Multi-Dimension Scaling

is a distance-preserving manifold learning method. All manifold learning algorithms assume the dataset lies on a smooth, non linear manifold of low dimension and that a mapping $f: \mathbb{R}^D \to \mathbb{R}^d$ (D>>d) can be found by preserving one or more properties of the higher dimension space. Distance preserving methods assume that a manifold can be defined by the pairwise distances of its points. In distance preserving methods, a low dimensional embedding is obtained from the higher dimension in such a way that pairwise distances between the points remain same. Some distance preserving methods preserve spatial distances (MDS) while some preserve graph distances.

MDS is not a single method but a family of methods. MDS takes a dissimilarity matrix D where D_{ij} represents the dissimilarity between points i and j and produces a mapping on a lower dimension, preserving the dissimilarities as closely as possible. The dissimilarity matrix could be observed or calculated from the given dataset.

MDS can be divided into two categories:

- Metric MDS Metric MDS is used for quantitative data and tries to preserve the original dissimilarity metrics.
- Non-Metric MDS Non-metric MDS is used for ordinal data. It tries to keep the
 order of dissimialrity metrics intact.

t-Distributed Stochastic Neighbor Embedding (t-SNE)

t-Distributed Stochastic Neighbor Embedding (t-SNE) is a non-linear technique for dimensionality reduction that is particularly well suited for the visualization of high-dimensional datasets. It is extensively applied in image processing, NLP, genomic data and speech processing. To keep things simple, here's a brief overview of working of t-SNE:

- The algorithms starts by calculating the probability of similarity of points in high-dimensional space and calculating the probability of similarity of points in the corresponding low-dimensional space. The similarity of points is calculated as the conditional probability that a point A would choose point B as its neighbor if neighbors were picked in proportion to their probability density under a Gaussian (normal distribution) centered at A.
- It then tries to minimize the difference between these conditional probabilities (or similarities) in higher-dimensional and lower-dimensional space for a perfect representation of data points in lower-dimensional space.

 To measure the minimization of the sum of difference of conditional probability t-SNE minimizes the sum of Kullback-Leibler divergence of overall data points using a gradient descent method.

In simpler terms, t-Distributed stochastic neighbor embedding (t-SNE) minimizes the divergence between two distributions: a distribution that measures pairwise similarities of the input objects and a distribution that measures pairwise similarities of the corresponding low-dimensional points in the embedding.

In this way, t-SNE maps the multi-dimensional data to a lower dimensional space and attempts to find patterns in the data by identifying observed clusters based on similarity of data points with multiple features. However, after this process, the input features are no longer identifiable, and you cannot make any inference based only on the output of t-SNE. Hence it is mainly a data exploration and visualization technique.

I recommend to familiarize with this amazing blogpost https://distill.pub/2016/misread-tsne/ which graphically shows traps associated with use of t-SNE and how hyperparameters selection can affect final embeding.

To better illustrate properties of individual methods of reducing dimensionality (from this and previous lab), create a set of points in the shape of a roulade. To do it:

- 1. Prepare a point generator for the circles in this generator, ensure that the radius decreases with the next steps (in this way you will get a spiral)
- 2. Treat the spiral as a cross-sectional solid, creating a croissant / crescent roll
- 3. Move the points in the roll with a slight noise to avoid their perfect placement
- 4. For better visualization, you can give individual points a color depending, e.g. on the distance from the center of the roulade
- 5. Generated roulade should resemble the picture below

```
In [ ]: from time import time
        import math
        import random
        # import mkl
        import glob
        import numpy as np
        import pandas as pd
        import seaborn as sn
        import matplotlib.pyplot as plt
        from scipy import stats
        from mpl_toolkits.mplot3d import Axes3D
        from PIL import Image
        from matplotlib.cbook import get sample data
        from matplotlib.offsetbox import TextArea, DrawingArea, OffsetImage, Annotat
        from IPython.display import Image
        import tensorflow as tf
        from tensorflow import keras
```

```
import warnings
warnings.filterwarnings("ignore")

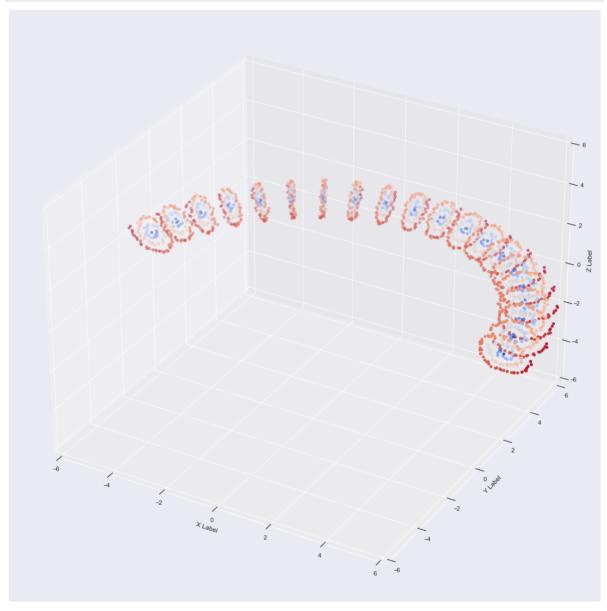
sn.set(color_codes=True)
np.random.seed(1234)
# mkl.set_num_threads(4)
%matplotlib inline
# %config InlineBackend.figure_format = 'retina'
plt.rcParams["figure.figsize"] = [20, 20]
```

Roulade points generator

```
In [ ]: def random spiral point(density=2):
            p = random.random() ** 0.5
            return p * math.cos(p * density * np.pi * 2), p * math.sin(p * density *
        def uniform spiral(density=3, steps=100):
            x, y = [], []
            for i in range(steps):
                x.append((i / steps) ** 0.5 * math.cos((i / steps) ** 0.5 * density
                y.append((i / steps) ** 0.5 * math.sin((i / steps) ** 0.5 * density
            return x, y
        def spiral2roll(xli, yli, width=7, angle=0.1):
            nx, ny, nz, d = [], [], []
            for x, y in zip(xli, yli):
                p = random.random()
                nx.append((width + x) * math.cos(angle * p * np.pi * 2))
                ny.append((width + x) * math.sin(angle * p * np.pi * 2))
                nz.append(y)
                d.append((x ** 2 + y ** 2) ** 0.5)
            return nx, ny, nz, d
        def uniform_roll(xli, yli, width=7, angle=0.25, density=5, noise_factor=0.05
            nx, ny, nz, d = [], [], []
            d1 = [((x ** 2 + y ** 2) ** 0.5)  for x, y in zip(xli, yli)]
            for i in range(density):
                nx.extend(
                     [(width + x) * math.cos(angle * i / density * np.pi * 2) + (rand
                     xli])
                ny.extend(
                     [(width + x) * math.sin(angle * i / density * np.pi * 2) + (rand
                     xli])
                nz.extend(yli)
                d.extend(d1)
            return nx, ny, nz, d
        def roll generator(to array=True, spiral density=3, spiral steps=20, width=7
            x, y = uniform spiral(density=spiral density, steps=spiral steps)
            x, y, z, d = uniform_roll(x, y, width=width, angle=angle, density=densit
            if to array:
                return np.array([x, y, z]).T, d
            else:
                return x, y, z, d
```

```
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
ax.scatter(x, y, z, c=d, cmap=plt.cm.coolwarm)
ax.set_xlabel('X Label')
ax.set_ylabel('Y Label')
ax.set_zlabel('Z Label')
ax.set_xlim([-6, 6])
ax.set_ylim([-6, 6])
ax.set_zlim([-6, 6])
plt.savefig('data/' + name)
if display is False:
    plt.close()
```

```
In []: xl, yl = uniform_spiral()
    x, y, z, d = uniform_roll(xl, yl, width=7, angle=0.5, density=20, noise_fact
    plot_roulade(x, y, z, d=d)
```



Visualize the prepared set of points by projecting onto a 2D plane, changing the following aspects in subsequent approaches:

- 1. Density of points generated, in terms of points per spiral
- 2. Distance between roll layers, layer density
- 3. Visualization method: PCA, KernelPCA, MDS, t-SNE

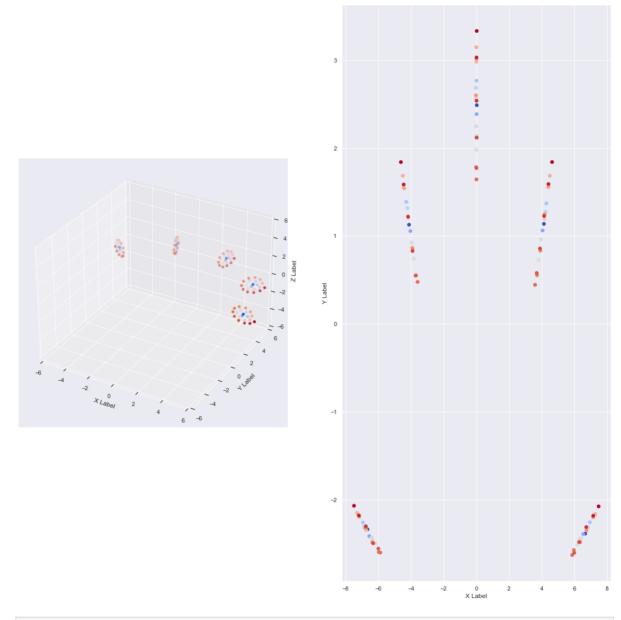
4. generate at least a few plots per method

Save each generated chart, you will later need it to embeding images

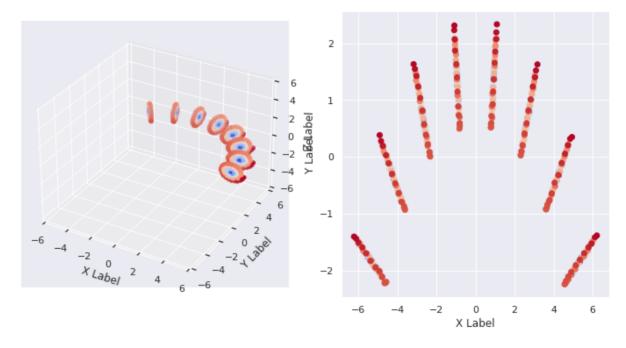
PCA implementation

```
In []: def show PCA(spiral density=3, spiral steps=20, width=7, angle=0.5, roll den
            fig = plt.figure()
            x, y, z, d = roll generator(to array=False, spiral density=spiral densit
                                         spiral steps=spiral steps, width=width,
                                         angle=angle, density=roll_density)
            from mpl toolkits.mplot3d import Axes3D
            # fig = plt.figure()
            ax = fig.add subplot(121, projection='3d')
            ax.scatter(x, y, z, c=d, cmap=plt.cm.coolwarm)
            ax.set xlabel('X Label')
            ax.set ylabel('Y Label')
            ax.set zlabel('Z Label')
            ax.set xlim([-6, 6])
            ax.set ylim([-6, 6])
            ax.set zlim([-6, 6])
            ax2 = fig.add subplot(122)
            points, d = roll_generator(to_array=True, spiral_density=spiral_density,
                                        spiral steps=spiral steps, width=width,
                                        angle=angle, density=roll density)
            from sklearn.decomposition import PCA
            embedding = PCA(n components=2)
            points_transformed = embedding.fit_transform(points)
            points transformed.shape
            points_transformed_t = points_transformed.T
            {\tt points\_transformed\_t.shape}
            ax2.scatter(points transformed t[0], points transformed t[1], c=d, cmap=
            ax2.set xlabel('X Label')
            ax2.set ylabel('Y Label')
            plt.rcParams["figure.figsize"] = [12, 6]
            extent = ax2.get window extent().transformed(fig.dpi scale trans.inverte
             fig savefig(f'pca spst{spiral steps} roldens{roll density} w{width} a{an
                         bbox inches=extent)
```

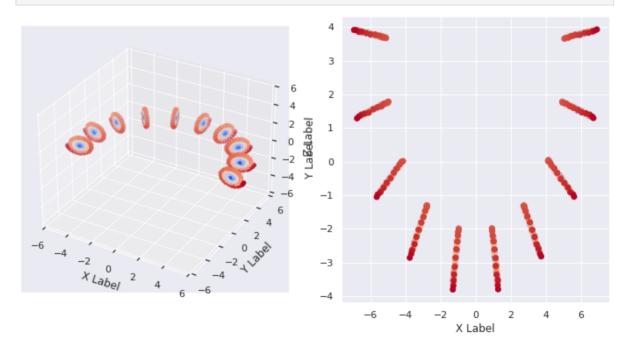
```
In [ ]: show_PCA()
```



In []: show_PCA(spiral_density=4, spiral_steps=50, width=6, angle=0.4, roll_density

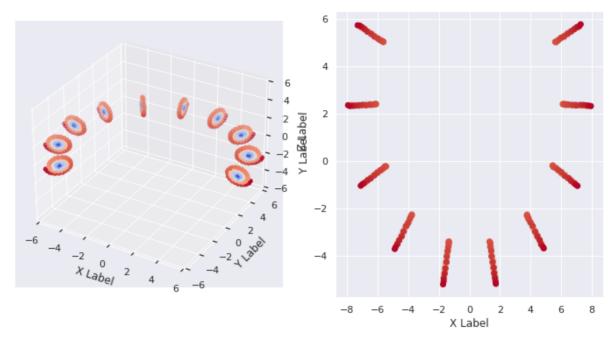


In []: show_PCA(spiral_density=4, spiral_steps=50, width=6, angle=0.60, roll_densit

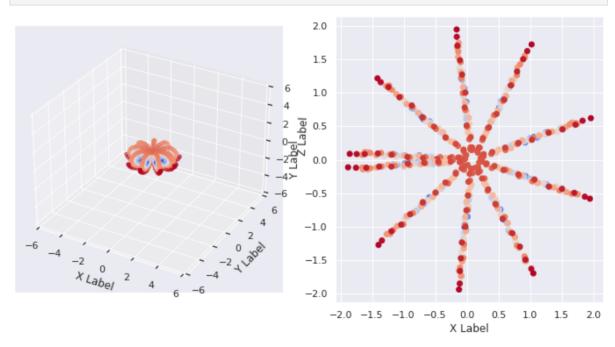


In []: show_PCA(spiral_density=4, spiral_steps=50, width=7, angle=0.70, roll_densit

28/03/2022, 00:57



In []: show_PCA(spiral_density=4, spiral_steps=50, width=1, angle=2.2, roll_density

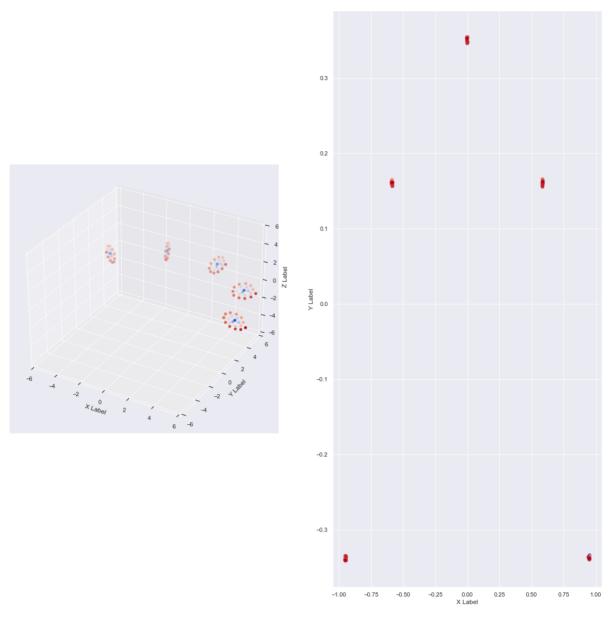


Patrzac na obrazki wygenrowane przez metode PCA, mozna odniesc wrazenie ze bierze ona pod uwagę tylko punkty w plaszczyznie x oraz y. W żaden sposob nie mamy zobrazowanej zalezności miedzy punktami na plaszczyznie z. Widzimy tak jakby rzut z gory.

KernelPCA implementation

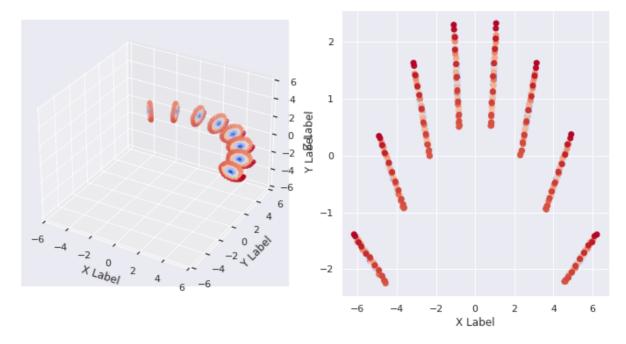
```
ax.set xlabel('X Label')
ax.set_ylabel('Y Label')
ax.set zlabel('Z Label')
ax.set xlim([-6, 6])
ax.set ylim([-6, 6])
ax.set zlim([-6, 6])
ax2 = fig.add subplot(122)
points, d = roll generator(to array=True, spiral density=spiral density,
                           spiral_steps=spiral_steps, width=width,
                           angle=angle, density=roll density)
from sklearn.decomposition import KernelPCA
embedding = KernelPCA(n components=2, degree=3, kernel='cosine', n jobs=
points transformed = embedding.fit transform(points)
points_transformed.shape
points_transformed_t = points_transformed.T
points transformed t.shape
ax2.scatter(points_transformed_t[0], points_transformed_t[1], c=d, cmap=
ax2.set xlabel('X Label')
ax2.set ylabel('Y Label')
plt.rcParams["figure.figsize"] = [12, 6]
extent = ax2.get window extent().transformed(fig.dpi scale trans.inverte
fig.savefig(f'kpca spst{spiral steps} roldens{roll density} w{width} a{a
            bbox inches=extent)
```

```
In [ ]: show_KernelPCA()
```

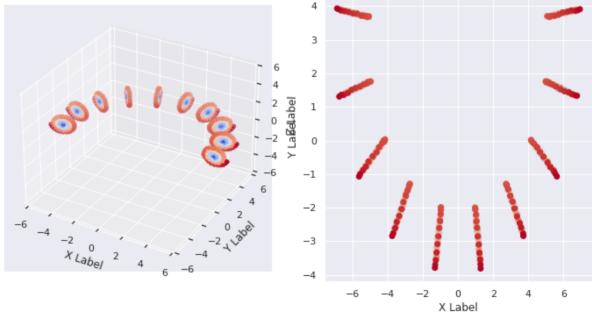


In []: show_KernelPCA(spiral_density=4, spiral_steps=50, width=5, angle=0.3, roll_d

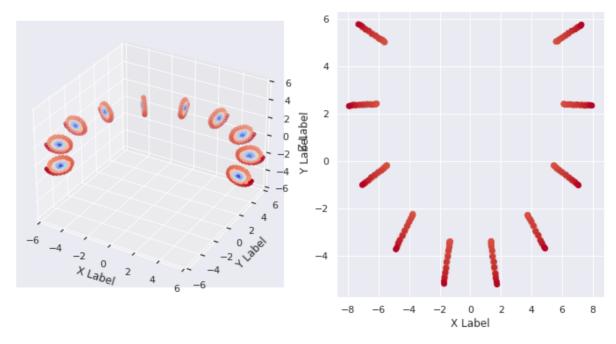
[n []: show_KernelPCA(spiral_density=4, spiral_steps=50, width=6, angle=0.4, roll_d



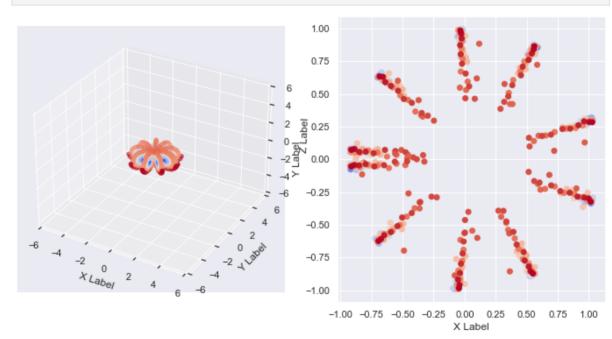
In []: show_KernelPCA(spiral_density=4, spiral_steps=50, width=6, angle=0.60, roll_



In []: show_KernelPCA(spiral_density=4, spiral_steps=50, width=7, angle=0.70, roll_





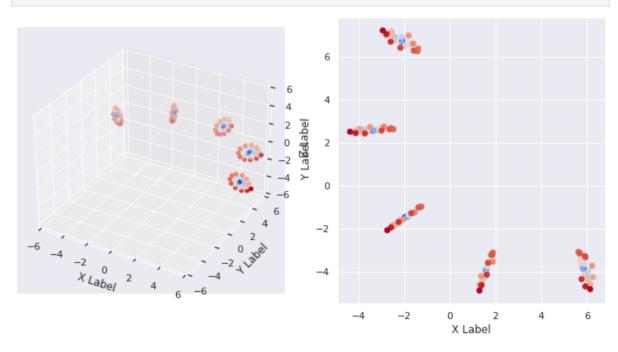


KernelPCA nie daje poprawy w stosunku do PCA, dla domyśnych parametrów. Zmiania parametrów nie jest pomocna - nadal nie widzimy odseparowanych niebieskich punktów

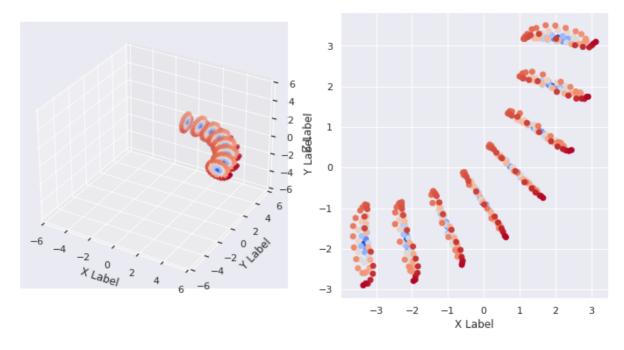
MDE implementation

```
ax.set_xlim([-6, 6])
ax.set_ylim([-6, 6])
ax.set_zlim([-6, 6])
ax2 = fig.add subplot(122)
points, d = roll generator(to array=True, spiral density=spiral density,
                           spiral steps=spiral steps, width=width,
                           angle=angle, density=roll density)
from sklearn.manifold import MDS
embedding = MDS(n components=2)
points_transformed = embedding.fit_transform(points)
points transformed.shape
points transformed t = points transformed.T
points transformed t.shape
ax2.scatter(points_transformed_t[0], points_transformed_t[1], c=d, cmap=
ax2.set xlabel('X Label')
ax2.set ylabel('Y Label')
plt.rcParams["figure.figsize"] = [12, 6]
extent = ax2.get_window_extent().transformed(fig.dpi_scale_trans.inverte
fig.savefig(f'mde_spst{spiral_steps}_roldens{roll_density}_w{width}_a{an
            bbox inches=extent)
```

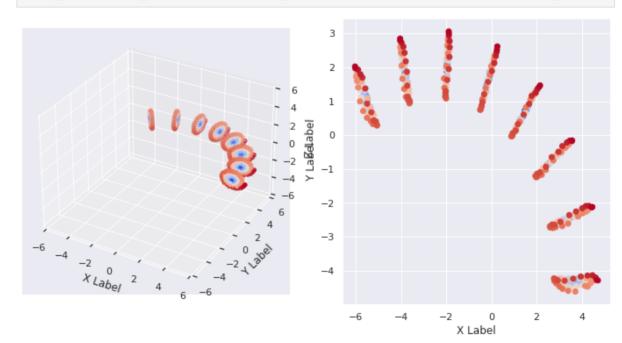
In []: show_MDE()



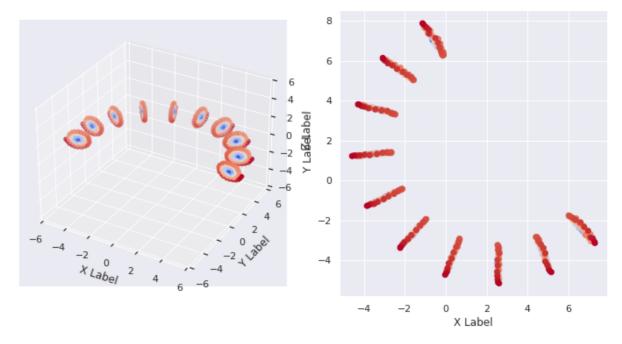
In []: show_MDE(spiral_density=4, spiral_steps=50, width=5, angle=0.3, roll_density



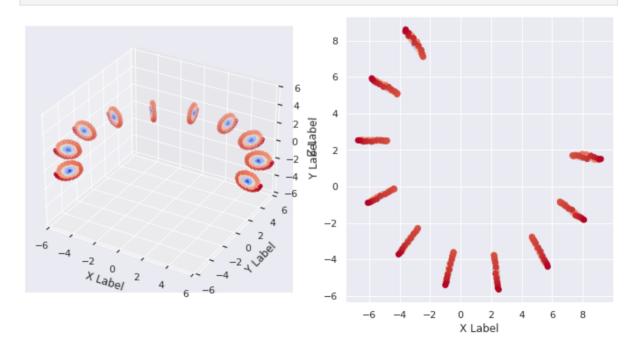
In []: show_MDE(spiral_density=4, spiral_steps=50, width=6, angle=0.4, roll_density



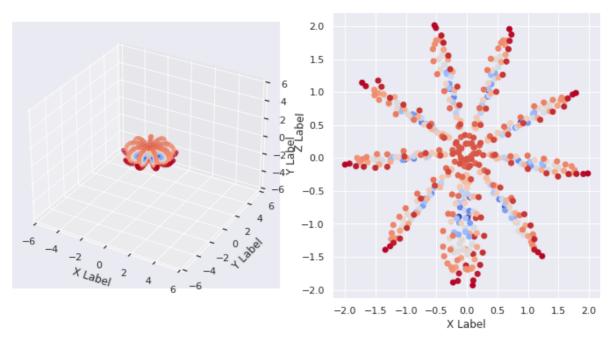
In []: show_MDE(spiral_density=4, spiral_steps=50, width=6, angle=0.60, roll_densit



In []: show_MDE(spiral_density=4, spiral_steps=50, width=7, angle=0.70, roll_densit



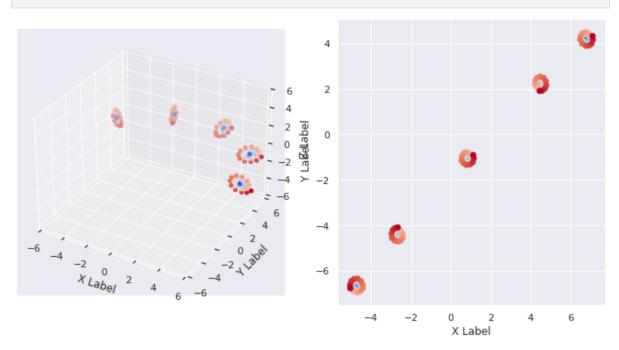
In []: show_MDE(spiral_density=4, spiral_steps=50, width=1, angle=2.2, roll_density



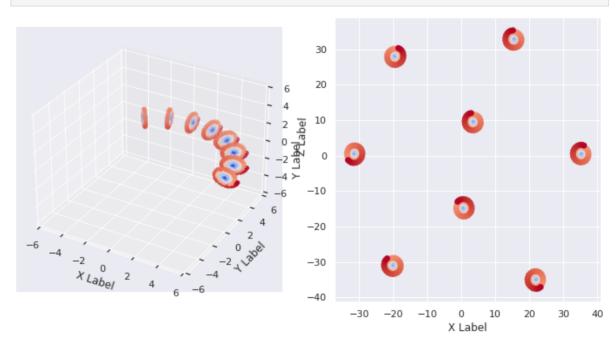
t-SNE implementation

```
In []: def show tSNE(spiral density=3, spiral steps=20, width=7, angle=0.5, roll de
                      metric='euclidean', perplexity=30):
            fig = plt.figure()
            x, y, z, d = roll generator(to array=False, spiral density=spiral densit
                                         spiral steps=spiral steps, width=width,
                                         angle=angle, density=roll_density)
            from mpl toolkits.mplot3d import Axes3D
            # fig = plt.figure()
            ax = fig.add subplot(121, projection='3d')
            ax.scatter(x, y, z, c=d, cmap=plt.cm.coolwarm)
            ax.set xlabel('X Label')
            ax.set ylabel('Y Label')
            ax.set zlabel('Z Label')
            ax.set_xlim([-6, 6])
            ax.set ylim([-6, 6])
            ax.set zlim([-6, 6])
            ax2 = fig.add subplot(122)
            points, d = roll_generator(to_array=True, spiral_density=spiral_density,
                                        spiral steps=spiral steps, width=width,
                                        angle=angle, density=roll density)
            from sklearn.manifold import TSNE
            points transformed = TSNE(n components=2, metric=metric, perplexity=perp
            points transformed t = points transformed.T
            ax2.scatter(points_transformed_t[0], points_transformed_t[1], c=d, cmap=
            ax2.set xlabel('X Label')
            ax2.set ylabel('Y Label')
            plt.rcParams["figure.figsize"] = [12, 6]
            extent = ax2.get window extent().transformed(fig.dpi scale trans.inverte
                 f'tsne n{n neighbors} spst{spiral steps} roldens{roll density} w{wid
                bbox_inches=extent)
            return points
```

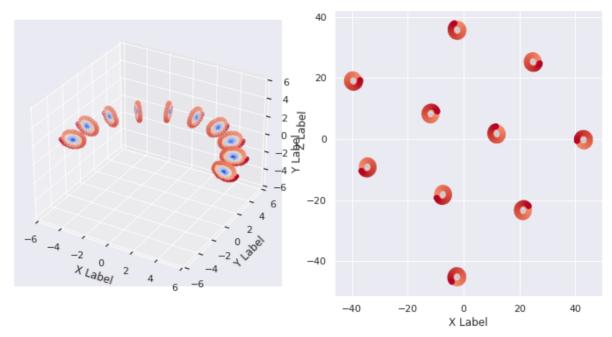
In []: points = show_tSNE()



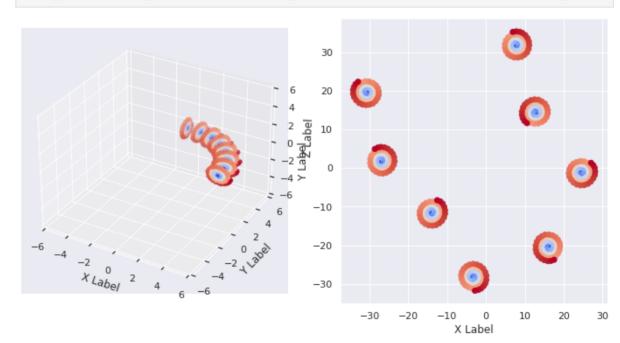
In []: show_tSNE(spiral_density=4, spiral_steps=50, width=6, angle=0.4, roll_densit



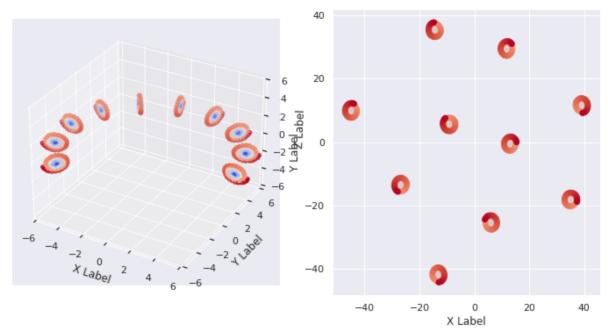
In []: show_tSNE(spiral_density=4, spiral_steps=50, width=6, angle=0.60, roll_densi



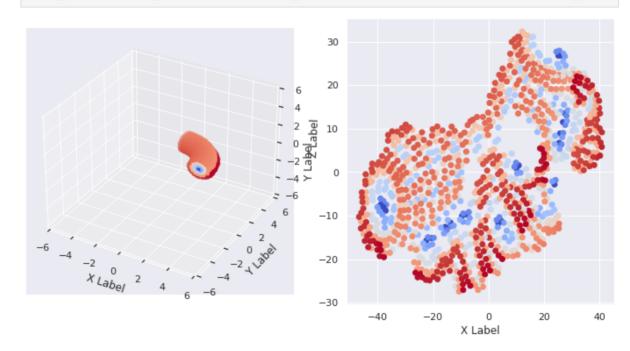
In []: show_tSNE(spiral_density=4, spiral_steps=50, width=5, angle=0.3, roll_densit



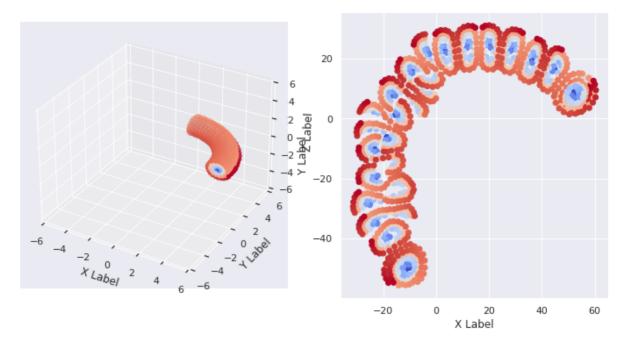
In []: show_tSNE(spiral_density=4, spiral_steps=50, width=7, angle=0.70, roll_densi



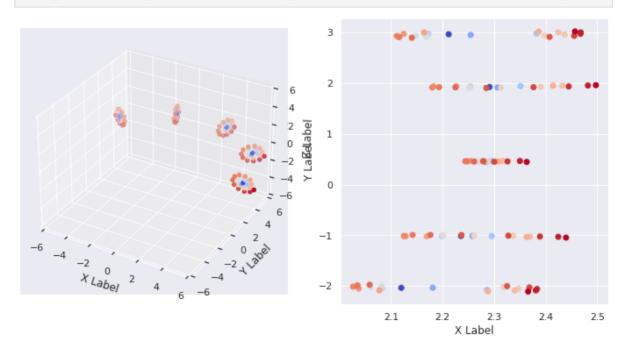
In []: show_tSNE(spiral_density=4, spiral_steps=50, width=3, angle=0.25, roll_densi



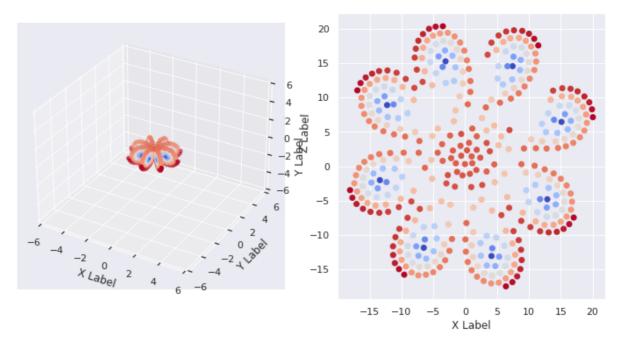
In []: show_tSNE(spiral_density=4, spiral_steps=50, width=5, angle=0.25, roll_densi



In []: show_tSNE(spiral_density=3, spiral_steps=20, width=7, angle=0.5, roll_densit



In []: show_tSNE(spiral_density=4, spiral_steps=50, width=1, angle=1, roll_density=

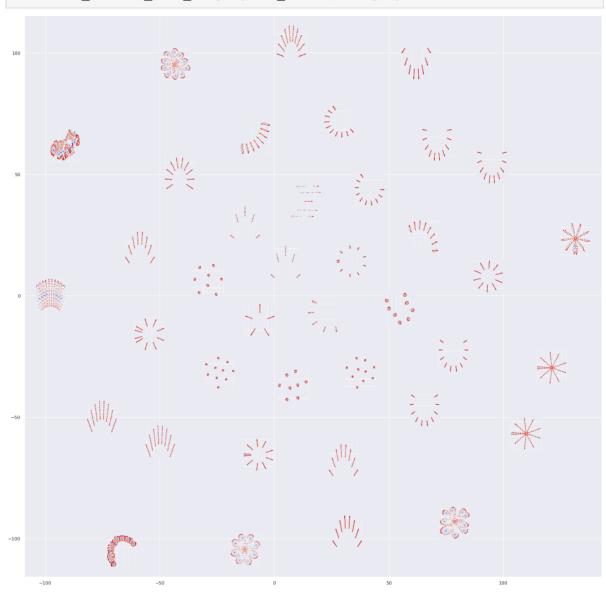


Zdecydowanie najlepsze efekty w porównaniu do poprzednich metod PCA i MDE. Rezult jest bardzo zalezny od wartosci uzytych parametrow, dobranie odpowiednich parametrow moze stanowic problem oraz trudnosci. W celu dobrania dobrych parametrow nalezy przeprowadzic wiele eksperymentow.

In this way, you should get a set of images showing the various available projections of the original roulade to the 2D plane. Treat these images as elements of a new data set, we treat image pixels as a high-dimensional vector. Use t-SNE to project the newly created set of 2d projection thumbnails into a 2-dimensional space.

```
In [ ]: import sklearn
        print(sklearn.neighbors.VALID METRICS['brute'])
        show tSNE(spiral density=3, spiral steps = 20, width=7, angle=0.5, roll dens
In [ ]: from PIL import Image
        import glob
In [ ]: def read images(flat=True):
            images = []
            for filename in glob.glob('data/*.png'):
                img=Image.open(filename)
                img as arr = np.asarray(img)
                if flat is True:
                     img as arr = img as arr.flatten()
                images.append(img as arr)
            return np.asarray(images)
        images = read images(False)
        flatten images = read images()
In [ ]: def execute tsne(images):
            from sklearn.manifold import TSNE
            points transformed = TSNE(n components=2, metric='euclidean', perplexity
            return points transformed
        tsne result = execute tsne(flatten images)
```

```
In []: visualize scatter with images(tsne result, images)
```



Na środku widzimy głównie obrazki z kernelPCA oraz PCA, które były bardzo podobne do siebie. Z samej prawej strony są te, które maja wypelniony srodek zdjecia. Na lewo strone trafily zdjecia o najmniej określonym ksztalcie.

homework - work with more complex data (higher dimensionality).

- use a basic machine learning set representing black and white scans of 32x32 pixel handwritten digits (MNIST)
- apply dimensionality reduction on these data using PCA, MDS and t-SNE methods

- Plot results
- Pick first 1000-2000 points as TSNE takes a lot of time for all samples

```
In [ ]: (x train, y train), (x test, y test) = tf.keras.datasets.mnist.load data(pat
        print(x train.shape)
        print(y train.shape)
        (60000, 28, 28)
        (60000,)
In [ ]: def plot 2d mnist(X, y):
             fig, plot = plt.subplots()
             # fig.set size inches(16, 16)
            plt.prism()
             for i in range(10):
                 digit indices = (y == i)
                 dim1 = X[digit_indices][:, 0]
                 dim2 = X[digit indices][:, 1]
                 plot.scatter(dim1, dim2)
            plot.set xticks(())
            plot.set yticks(())
            plt.tight layout()
            plt.legend(labels = [i for i in range(10)])
             plt.show()
In [ ]: # narrow down sample size
        n \text{ samples} = 1500
        y train small = y train[:n samples]
        x train small = x train[:n samples]
        (1500, 784)
Out[ ]:
In [ ]:
        np.unique(y train small, return counts=True) # sprawdzenie czy podzbiór ma z
Out[]: (array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9], dtype=uint8),
         array([140, 172, 144, 142, 160, 137, 141, 177, 134, 153]))
In [ ]: #PCA
        def mnist PCA(x):
             from sklearn.decomposition import PCA
             embedding = PCA(n components=2)
            x transformed = embedding.fit transform(x)
             print(x transformed.shape)
            return(x transformed)
In [ ]: print(x train small.shape)
        x train small 2d = x train small reshape(-1, 28 * 28)
        print(x train small 2d.shape)
        (1500, 28, 28)
        (1500, 784)
In []: transformed x = mnist PCA(x train small 2d)
        plot 2d mnist(transformed x, y train small)
        (1500, 2)
```

28/03/2022, 00:57

PCA



```
In []: #MDS
    def mnist_MDE(x_train):
        from sklearn.manifold import MDS
        embedding = MDS(n_components=2)
        points_transformed = embedding.fit_transform(x_train)
        return points_transformed

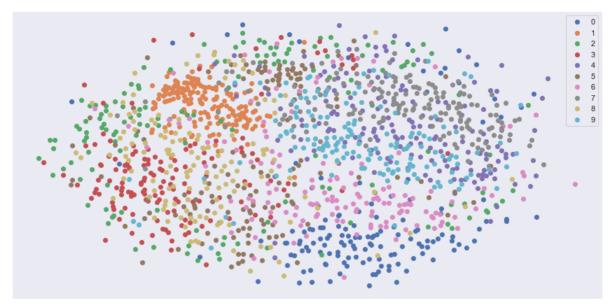
transformed_x_MDE = mnist_MDE(x_train_small_2d)
```

In []: plot_2d_mnist(transformed_x_MDE, y_train_small)



```
In []: def mnist_MDE(x_train):
    from sklearn.manifold import MDS
    embedding = MDS(n_components=2, max_iter=400, verbose=1, n_jobs=-1)
    points_transformed = embedding.fit_transform(x_train)
    return points_transformed

transformed_x_MDE = mnist_MDE(x_train_small_2d)
    plot_2d_mnist(transformed_x_MDE, y_train_small)
```



```
In [ ]: transformed_x_MDE = mnist_MDE(x_train.reshape(-1, 28 * 28))
    plot_2d_mnist(transformed_x_MDE, y_train)
```

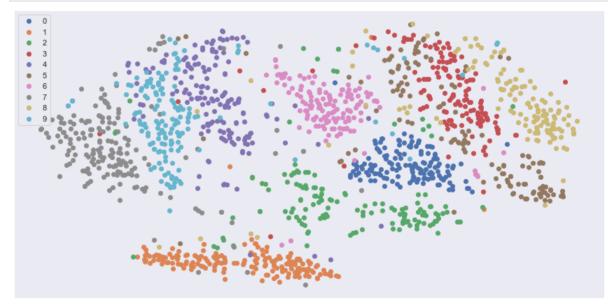
```
In []: # t-SNE
    def tsne_mnist(x_train, perplexity=30):
        from sklearn.manifold import TSNE
        points_transformed = TSNE(n_components=2, metric='euclidean', perplexity
        return points_transformed
    tsne_x_train = tsne_mnist(x_train_small_2d)
    plot_2d_mnist(tsne_x_train, y_train_small)
```



```
In []: def tsne_mnist(x_train, perplexity=30):
    from sklearn.manifold import TSNE
    points_transformed = TSNE(n_components=2, metric='cosine', perplexity=pe
    return points_transformed
    tsne_x_train = tsne_mnist(x_train_small_2d)
    plot_2d_mnist(tsne_x_train, y_train_small)
```



```
In []: def tsne_mnist(x_train, perplexity=100):
    from sklearn.manifold import TSNE
    points_transformed = TSNE(n_components=2, metric='cosine', perplexity=pe
    return points_transformed
    tsne_x_train = tsne_mnist(x_train_small_2d)
    plot_2d_mnist(tsne_x_train, y_train_small)
```



Najlepiej wypadała metoda tSNE, widzimy wyraźną klasteryzajcę, odpowiednio dobrane parametry mogą jeszcze dalej nieznacznie poprawić jakość danych. Metody PCA i MDE wypałdy znacznie gorzej – wielie liczb jest rozproszonych niemal po całym wykresie – dobrze klasteryzują liczbę 1. W przypadku MDE nie widać poprawy przy manipulacji parametrami. W PCA nie za bardzo jest czym manipulować, na pewno w porównaniu do MDE lepiej radzi sobie z klateryzajcą 0.