Dimensionality Reduction Exercises

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Learning Objectives

- Explain and Apply Principal Component Analysis (PCA)
- Explain Multidimensional Scaling (MDS)
- Apply Intel® Extension for Scikit-learn* to leverage underlying compute capabilities of hardware

scikit-learn*

Frameworks provide structure that Data Scientists use to build code. Frameworks are more than just libraries, because in addition to callable code, frameworks influence how code is written.

A main virtue of using an optimized framework is that code runs faster. Code that runs faster is just generally more convenient but when we begin looking at applied data science and AI models, we can see more material benefits. Here you will see how optimization, particularly hyperparameter optimization can benefit more than just speed.

These exercises will demonstrate how to apply **the Intel® Extension for Scikit-learn*,** a seamless way to speed up your Scikit-learn application. The acceleration is achieved through the use of the Intel® oneAPI Data Analytics Library (oneDAL). Patching is the term used to extend scikit-learn with Intel optimizations and makes it a well-suited machine learning framework for dealing with real-life problems.

To get optimized versions of many Scikit-learn algorithms using a patch() approach consisting of adding these lines of code after importing sklearn:

- **from sklearnex import patch_sklearn**
- **patch_sklearn()**

This exercise relies on installation of Intel® Extension for Scikit-learn*

If you have not already done so, follow the instructions from Week 1 for instructions

Introduction

We will be using customer data from a Portuguese wholesale distributor for clustering. This data file is called `Wholesale_Customers_Data`.

It contains the following features:

- Fresh: annual spending (m.u.) on fresh products
- Milk: annual spending (m.u.) on milk products
- Grocery: annual spending (m.u.) on grocery products
- Frozen: annual spending (m.u.) on frozen products
- Detergents_Paper: annual spending (m.u.) on detergents and paper products
- Delicatessen: annual spending (m.u.) on delicatessen products
- Channel: customer channel (1: hotel/restaurant/cafe or 2: retail)
- Region: customer region (1: Lisbon, 2: Porto, 3: Other)

In this data, the values for all spending are given in an arbitrary unit (m.u. = monetary unit).

```
from __future__ import print_function
import os
data_path = ['data']

from sklearn.preprocessing import MinMaxScaler
from sklearn.preprocessing import FunctionTransformer
from sklearn.pipeline import Pipeline
from sklearn.decomposition import PCA
from sklearn.decomposition import KernelPCA
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import mean_squared_error
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import StratifiedShuffleSplit
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import accuracy_score

from sklearnex import patch_sklearn
patch_sklearn()
```

```
Intel(R) Extension for Scikit-learn* enabled (https://github.com/intel/scikit-learn-intelex)
```

Question 1

- Import the data and check the data types.
- Drop the channel and region columns as they won't be used.
- Convert the remaining columns to floats if necessary.
- Copy this version of the data (using the `copy` method) to a variable to preserve it. We will be using it later.

```
import pandas as pd
import numpy as np

filepath = os.sep.join(data_path + ['Wholesale_Customers_Data.csv'])
data = pd.read_csv(filepath, sep=',')
```

```
data.shape
```

```
(440, 8)
```

```
data.head()
```

	Channel	Region	Fresh	Milk	Grocery	Frozen	Detergents_Paper	Delicassen
0	2	3	12669	9656	7561	214	2674	1338
1	2	3	7057	9810	9568	1762	3293	1776
2	2	3	6353	8808	7684	2405	3516	7844
3	1	3	13265	1196	4221	6404	507	1788
4	2	3	22615	5410	7198	3915	1777	5185

```
data = data.drop(['Channel', 'Region'], axis=1)
```

```
data.dtypes
```

```
Fresh               int64
Milk                int64
Grocery             int64
Frozen              int64
Detergents_Paper    int64
Delicassen          int64
dtype: object
```

```
# Convert to floats
for col in data.columns:
    data[col] = data[col].astype(float)
```

Preserve the original data.

```
data_orig = data.copy()
```

Question 2

As with the previous lesson, we need to ensure the data is scaled and (relatively) normally distributed.

- Examine the correlation and skew.
- Perform any transformations and scale data using your favorite scaling method.
- View the pairwise correlation plots of the new data.

```
corr_mat = data.corr()

# Strip the diagonal for future examination
for x in range(corr_mat.shape[0]):
    corr_mat.iloc[x,x] = 0.0

corr_mat
```

	Fresh	Milk	Grocery	Frozen	Detergents_Paper	Delicassen
Fresh	0.000000	0.100510	-0.011854	0.345881	-0.101953	0.244690
Milk	0.100510	0.000000	0.728335	0.123994	0.661816	0.406368
Grocery	-0.011854	0.728335	0.000000	-0.040193	0.924641	0.205497
Frozen	0.345881	0.123994	-0.040193	0.000000	-0.131525	0.390947
Detergents_Paper	-0.101953	0.661816	0.924641	-0.131525	0.000000	0.069291
Delicassen	0.244690	0.406368	0.205497	0.390947	0.069291	0.000000

As before, the two categories with their respective most strongly correlated variable.

```
corr_mat.abs().idxmax()
```

```
Fresh                         Frozen
Milk                         Grocery
Grocery             Detergents_Paper
Frozen                    Delicassen
Detergents_Paper             Grocery
Delicassen                      Milk
dtype: object
```

Examine the skew values and log transform. Looks like all of them need it.

```
log_columns = data.skew().sort_values(ascending=False)
log_columns = log_columns.loc[log_columns > 0.75]

log_columns
```

```
Delicassen          11.151586
Frozen               5.907986
Milk                 4.053755
Detergents_Paper     3.631851
Grocery              3.587429
Fresh                2.561323
dtype: float64
```

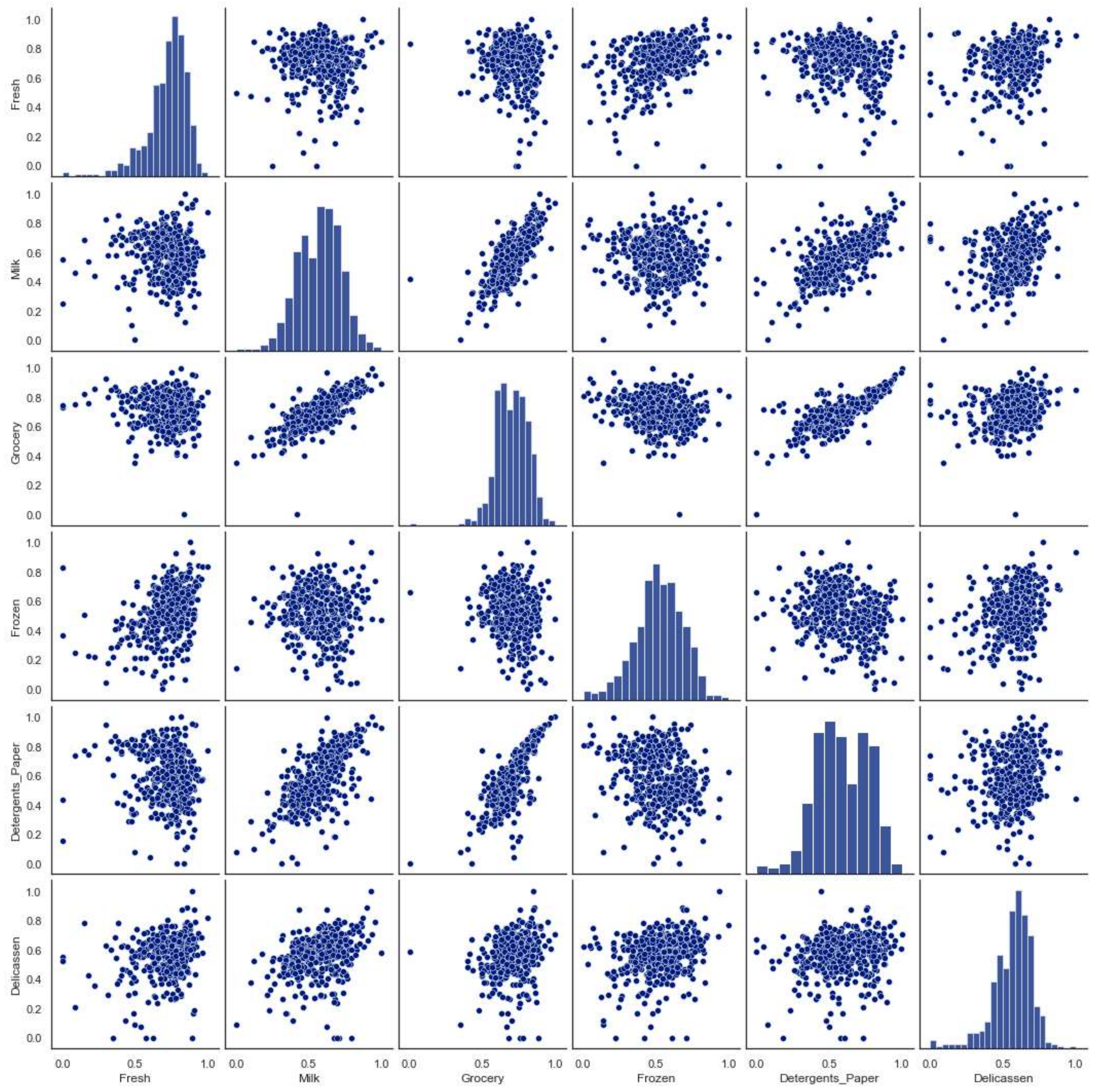
```
# The log transformations
for col in log_columns.index:
    data[col] = np.log1p(data[col])
```

Scale the data again. Let's use `MinMaxScaler` this time just to mix things up.

```
mms = MinMaxScaler()

for col in data.columns:
    data[col] = mms.fit_transform(data[[col]]).squeeze()
```

Visualize the relationship between the variables.

```
import seaborn as sns
import matplotlib.pyplot as plt

%matplotlib inline


sns.set_context('notebook')
sns.set_palette('dark')
sns.set_style('white')

sns.pairplot(data);
```


Fresh
Milk
Grocery
Frozen
Detergents_Paper
Delicassen
0.0
0.2
0.4
0.6
0.8
1.0
0.5

Question 3

- Using Scikit-learn's pipeline function, recreate the data pre-processing scheme above (transformation and scaling) using a pipeline. If you used a non-Scikit learn function to transform the data (e.g. NumPy's log function), checkout the custom transformer class called `FunctionTransformer`.
- Use the pipeline to transform the original data that was stored at the end of question 1.
- Compare the results to the original data to verify that everything worked.

Hint: Scikit-learn has a more flexible `Pipeline` function and a shortcut version called `make_pipeline`. Either can be used. Also, if different transformations need to be performed on the data, a `FeatureUnion` can be used.

```
# The custom NumPy log transformer
log_transformer = FunctionTransformer(np.log1p)

# The pipeline
estimators = [('log1p', log_transformer), ('minmaxscale', MinMaxScaler())]
pipeline = Pipeline(estimators)

# Convert the original data
data_pipe = pipeline.fit_transform(data_orig)
```

The results are identical. Note that machine learning models and grid searches can also be added to the pipeline (and in fact, usually are.)

```
np.allclose(data_pipe, data)
```

```
    True
```

Question 4

- Perform PCA with `n_components` ranging from 1 to 5.
- Store the amount of explained variance for each number of dimensions.
- Also store the feature importance for each number of dimensions. *Hint:* PCA doesn't explicitly provide this after a model is fit, but the `components_` properties can be used to determine something that approximates importance. How you decided to do so is entirely up to you.
- Plot the explained variance and feature importances.

```
pca_list = list()
feature_weight_list = list()

# Fit a range of PCA models

for n in range(1, 6):

    # Create and fit the model
    PCAmod = PCA(n_components=n)
    PCAmod.fit(data)

    # Store the model and variance
    pca_list.append(pd.Series({'n':n, 'model':PCAmod,
                               'var': PCAmod.explained_variance_ratio_.sum()}))

    # Calculate and store feature importances
    abs_feature_values = np.abs(PCAmod.components_).sum(axis=0)
    feature_weight_list.append(pd.DataFrame({'n':n,
                                             'features': data.columns,
                                             'values':abs_feature_values/abs_feature_values.sum(

pca_df = pd.concat(pca_list, axis=1).T.set_index('n')
pca_df
```

n	model	var
1	PCA(n_components=1)	0.448011
2	PCA(n_components=2)	0.720990
3	PCA(n_components=3)	0.827534
4	PCA(n_components=4)	0.923045
5	PCA(n_components=5)	0.979574

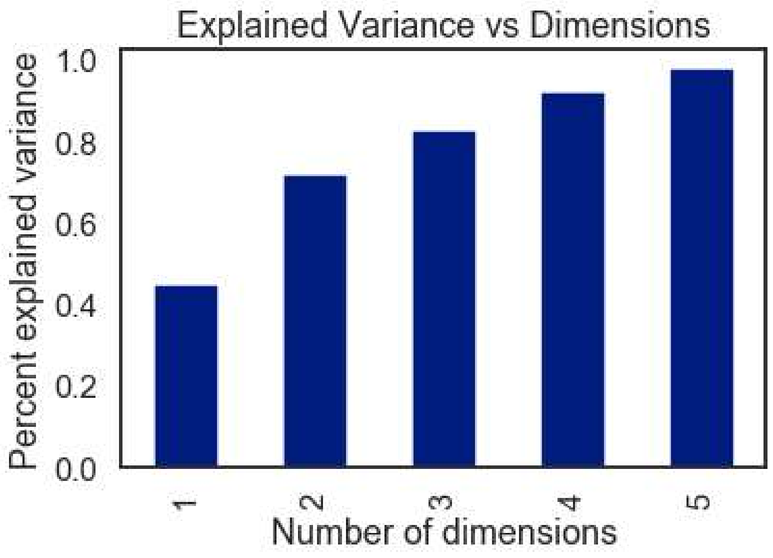
Create a table of feature importances for each data column.

```
features_df = (pd.concat(feature_weight_list)
               .pivot(index='n', columns='features', values='values'))

features_df
```

features n	Delicassen	Detergents_Paper	Fresh	Frozen	Grocery	Milk
1	0.071668	0.335487	0.060620	0.095979	0.190236	0.246010
2	0.151237	0.177519	0.158168	0.222172	0.112032	0.178872
3	0.165518	0.145815	0.211434	0.268363	0.084903	0.123967
4	0.224259	0.149981	0.239527	0.214275	0.070971	0.100987
5	0.211840	0.182447	0.196382	0.178104	0.067338	0.163888

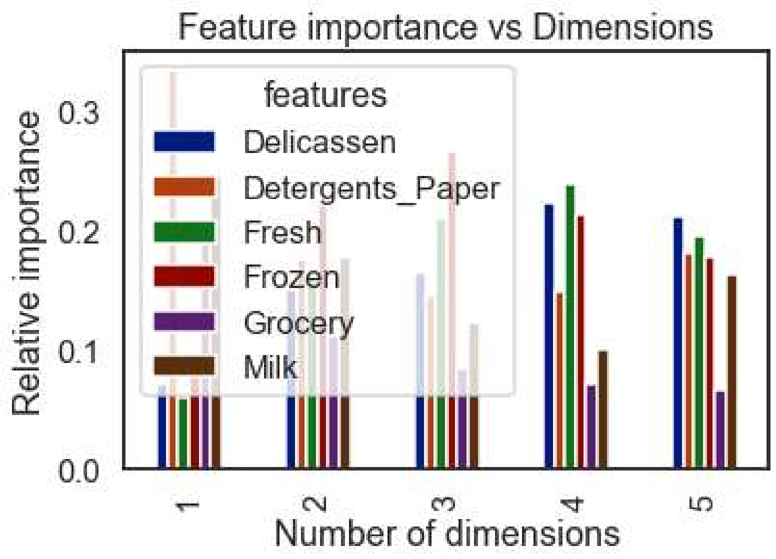
Create a plot of explained variances.

```
sns.set_context('talk')

ax = pca_df['var'].plot(kind='bar')

ax.set(xlabel='Number of dimensions',
       ylabel='Percent explained variance',
       title='Explained Variance vs Dimensions');
```



And here's a plot of feature importances.

```
ax = features_df.plot(kind='bar')

ax.set(xlabel='Number of dimensions',
       ylabel='Relative importance',
       title='Feature importance vs Dimensions');
```



Question 5

- Fit a `KernelPCA` model with `kernel='rbf'`. You can choose how many components and what values to use for the other parameters.
- If you want to tinker some more, use `GridSearchCV` to tune the parameters of the `KernelPCA` model.

The second step is tricky since grid searches are generally used for supervised machine learning methods and rely on scoring metrics, such as accuracy, to determine the best model. However, a custom scoring function can be written for `GridSearchCV`, where larger is better for the outcome of the scoring function.

What would such a metric involve for PCA? What about percent of explained variance? Or perhaps the negative mean squared error on the data once it has been transformed and then inversely transformed?

```
# Custom scorer--use negative rmse of inverse transform
def scorer(pcamodel, X, y=None):

    try:
        X_val = X.values
    except:
        X_val = X

    # Calculate and inverse transform the data
    data_inv = pcamodel.fit(X_val).transform(X_val)
    data_inv = pcamodel.inverse_transform(data_inv)

    # The error calculation
    mse = mean_squared_error(data_inv.ravel(), X_val.ravel())

    # Larger values are better for scorers, so take negative value
    return -1.0 * mse

# The grid search parameters
param_grid = {'gamma':[0.001, 0.01, 0.05, 0.1, 0.5, 1.0],
              'n_components': [2, 3, 4]}

# The grid search
kernelPCA = GridSearchCV(KernelPCA(kernel='rbf', fit_inverse_transform=True),
                         param_grid=param_grid,
                         scoring=scorer,
                         n_jobs=-1)


kernelPCA = kernelPCA.fit(data)

kernelPCA.best_estimator_
```

```
KernelPCA(fit_inverse_transform=True, gamma=1.0, kernel='rbf', n_components=4)
```

```
filepath = os.sep.join(data_path + ['Human_Activity_Recognition_Using_Smartphones_Data.csv'])
data2 = pd.read_csv(filepath, sep=',')
```

Let's explore how our model accuracy may change if we include a `PCA` in our model building pipeline

```
X = data2.drop('Activity', axis=1)
y = data2.Activity
sss = StratifiedShuffleSplit(n_splits=5, random_state=42)

# From the previous question build the code for this question
def get_avg_score(n):
    pipe = [
        ('scaler', MinMaxScaler()),
        ('pca', PCA(n_components=n)),
        ('estimator', LogisticRegression(max_iter=295, C=.001, penalty='l2'))
    ]
    pipe = Pipeline(pipe)
    scores = []
    for train_index, test_index in sss.split(X, y):
        X_train, X_test = X.loc[train_index], X.loc[test_index]
        y_train, y_test = y.loc[train_index], y.loc[test_index]
        pipe.fit(X_train, y_train)
        scores.append(accuracy_score(y_test, pipe.predict(X_test)))
    return np.mean(scores)
```