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December 19, 2024

[1]:
```
import numpy as np
import pandas as pd

import random
import os
from tqdm import tqdm
from itertools import product
import time
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler, StandardScaler
```

[2]:
```
print(plt.style.available)
```

```
['Solarize_Light2', '_classic_test_patch', '_mpl-gallery', '_mpl-gallery-
nogrid', 'bmh', 'classic', 'dark_background', 'fast', 'fivethirtyeight',
'ggplot', 'grayscale', 'seaborn-v0_8', 'seaborn-v0_8-bright',
'seaborn-v0_8-colorblind', 'seaborn-v0_8-dark', 'seaborn-v0_8-dark-palette',
'seaborn-v0_8-darkgrid', 'seaborn-v0_8-deep', 'seaborn-v0_8-muted',
'seaborn-v0_8-notebook', 'seaborn-v0_8-paper', 'seaborn-v0_8-pastel',
'seaborn-v0_8-poster', 'seaborn-v0_8-talk', 'seaborn-v0_8-ticks',
'seaborn-v0_8-white', 'seaborn-v0_8-whitegrid', 'tableau-colorblind10']
```

[3]:
```
plt.style.use('_classic_test_patch')
```

[4]:
```
df = pd.read_csv('dataset.csv')
df = df.drop(columns=['Unnamed: 0'])
df.head(3)
```

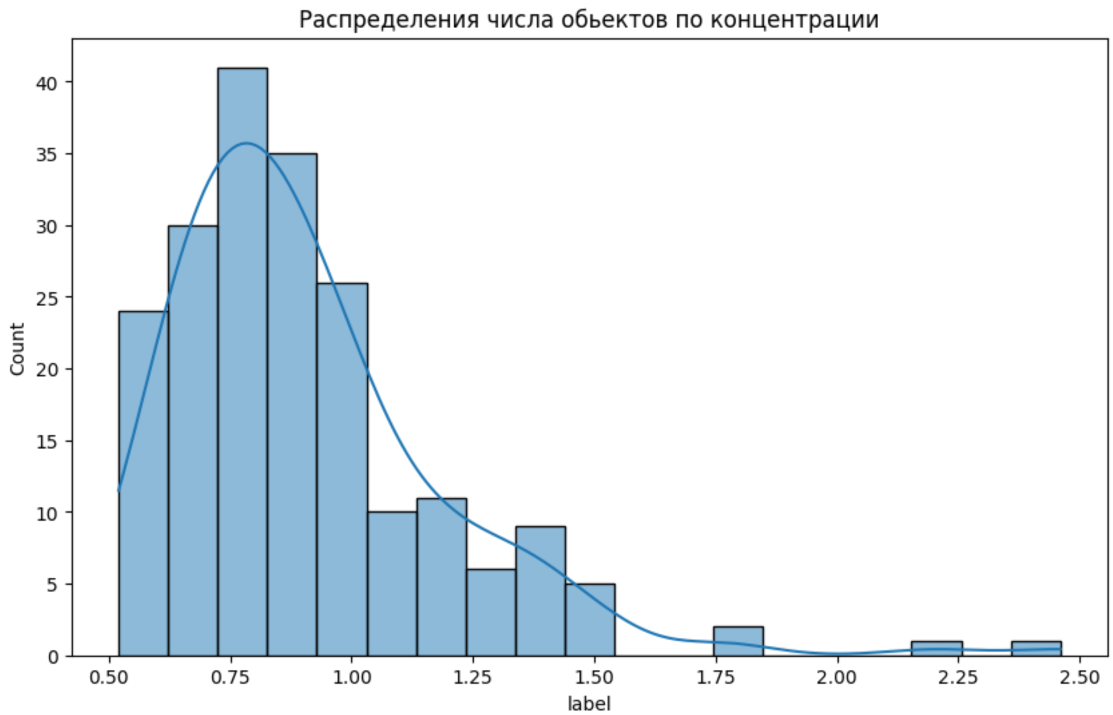
[4]:
```
   label         S        Ag        Cr     Fe_Ka     Fe_Kb     Ar_Kb  \
0   1.75  0.231535  0.313065  0.545376  0.721069  0.729788  0.285071
1   1.47  0.012676  0.116311  0.793318  0.991717  0.989997  0.065601
2   1.39  0.037654  0.160137  0.827570  0.974607  0.979088  0.065373

      Ca_Ka     Ni_Ka     Ni_kb     Cu_Ka     Cu_Kb     Zn_Ka     Zn_Kb  \
0  0.492815  0.303459  0.500176  0.187549  0.201640  0.737144  0.737183
1  0.511980  0.064954  0.516423  0.187322  0.193414  0.920373  0.906333
```

```
2  0.563065  0.118139  0.494226  0.163690  0.181668  0.895705  0.885828

      Pb_La     Pb_Lb        Ti       Nkr        Kr
0  0.737475  0.556190  0.685554  0.193391  0.202682
1  0.812522  0.473542  0.929378  0.019910  0.027779
2  0.788664  0.399465  0.936216  0.019138  0.029954
```

[5]:
```python
scaler = MinMaxScaler()
scaled_data = scaler.fit_transform(df)
scaled_df = pd.DataFrame(scaled_data, columns=df.columns)
scaled_df.head()
```

[5]:
```
      label         S        Ag        Cr     Fe_Ka     Fe_Kb     Ar_Kb  \
0  0.634021  0.231535  0.313065  0.545376  0.721069  0.729788  0.285071
1  0.489691  0.012676  0.116311  0.793318  0.991717  0.989997  0.065601
2  0.448454  0.037654  0.160137  0.827570  0.974607  0.979088  0.065373
3  1.000000  0.048364  0.058915  0.764076  1.000000  1.000000  0.056061
4  0.865979  0.009517  0.099478  0.712293  0.966873  0.968154  0.091002

      Ca_Ka     Ni_Ka     Ni_kb     Cu_Ka     Cu_Kb     Zn_Ka     Zn_Kb  \
0  0.492815  0.303459  0.500176  0.187549  0.201640  0.737144  0.737183
1  0.511980  0.064954  0.516423  0.187322  0.193414  0.920373  0.906333
2  0.563065  0.118139  0.494226  0.163690  0.181668  0.895705  0.885828
3  0.652656  0.108286  0.443447  0.212785  0.224492  0.906779  0.903560
4  0.756323  0.121018  0.450786  0.191769  0.196904  0.908752  0.892736

      Pb_La     Pb_Lb        Ti       Nkr        Kr
0  0.737475  0.556190  0.685554  0.193391  0.202682
1  0.812522  0.473542  0.929378  0.019910  0.027779
2  0.788664  0.399465  0.936216  0.019138  0.029954
3  0.836439  0.464816  0.977572  0.015380  0.019553
4  0.789741  0.479420  0.851971  0.016130  0.019575
```

[6]:
```python
plt.figure(figsize=(10, 6))
sns.histplot(df['label'], kde=True)
plt.title('                          ')
plt.show()
```

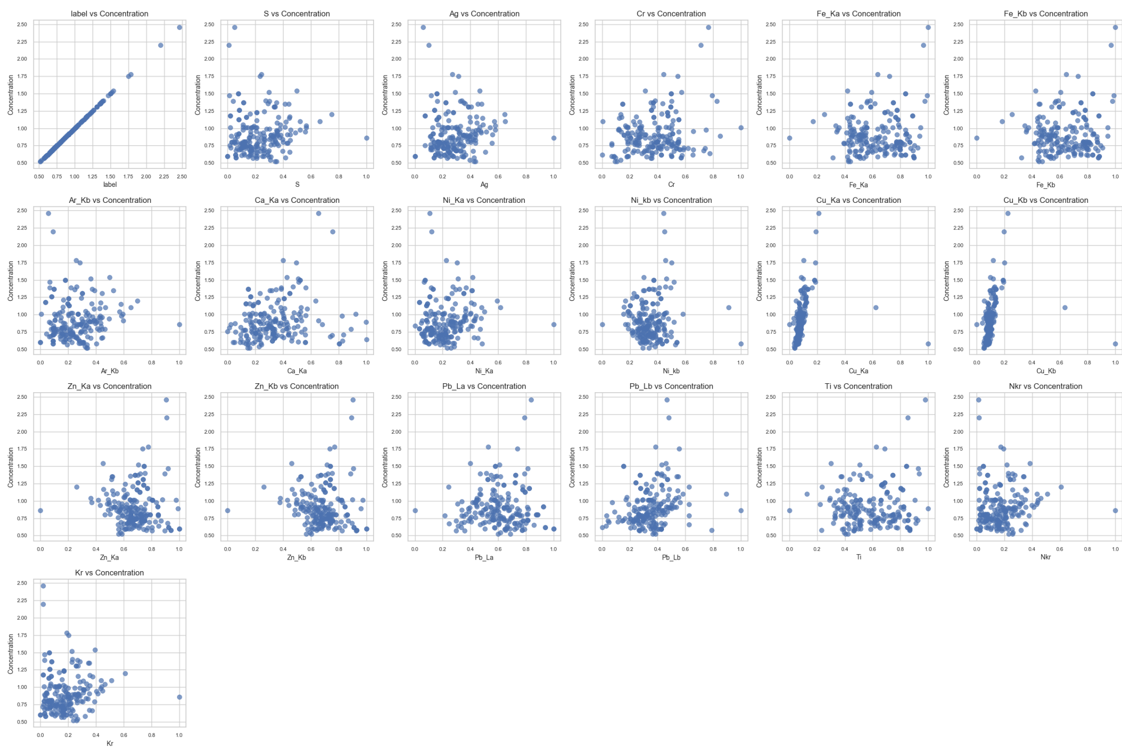


[7]:
```
df.columns
```

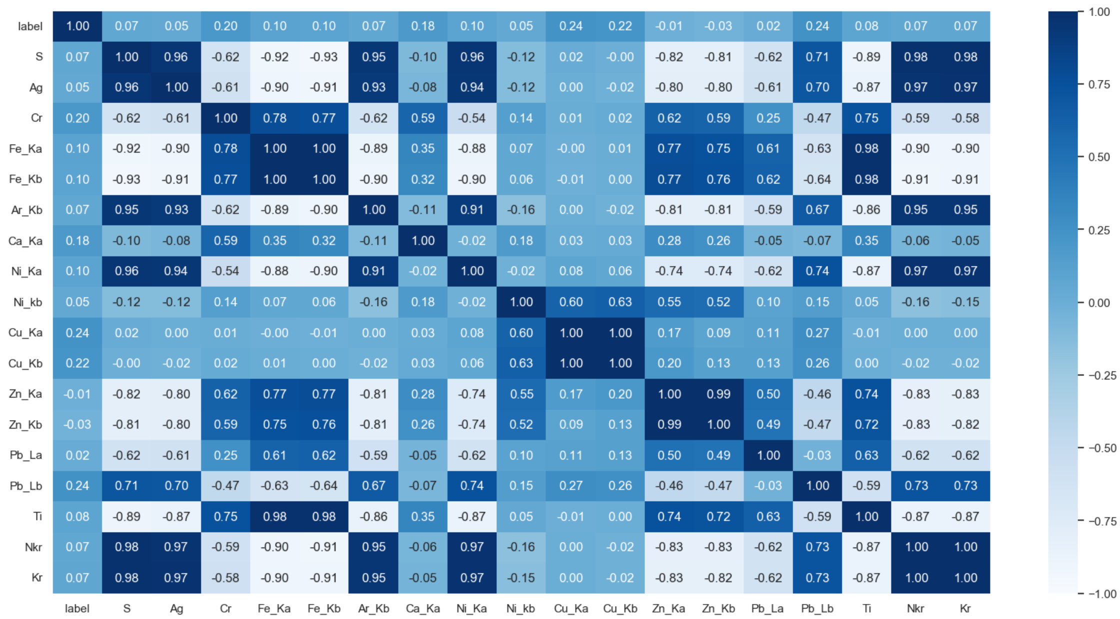
[7]:
```
Index(['label', 'S', 'Ag', 'Cr', 'Fe_Ka', 'Fe_Kb', 'Ar_Kb', 'Ca_Ka', 'Ni_Ka',
       'Ni_kb', 'Cu_Ka', 'Cu_Kb', 'Zn_Ka', 'Zn_Kb', 'Pb_La', 'Pb_Lb', 'Ti',
       'Nkr', 'Kr'],
      dtype='object')
```

[8]:
```
import math
features = ['label', 'S', 'Ag', 'Cr', 'Fe_Ka', 'Fe_Kb', 'Ar_Kb', 'Ca_Ka',␣
 ↪'Ni_Ka',
       'Ni_kb', 'Cu_Ka', 'Cu_Kb', 'Zn_Ka', 'Zn_Kb', 'Pb_La', 'Pb_Lb', 'Ti',
       'Nkr', 'Kr']
n_cols = 6
n_features = len(features)
n_rows = math.ceil(n_features / n_cols)

sns.set(style="whitegrid")


fig, axes = plt.subplots(n_rows, n_cols, figsize=(n_cols * 4, n_rows * 4))
axes = axes.flatten()

for i, feature in enumerate(features):
```

```
    sns.scatterplot(data=df, x=feature, y='label', ax=axes[i], s=50, alpha=0.7,␣
↪edgecolor=None)
    axes[i].set_title(f'{feature} vs Concentration', fontsize=12)
    axes[i].set_xlabel(feature, fontsize=10)
    axes[i].set_ylabel('Concentration', fontsize=10)
    axes[i].tick_params(axis='both', which='major', labelsize=8)

for ax in axes[n_features:]:
    ax.set_visible(False)

plt.tight_layout()
plt.show()
```



[9]:
```
correlation_matrix = scaled_df.corr()

plt.figure(figsize=(20, 10))
sns.heatmap(correlation_matrix, annot=True,
            cmap='Blues', fmt='.2f', vmin=-1, vmax=1)
plt.show()
```



[10]:
```
from sklearn.model_selection import train_test_split

X = scaled_df[features]
y = scaled_df['label']

X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=4)
```

[11]:
```
train_data = [(np.array(x).reshape(-1, 1), y)
                 for x, y in zip(X_train.values.tolist(), y_train.values.
 ↪tolist())]
test_data = [(np.array(x).reshape(-1, 1), y)
                 for x, y in zip(X_test.values.tolist(), y_test.values.tolist())]
```

[12]:
```
def set_seed(seed_value=42):
    random.seed(seed_value)
    np.random.seed(seed_value)
```

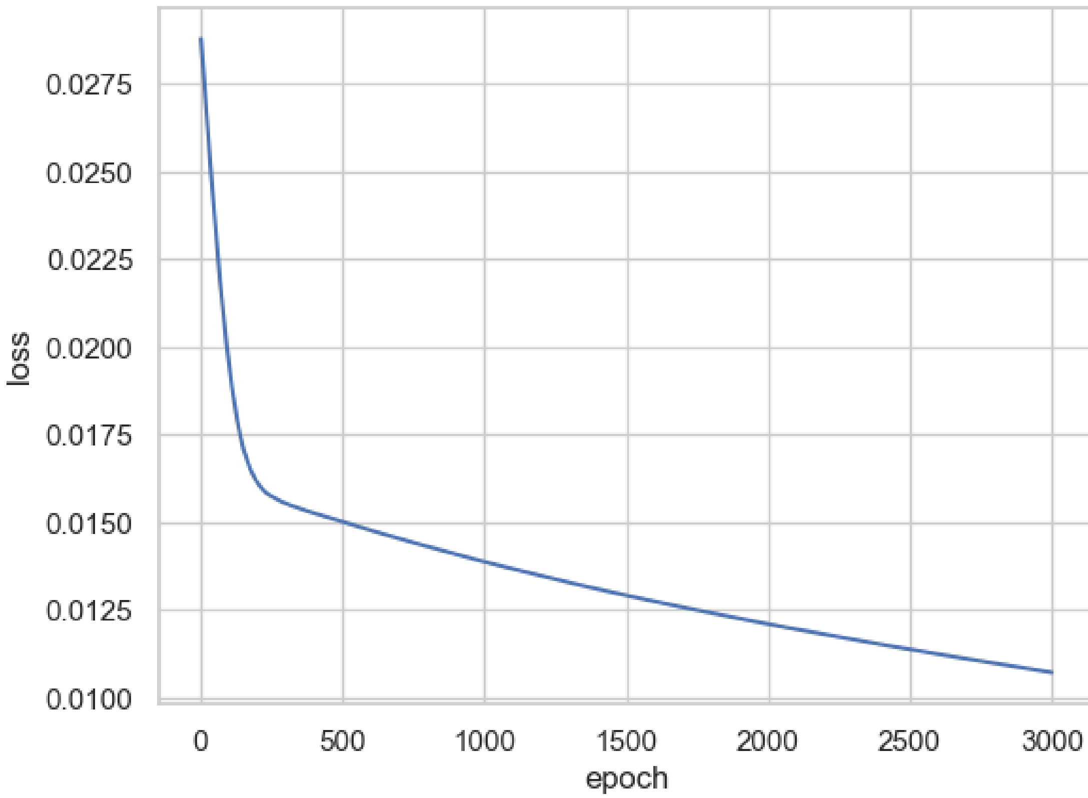
[13]:
```
class Network(object):

    def __init__(self, sizes):
        set_seed(42)
        self.num_layers = len(sizes)
        self.sizes = sizes
        self.biases = [np.random.randn(y, 1) for y in sizes[1:]]
        self.weights = [np.random.randn(y, x)
                        for x, y in zip(sizes[:-1], sizes[1:])]
```

```
def feedforward(self, a):
    for b, w in zip(self.biases, self.weights):
        a = self.sigmoid(np.dot(w, a) + b)
    return a

def SGD(self, training_data, epochs, mini_batch_size, eta, test_data=None):
    set_seed(42)
    n = len(training_data)
    epoch_losses = []

    for j in range(epochs):
        random.shuffle(training_data)
        mini_batches = [training_data[k:k + mini_batch_size]
                        for k in range(0, n, mini_batch_size)]
        for mini_batch in mini_batches:
            self.update_mini_batch(mini_batch, eta)

        epoch_loss = self.calculate_loss(training_data)
        epoch_losses.append(epoch_loss)

    return epoch_losses

def update_mini_batch(self, mini_batch, eta):
    nabla_b = [np.zeros(b.shape) for b in self.biases]
    nabla_w = [np.zeros(w.shape) for w in self.weights]
    for x, y in mini_batch:
        delta_nabla_b, delta_nabla_w = self.backprop(x, y)
        nabla_b = [nb + dnb for nb, dnb in zip(nabla_b, delta_nabla_b)]
        nabla_w = [nw + dnw for nw, dnw in zip(nabla_w, delta_nabla_w)]
    self.weights = [w - (eta / len(mini_batch)) *
                    nw for w, nw in zip(self.weights, nabla_w)]
    self.biases = [b - (eta / len(mini_batch)) * nb for b,
                   nb in zip(self.biases, nabla_b)]

def backprop(self, x, y):
    nabla_b = [np.zeros(b.shape) for b in self.biases]
    nabla_w = [np.zeros(w.shape) for w in self.weights]

    activation = x
    activations = [x]
    zs = []
    for b, w in zip(self.biases, self.weights):
        z = np.dot(w, activation) + b
        zs.append(z)
        activation = self.sigmoid(z)
        activations.append(activation)
```

```
        delta = self.cost_derivative(
            activations[-1], y) * self.sigmoid_prime(zs[-1])
        nabla_b[-1] = delta
        nabla_w[-1] = np.dot(delta, activations[-2].transpose())

        for l in range(2, self.num_layers):
            z = zs[-l]
            sp = self.sigmoid_prime(z)
            delta = np.dot(self.weights[-l + 1].transpose(), delta) * sp
            nabla_b[-l] = delta
            nabla_w[-l] = np.dot(delta, activations[-l - 1].transpose())
        return (nabla_b, nabla_w)

    def evaluate(self, test_data):
        test_results = [(np.argmax(self.feedforward(x)), y)
                        for (x, y) in test_data]
        return sum(int(x == y) for (x, y) in test_results)

    def cost_derivative(self, output_activations, y):
        return (output_activations - y)

    def sigmoid(self, z):
        return 1.0 / (1.0 + np.exp(-z))

    def sigmoid_prime(self, z):
        return self.sigmoid(z) * (1 - self.sigmoid(z))

    def calculate_loss(self, data):
        loss = 0
        for x, y in data:
            output = self.feedforward(x)
            loss += np.sum((output - y) ** 2)
        return loss / len(data)
```

[14]:
```
net = Network([len(features), 50, 25, 1])
epoch_losses = net.SGD(train_data, epochs=3000,
                       mini_batch_size=64, eta=0.01, test_data=test_data)
```

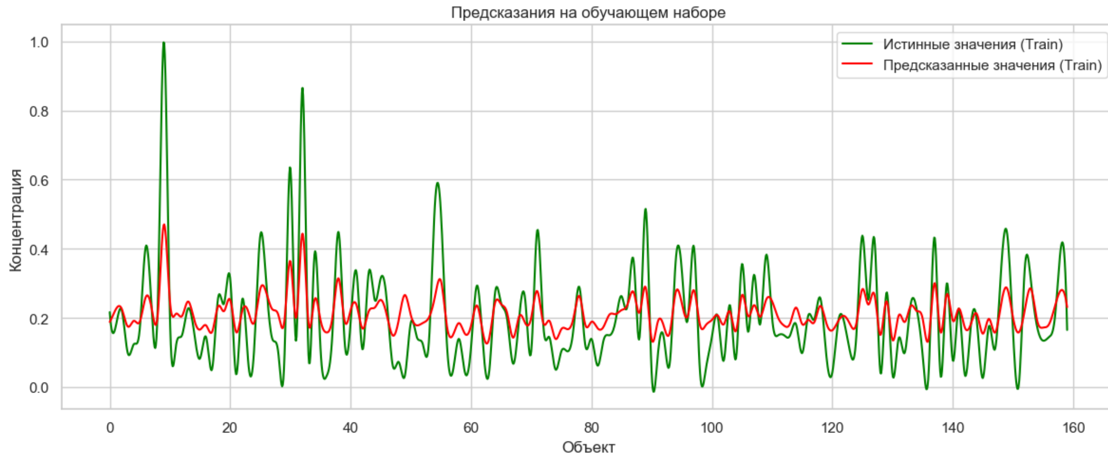
[15]:
```
plt.plot(range(1, len(epoch_losses) + 1), epoch_losses)
plt.xlabel('epoch')
plt.ylabel('loss')
plt.grid(True)
plt.show()
```



[16]:
```
from scipy.interpolate import make_interp_spline
import numpy as np
import matplotlib.pyplot as plt

def get_predictions(model, data):
    predictions = []
    for x, _ in data:
        predictions.append(model.feedforward(x))
    return predictions

def plot_predictions(train_data, train_predictions, test_data,␣
 ↪test_predictions):
    #
    train_true_values = [y for _, y in train_data]
    train_predicted_values = [pred[0] for pred in train_predictions]

    #
    test_true_values = [y for _, y in test_data]
    test_predicted_values = [pred[0] for pred in test_predictions]

    #
```

```python
def smooth_line(values):
    x_original = np.arange(len(values))
    x_new = np.linspace(0, len(values) - 1, len(values) * 10)  #

    spline = make_interp_spline(x_original, values, k=3)  #
    return x_new, spline(x_new)

#
train_x_smooth, train_true_smooth = smooth_line(train_true_values)
_, train_predicted_smooth = smooth_line(train_predicted_values)

#
test_x_smooth, test_true_smooth = smooth_line(test_true_values)
_, test_predicted_smooth = smooth_line(test_predicted_values)

#
plt.figure(figsize=(12, 10))

#
plt.subplot(2, 1, 1)
plt.plot(train_x_smooth, train_true_smooth, label='          (Train)', color='green')
plt.plot(train_x_smooth, train_predicted_smooth, label='            (Train)', color='red')
plt.title('                  ')
plt.xlabel('    ')
plt.ylabel('       ')
plt.legend()
plt.grid(True)

#
plt.subplot(2, 1, 2)
plt.plot(test_x_smooth, test_true_smooth, label='          (Test)', color='green')
plt.plot(test_x_smooth, test_predicted_smooth, label='            (Test)', color='red')
plt.title('                  ')
plt.xlabel('    ')
plt.ylabel('       ')
plt.legend()
plt.grid(True)

#
plt.tight_layout()
plt.show()
```

[17]:
```
test_predictions = get_predictions(net, test_data)
train_predictions = get_predictions(net, train_data)
plot_predictions(train_data, train_predictions, test_data, test_predictions)
```



[18]:
```
correlation_matrix = scaled_df.drop(columns=['label']).corr()
label_correlation = scaled_df.corr()['label']
columns_to_drop = set()
for col1 in correlation_matrix.columns:
    for col2 in correlation_matrix.columns:
        if col1 != col2 and (correlation_matrix.loc[col1, col2] > 0.8):
            if label_correlation[col1] >= label_correlation[col2]:
                columns_to_drop.add(col2)
            else:
                columns_to_drop.add(col1)

filtered_df = scaled_df.drop(columns=columns_to_drop)

filtered_df.head()
```

```
[18]:       label        Cr     Fe_Ka     Ca_Ka     Ni_Ka     Ni_kb     Cu_Ka  \
0  0.634021  0.545376  0.721069  0.492815  0.303459  0.500176  0.187549
1  0.489691  0.793318  0.991717  0.511980  0.064954  0.516423  0.187322
2  0.448454  0.827570  0.974607  0.563065  0.118139  0.494226  0.163690
3  1.000000  0.764076  1.000000  0.652656  0.108286  0.443447  0.212785
4  0.865979  0.712293  0.966873  0.756323  0.121018  0.450786  0.191769

      Zn_Ka     Pb_La     Pb_Lb
0  0.737144  0.737475  0.556190
1  0.920373  0.812522  0.473542
2  0.895705  0.788664  0.399465
3  0.906779  0.836439  0.464816
4  0.908752  0.789741  0.479420
```

```
[19]: filtered_df.columns
```

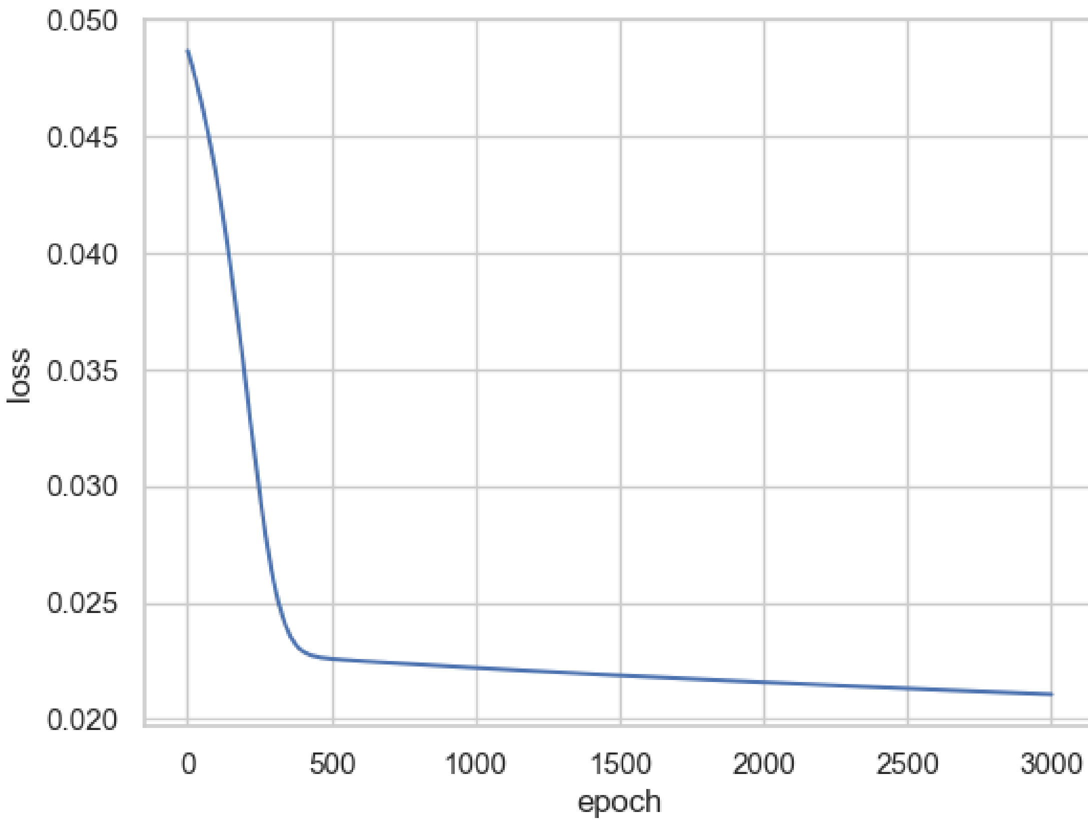
```
[19]: Index(['label', 'Cr', 'Fe_Ka', 'Ca_Ka', 'Ni_Ka', 'Ni_kb', 'Cu_Ka', 'Zn_Ka',
             'Pb_La', 'Pb_Lb'],
            dtype='object')
```

```
[20]: features = ['Cr', 'Fe_Ka', 'Ca_Ka', 'Ni_Ka', 'Ni_kb', 'Cu_Ka', 'Zn_Ka','Pb_La',␣
       ↪'Pb_Lb']
      X = filtered_df[features]
      y = filtered_df['label']

      X_train, X_test, y_train, y_test = train_test_split(
          X, y, test_size=0.2, random_state=4)
```

```
[21]: train_data = [(np.array(x).reshape(-1, 1), y)
                          for x, y in zip(X_train.values.tolist(), y_train.values.
       ↪tolist())]
      test_data = [(np.array(x).reshape(-1, 1), y)
                      for x, y in zip(X_test.values.tolist(), y_test.values.tolist())]
```

```
[22]: net = Network([len(features), 50, 25, 1])
      epoch_losses = net.SGD(train_data, epochs=3000,
                             mini_batch_size=64, eta=0.01, test_data=test_data)
```

```
[23]: plt.plot(range(1, len(epoch_losses) + 1), epoch_losses)
      plt.xlabel('epoch')
      plt.ylabel('loss')
      plt.grid(True)
      plt.show()
```



[24]:
```
test_predictions = get_predictions(net, test_data)
train_predictions = get_predictions(net, train_data)
plot_predictions(train_data, train_predictions, test_data, test_predictions)
```


Предсказания на обучающем наборе
Истинные значения (Train)
Предсказанные значения (Train)
Концентрация
Объект


Предсказания на тестовом наборе
Истинные значения (Test)
Предсказанные значения (Test)
Концентрация
Событие