size: 256
5-fold validation | avg train loss: 0.196589, avg valid loss: 0.200509
(63) parameters: [lr: 0.1, weight_decay: 0.0, batch_size: 512
5-fold validation | avg train loss: 0.195523, avg valid loss: 0.201231
(64) parameters: [lr: 0.1, weight_decay: 0.0001, batch_size: 128
5-fold validation | avg train loss: 0.201737, avg valid loss: 0.202214
(65) parameters: [lr: 0.1, weight_decay: 0.0001, batch_size: 256
5-fold validation | avg train loss: 0.197256, avg valid loss: 0.199964
(66) parameters: [lr: 0.1, weight_decay: 0.0001, batch_size: 512
5-fold validation | avg train loss: 0.196724, avg valid loss: 0.202070
(67) parameters: [lr: 0.1, weight_decay: 0.001, batch_size: 128
5-fold validation | avg train loss: 0.201608, avg valid loss: 0.202680
(68) parameters: [lr: 0.1, weight_decay: 0.001, batch_size: 256
5-fold validation | avg train loss: 0.199682, avg valid loss: 0.202253
(69) parameters: [lr: 0.1, weight decay: 0.001, batch size: 512
5-fold validation | avg train loss: 0.199342, avg valid loss: 0.201148
(70) parameters: [lr: 0.1, weight decay: 0.01, batch size: 128
5-fold validation | avg train loss: 0.207274, avg valid loss: 0.207901
(71) parameters: [lr: 0.1, weight decay: 0.01, batch size: 256
5-fold validation | avg train loss: 0.206827, avg valid loss: 0.206642
(72) parameters: [lr: 0.1, weight_decay: 0.01, batch_size: 512
5-fold validation | avg train loss: 0.204791, avg valid loss: 0.205632
(73) parameters: [lr: 0.1, weight_decay: 0.1, batch_size: 128
5-fold validation | avg train loss: 0.248859, avg valid loss: 0.249969
(74) parameters: [lr: 0.1, weight_decay: 0.1, batch_size: 256
5-fold validation | avg train loss: 0.250916, avg valid loss: 0.250867
(75) parameters: [lr: 0.1, weight_decay: 0.1, batch_size: 512
5-fold validation | avg train loss: 0.254152, avg valid loss: 0.254757
(76) parameters: [lr: 0.9, weight_decay: 0.0, batch_size: 128
5-fold validation | avg train loss: 0.207804, avg valid loss: 0.207646
(77) parameters: [lr: 0.9, weight_decay: 0.0, batch_size: 256
5-fold validation | avg train loss: 0.208305, avg valid loss: 0.209196
(78) parameters: [lr: 0.9, weight_decay: 0.0, batch_size: 512
5-fold validation | avg train loss: 0.209092, avg valid loss: 0.209639
(79) parameters: [lr: 0.9, weight_decay: 0.0001, batch_size: 128
5-fold validation | avg train loss: 0.209461, avg valid loss: 0.211060
(80) parameters: [lr: 0.9, weight_decay: 0.0001, batch_size: 256
5-fold validation | avg train loss: 0.207885, avg valid loss: 0.209405
(81) parameters: [lr: 0.9, weight_decay: 0.0001, batch_size: 512
5-fold validation | avg train loss: 0.207840, avg valid loss: 0.208355
(82) parameters: [lr: 0.9, weight_decay: 0.001, batch_size: 128
5-fold validation | avg train loss: 0.212642, avg valid loss: 0.211905
(83) parameters: [lr: 0.9, weight_decay: 0.001, batch_size: 256
```

```
5-fold validation | avg train loss: 0.210145, avg valid loss: 0.209065 (84) parameters: [lr: 0.9, weight_decay: 0.001, batch_size: 512 5-fold validation | avg train loss: 0.208735, avg valid loss: 0.208856 (85) parameters: [lr: 0.9, weight_decay: 0.01, batch_size: 128 5-fold validation | avg train loss: 0.216780, avg valid loss: 0.215818 (86) parameters: [lr: 0.9, weight_decay: 0.01, batch_size: 256 5-fold validation | avg train loss: 0.217214, avg valid loss: 0.214920 (87) parameters: [lr: 0.9, weight_decay: 0.01, batch_size: 512 5-fold validation | avg train loss: 0.207690, avg valid loss: 0.208377 (88) parameters: [lr: 0.9, weight_decay: 0.1, batch_size: 128 5-fold validation | avg train loss: 0.259336, avg valid loss: 0.259840 (89) parameters: [lr: 0.9, weight_decay: 0.1, batch_size: 256 5-fold validation | avg train loss: 0.259901, avg valid loss: 0.261866 (90) parameters: [lr: 0.9, weight_decay: 0.1, batch_size: 512 5-fold validation | avg train loss: 0.258650, avg valid loss: 0.258868
```

The neural network performs better with the following combination of hyperparameters' values:

```
[]: best_nn = hyperparams.loc[[(hyperparams["avg valid loss"]).idxmin()]]
best_nn.head()
```

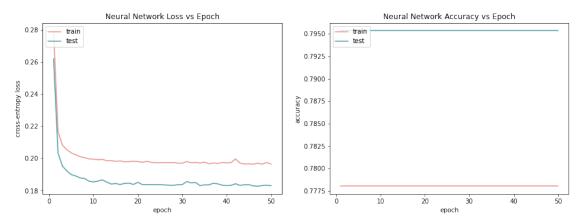
```
[]: learning rate weight decay batch size avg train loss avg valid loss 30 0.01 0.0 128.0 0.194717 0.198043
```

6 Training & Testing

Finally, the neural network is trained on training data with **tuned hyperparameters**, and then applied on test data in order to predict the rating of new and not-seen-so-far Sephora products.

```
[]: # Train & Test
     net = get_net(num_nodes1, num_nodes2)
     net.apply(init_weights)
     train_ls, test_ls, acc_train_ls, acc_test_ls = train(net, train_features,_
     →train_labels, test_features, test_labels,
                                                          num_epochs, learning_rate,
     →weight_decay, batch_size)
     # Neural network performance visualization
     fig, (ax1, ax2) = plt.subplots(1,2, figsize=(15,5))
     ax1.plot(np.arange(1, num_epochs + 1), np.array(train_ls), color="#eb9089")
     ax1.plot(np.arange(1, num_epochs + 1), np.array(test_ls), color="#4c9ca6")
     ax1.set_title('Neural Network Loss vs Epoch')
     ax1.set(xlabel='epoch', ylabel='cross-entropy loss')
     ax1.legend(['train', 'test'], loc='upper left')
     ax2.plot(np.arange(1, num_epochs + 1), np.array(acc_train_ls), color="#eb9089")
     ax2.plot(np.arange(1, num_epochs + 1), np.array(acc_test_ls), color="#4c9ca6")
     ax2.set_title('Neural Network Accuracy vs Epoch')
```

```
ax2.set(xlabel='epoch', ylabel='accuracy')
ax2.legend(['train', 'test'], loc='upper left')
plt.show()
```



```
[]: # Loss & accuracy over epochs overview
for i in range(1, num_epochs):
    print(f'Epoch {i}')
    print(f' train loss {float(train_ls[i]):.4f}, train accuracy
    →{float(acc_train_ls[i]):.4f}')
    print(f' test loss {float(test_ls[i]):.4f}, test accuracy
    →{float(acc_test_ls[i]):.4f}')
    print("")
```

Epoch 1 train loss 0.2166, train

train loss 0.2166, train accuracy 0.7780 test loss 0.2033, test accuracy 0.7953

Epoch 2

train loss 0.2081, train accuracy 0.7780 test loss 0.1951, test accuracy 0.7953

Epoch 3

train loss 0.2054, train accuracy 0.7780 test loss 0.1922, test accuracy 0.7953

Epoch 4

train loss 0.2034, train accuracy 0.7780 test loss 0.1899, test accuracy 0.7953

Epoch 5

train loss 0.2022, train accuracy 0.7780 test loss 0.1891, test accuracy 0.7953

Epoch 6

train loss 0.2011, train accuracy 0.7780 test loss 0.1879, test accuracy 0.7953

Epoch 7

train loss 0.2005, train accuracy 0.7780 test loss 0.1875, test accuracy 0.7953

Epoch 8

train loss 0.1997, train accuracy 0.7780 test loss 0.1858, test accuracy 0.7953

Epoch 9

train loss 0.1996, train accuracy 0.7780 test loss 0.1853, test accuracy 0.7953

Epoch 10

train loss 0.1991, train accuracy 0.7780 test loss 0.1859, test accuracy 0.7953

Epoch 11

train loss 0.1994, train accuracy 0.7780 test loss 0.1866, test accuracy 0.7953

Epoch 12

train loss 0.1985, train accuracy 0.7780 test loss 0.1852, test accuracy 0.7953

Epoch 13

train loss 0.1986, train accuracy 0.7780 test loss 0.1840, test accuracy 0.7953

Epoch 14

train loss 0.1982, train accuracy 0.7780 test loss 0.1843, test accuracy 0.7953

Epoch 15

train loss 0.1984, train accuracy 0.7780 test loss 0.1838, test accuracy 0.7953

Epoch 16

train loss 0.1979, train accuracy 0.7780 test loss 0.1844, test accuracy 0.7953

Epoch 17

train loss 0.1979, train accuracy 0.7780 test loss 0.1846, test accuracy 0.7953

Epoch 18

train loss 0.1983, train accuracy 0.7780 test loss 0.1838, test accuracy 0.7953

Epoch 19

train loss 0.1980, train accuracy 0.7780 test loss 0.1851, test accuracy 0.7953

Epoch 20

train loss 0.1976, train accuracy 0.7780 test loss 0.1837, test accuracy 0.7953

Epoch 21

train loss 0.1981, train accuracy 0.7780 test loss 0.1838, test accuracy 0.7953

Epoch 22

train loss 0.1976, train accuracy 0.7780 test loss 0.1837, test accuracy 0.7953

Epoch 23

train loss 0.1973, train accuracy 0.7780 test loss 0.1837, test accuracy 0.7953

Epoch 24

train loss 0.1973, train accuracy 0.7780 test loss 0.1837, test accuracy 0.7953

Epoch 25

train loss 0.1974, train accuracy 0.7780 test loss 0.1835, test accuracy 0.7953

Epoch 26

train loss 0.1973, train accuracy 0.7780 test loss 0.1833, test accuracy 0.7953

Epoch 27

train loss 0.1975, train accuracy 0.7780 test loss 0.1832, test accuracy 0.7953

Epoch 28

train loss 0.1970, train accuracy 0.7780 test loss 0.1836, test accuracy 0.7953

Epoch 29

train loss 0.1970, train accuracy 0.7780 test loss 0.1837, test accuracy 0.7953

Epoch 30

train loss 0.1980, train accuracy 0.7780 test loss 0.1856, test accuracy 0.7953

Epoch 31

train loss 0.1973, train accuracy 0.7780 test loss 0.1847, test accuracy 0.7953

Epoch 32

train loss 0.1975, train accuracy 0.7780 test loss 0.1850, test accuracy 0.7953

Epoch 33

train loss 0.1971, train accuracy 0.7780 test loss 0.1830, test accuracy 0.7953

Epoch 34

train loss 0.1977, train accuracy 0.7780 test loss 0.1835, test accuracy 0.7953

Epoch 35

train loss 0.1966, train accuracy 0.7780 test loss 0.1835, test accuracy 0.7953

Epoch 36

train loss 0.1971, train accuracy 0.7780 test loss 0.1845, test accuracy 0.7953

Epoch 37

train loss 0.1968, train accuracy 0.7780 test loss 0.1842, test accuracy 0.7953

Epoch 38

train loss 0.1974, train accuracy 0.7780 test loss 0.1833, test accuracy 0.7953

Epoch 39

train loss 0.1972, train accuracy 0.7780 test loss 0.1831, test accuracy 0.7953

Epoch 40

train loss 0.1974, train accuracy 0.7780 test loss 0.1833, test accuracy 0.7953

Epoch 41

train loss 0.1997, train accuracy 0.7780 test loss 0.1842, test accuracy 0.7953

```
Epoch 42
     train loss 0.1970, train accuracy 0.7780
     test loss 0.1832, test accuracy 0.7953
    Epoch 43
     train loss 0.1965, train accuracy 0.7780
     test loss 0.1836, test accuracy 0.7953
    Epoch 44
     train loss 0.1966, train accuracy 0.7780
     test loss 0.1836, test accuracy 0.7953
    Epoch 45
     train loss 0.1964, train accuracy 0.7780
     test loss 0.1829, test accuracy 0.7953
    Epoch 46
     train loss 0.1970, train accuracy 0.7780
     test loss 0.1827, test accuracy 0.7953
    Epoch 47
     train loss 0.1964, train accuracy 0.7780
     test loss 0.1831, test accuracy 0.7953
    Epoch 48
     train loss 0.1974, train accuracy 0.7780
     test loss 0.1833, test accuracy 0.7953
    Epoch 49
     train loss 0.1965, train accuracy 0.7780
     test loss 0.1830, test accuracy 0.7953
[]: # Apply neural network to test set
     preds = net(test_features).detach()
     _, predicted = torch.max(preds.data,1)
     # Reformat
     predictions = pd.Series(predicted.reshape(1, -1)[0])
     test_labels = pd.DataFrame(test_labels)
     # Confusion matrix test
     cm = confusion_matrix(test_labels, predictions)
     print("Confusion Matrix")
     print(cm)
     # Show some results
```

```
df_results = pd.concat([products, predictions, test_labels], axis=1)
df_results.columns = ['Sephora Products', 'Predicted Rating', 'True Rating']
df_results.head(10)
```

```
Confusion Matrix
0
           0
                      1
                            0]
 0
           0
                 0
                     14
                            0]
                            0]
 0
           0
                 0
                    230
 0
           0
                 0 1162
                            0]
 Γ
     0
           0
                 0
                            0]]
                     54
```

[]:		Sephora Products		True Rating
	0	Thickening Volume Conditioner		2
	1	Blossom & Bloom Ginseng + Biotin Volumizing C		3
	2	Sugar Lemon	•••	3
;	3	Rice Dry Oil	•••	3
	4	Retinol Fusion PM	•••	3
	5	Brow Tech Matte Pencil	•••	3
	6	Squalane + Antioxidant Cleansing Oil	•••	3
•	7	Bamboo Body Lotion		3
;	8	Blond Absolu Hydrating Illuminating Shampoo		3
	9	Encre Interdite 24 Hour Lip Stain		2

[10 rows x 3 columns]

Ultimately, the trained neural network performs with a *loss* of approximately **0.18** and an *accuracy* of **0.80** on test set. The learning curve seems to flatten out soon, already after a few epochs (less than 10). Also, and strangely, the neural network performs better on test set than train set, which is likely due to the unbalanced classes. In fact, we can observe from the *confusion matrix* how the model classifies all the observations as belonging to class 3 ("4 Stars") - which is the one the net is able to predict best.

A more balanced train set, with more observations belonging to the other classes (especially class 0 and 1) would presumably have allowed a greater level of accuracy to be achieved.

Furthermore from the plot displaying the *accuracy*, we can observe how the neural network has basically no growth over the epochs: it remains almost stable, both for train and test set. We can assume that the growth is really minimal at the decimal level, and that the neural network already starts at its best.