PCA - An example on Exploratory Data Analysis

In this notebook you will:

- Replicate Andrew's example on PCA
- Visualize how PCA works on a 2-dimensional small dataset and that not every projection is "good"
- Visualize how a 3-dimensional data can also be contained in a 2-dimensional subspace
- Use PCA to find hidden patterns in a high-dimensional dataset

Importing the libraries

In [1]:
```
import pandas as pd
import numpy as np
from sklearn.decomposition import PCA
from pca_utils import plot_widget
from bokeh.io import show, output_notebook
from bokeh.plotting import figure
import matplotlib.pyplot as plt
import plotly.offline as py
```

In [2]:
```
py.init_notebook_mode()
```

In [3]:
```
output_notebook()
```

(https://bokeh.org) Loading BokehJS ...

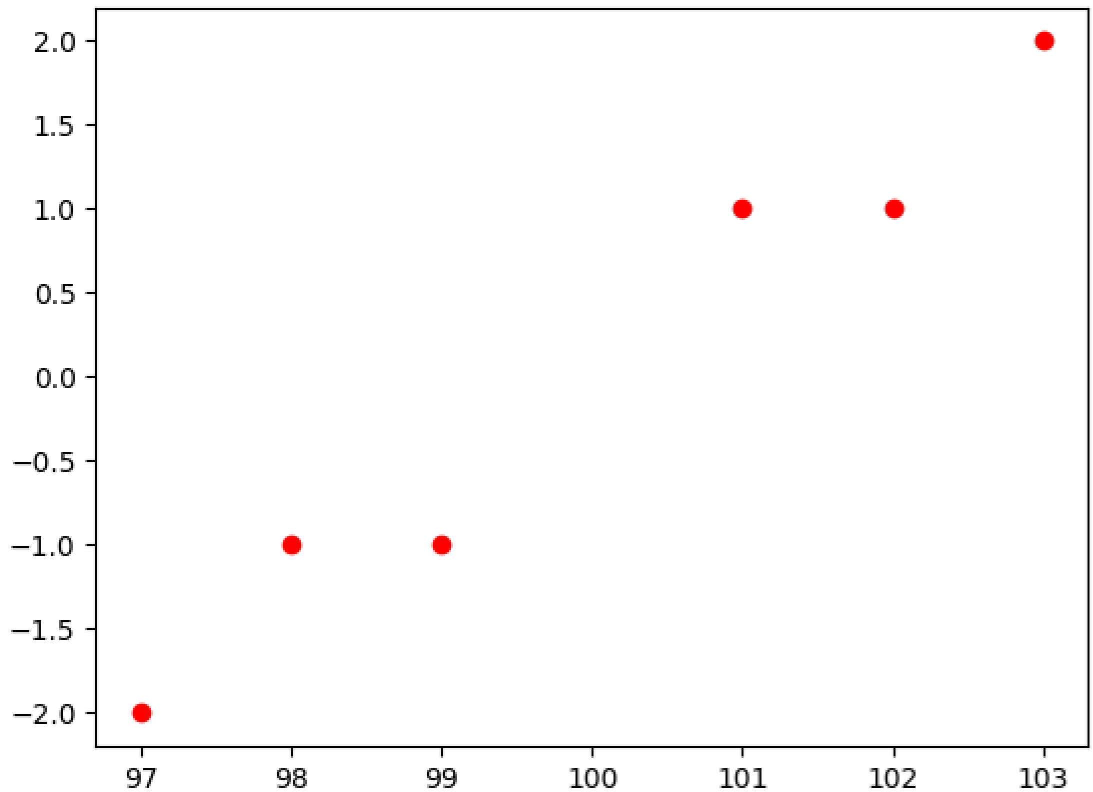
Lecture Example

We are going work on the same example that Andrew has shown in the lecture.

In [4]:
```
X = np.array([[ 99,  -1],
       [ 98,  -1],
       [ 97,  -2],
       [101,   1],
       [102,   1],
       [103,   2]])
```

In [5]:
```
plt.plot(X[:,0], X[:,1], 'ro')
```

Out[5]: [<matplotlib.lines.Line2D at 0x7f0c800ddfd0>]



In [6]:
```
# Loading the PCA algorithm
pca_2 = PCA(n_components=2)
pca_2
```

Out[6]: PCA(n_components=2)

In [7]:
```
# Let's fit the data. We do not need to scale it, since sklearn's implement
pca_2.fit(X)
```

Out[7]: PCA(n_components=2)

In [8]:
```
pca_2.explained_variance_ratio_
```

Out[8]: array([0.99244289, 0.00755711])

The coordinates on the first principal component (first axis) are enough to retain 99.24% of the information ("explained variance"). The second principal component adds an additional 0.76% of the information ("explained variance") that is not stored in the first principal component coordinates.

In [9]:
```python
X_trans_2 = pca_2.transform(X)
X_trans_2
```

Out[9]:
```
array([[ 1.38340578,  0.2935787 ],
       [ 2.22189802, -0.25133484],
       [ 3.6053038 ,  0.04224385],
       [-1.38340578, -0.2935787 ],
       [-2.22189802,  0.25133484],
       [-3.6053038 , -0.04224385]])
```

Think of column 1 as the coordinate along the first principal component (the first new axis) and column 2 as the coordinate along the second principal component (the second new axis).

You can probably just choose the first principal component since it retains 99% of the information (explained variance).

In [10]:
```python
pca_1 = PCA(n_components=1)
pca_1
```

Out[10]:
```
PCA(n_components=1)
```

In [11]:
```python
pca_1.fit(X)
pca_1.explained_variance_ratio_
```

Out[11]:
```
array([0.99244289])
```

In [12]:
```python
X_trans_1 = pca_1.transform(X)
X_trans_1
```

Out[12]:
```
array([[ 1.38340578],
       [ 2.22189802],
       [ 3.6053038 ],
       [-1.38340578],
       [-2.22189802],
       [-3.6053038 ]])
```

Notice how this column is just the first column of `X_trans_2` .

If you had 2 features (two columns of data) and choose 2 principal components, then you'll keep all the information and the data will end up the same as the original.

In [13]:
```python
X_reduced_2 = pca_2.inverse_transform(X_trans_2)
X_reduced_2
```

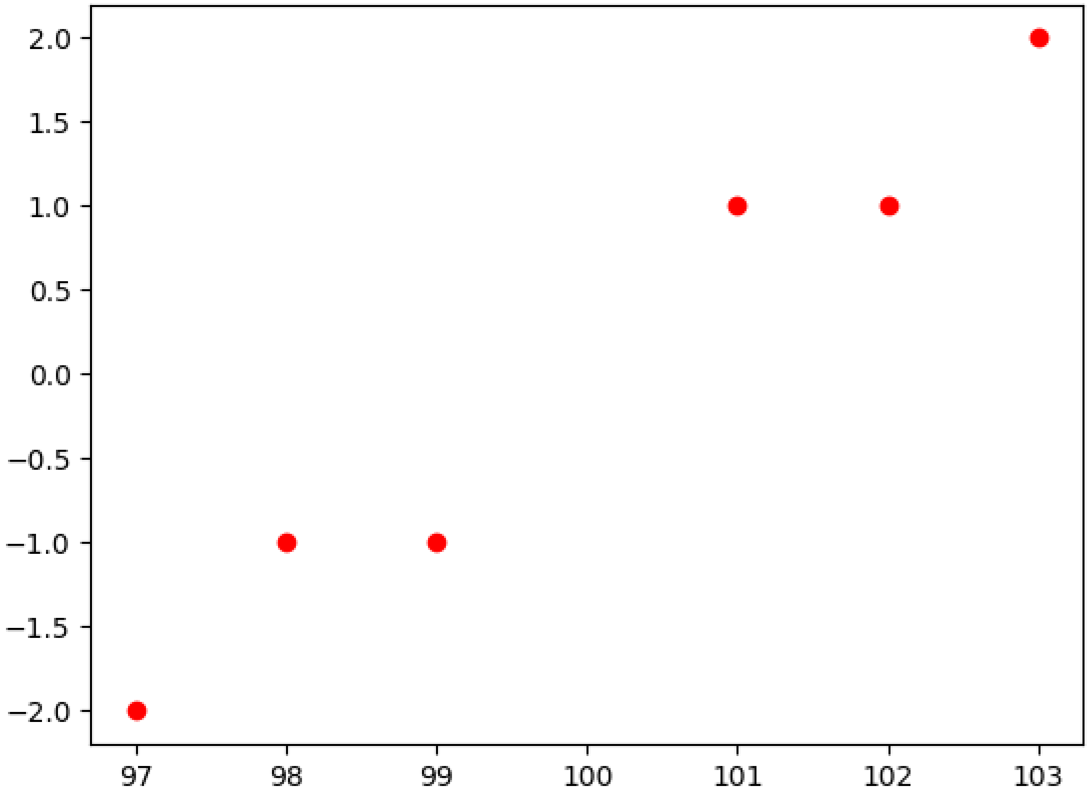
Out[13]:
```
array([[ 99.,  -1.],
       [ 98.,  -1.],
       [ 97.,  -2.],
       [101.,   1.],
       [102.,   1.],
       [103.,   2.]])
```

In [14]:

```
plt.plot(X_reduced_2[:,0], X_reduced_2[:,1], 'ro')
```

Out[14]:

```
[<matplotlib.lines.Line2D at 0x7f0c7b1d78d0>]
```



Reduce to 1 dimension instead of 2

In [15]:

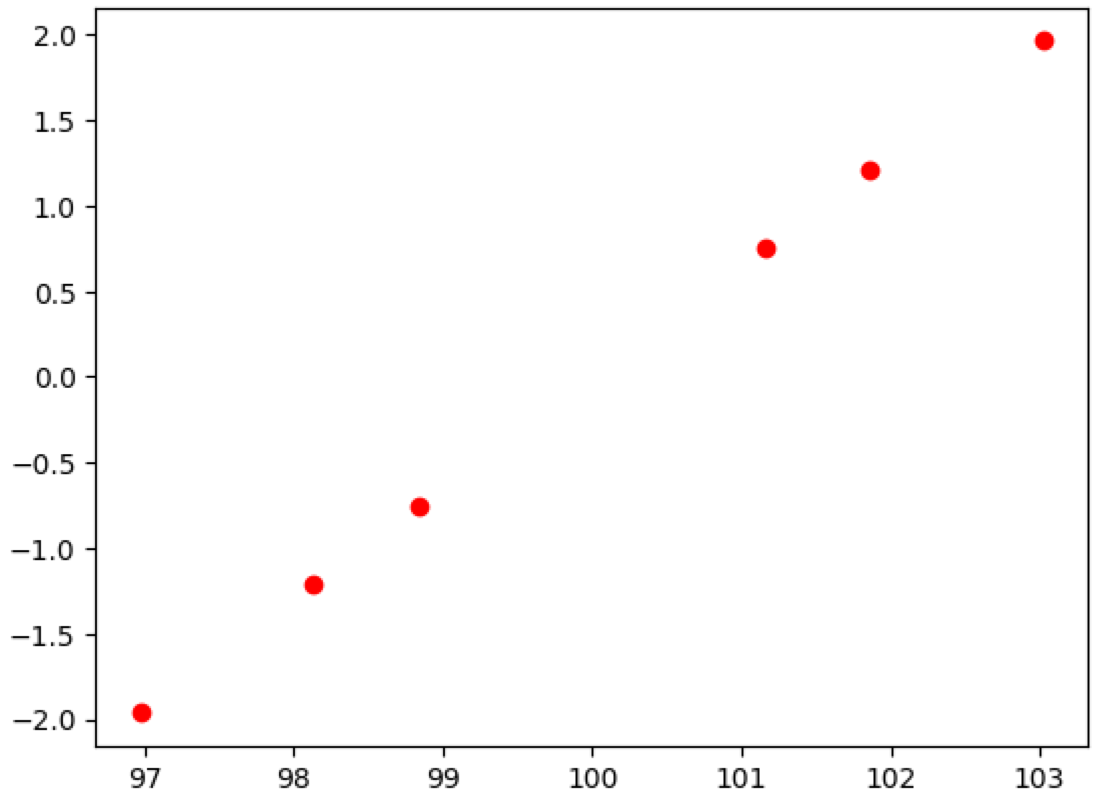
```
X_reduced_1 = pca_1.inverse_transform(X_trans_1)
X_reduced_1
```

Out[15]:

```
array([[ 98.84002499,  -0.75383654],
       [ 98.13695576,  -1.21074232],
       [ 96.97698075,  -1.96457886],
       [101.15997501,   0.75383654],
       [101.86304424,   1.21074232],
       [103.02301925,   1.96457886]])
```

In [16]:
```
plt.plot(X_reduced_1[:,0], X_reduced_1[:,1], 'ro')
```

Out[16]: [<matplotlib.lines.Line2D at 0x7f0c7b1638d0>]



Notice how the data are now just on a single line (this line is the single principal component that was used to describe the data; and each example had a single "coordinate" along that axis to describe its location.

Visualizing the PCA algorithm

Let's define 10 points in the plane and use them as an example to visualize how we can compress this points in 1 dimension. You will see that there are good ways and bad ways.

In [17]:
```
X = np.array([[-0.83934975, -0.21160323],
       [ 0.67508491,  0.25113527],
       [-0.05495253,  0.36339613],
       [-0.57524042,  0.24450324],
       [ 0.58468572,  0.95337657],
       [ 0.5663363 ,  0.07555096],
       [-0.50228538, -0.65749982],
       [-0.14075593,  0.02713815],
       [ 0.2587186 , -0.26890678],
       [ 0.02775847, -0.77709049]])
```

In [18]:
```python
p = figure(title = '10-point scatterplot', x_axis_label = 'x-axis', y_axis_
p.scatter(X[:,0],X[:,1],marker = 'o', color = '#C00000', size = 5) ## Add t

## Some visual adjustments
p.grid.visible = False
p.grid.visible = False
p.outline_line_color = None
p.toolbar.logo = None
p.toolbar_location = None
p.xaxis.axis_line_color = "#f0f0f0"
p.xaxis.axis_line_width = 5
p.yaxis.axis_line_color = "#f0f0f0"
p.yaxis.axis_line_width = 5

## Shows the figure
show(p)
```

The next code will generate a widget where you can see how different ways of compressing this data into 1-dimensional datapoints will lead to different ways on how the points are spread in this new space. The line generated by PCA is the line that keeps the points as far as possible from each other.

You can use the slider to rotate the black line through its center and see how the points' projection onto the line will change as we rotate the line.

You can notice that there are projections that place different points in almost the same point, and there are projections that keep the points as separated as they were in the plane.

In [19]:
```python
plot_widget()
```

```
HBox(children=(FigureWidget({
    'data': [{'hovertemplate': 'x=%{x}<br>y=%{y}<extra></extra>',
              …
```

Visualization of a 3-dimensional dataset

In this section we will see how some 3 dimensional data can be condensed into a 2 dimensional space.

In [20]:
```python
from pca_utils import random_point_circle, plot_3d_2d_graphs
```

In [21]:
```python
X = random_point_circle(n = 150)
```

In [22]:
```python
deb = plot_3d_2d_graphs(X)
```

In [23]:
```python
deb.update_layout(yaxis2 = dict(title_text = 'test', visible=True))
```

Using PCA in Exploratory Data Analysis

Let's load a toy dataset with 500 samples and 1000 features.

In [24]:
```python
df = pd.read_csv("toy_dataset.csv")
```

In [25]:

```
df.head()
```

Out[25]:

	feature_0	feature_1	feature_2	feature_3	feature_4	feature_5	feature_6	feature_
0	27.422157	-29.662712	-23.297163	-15.161935	0.345581	3.706750	-5.507209	-46.9924
1	3.489482	-19.153551	-14.636424	14.688258	20.114204	13.532852	34.298084	22.9825
2	4.293509	22.691579	-1.045155	-8.740350	12.401082	31.362987	-18.831206	-35.3845
3	-2.139348	23.158754	-26.241206	19.426465	9.472049	8.453948	0.637211	-26.6759
4	-35.251034	27.281816	-29.470282	-21.786865	11.806822	58.655133	5.375230	59.7406

5 rows × 1000 columns

This is a dataset with 1000 features.

Let's try to see if there is a pattern in the data. The following function will randomly sample 100 pairwise tuples (x,y) of features, so we can scatter-plot them.

In [29]:

```
def get_pairs(n = 100):
    from random import randint
    i = 0
    tuples = []
    while i < 100:
        x = df.columns[randint(0,999)]
        y = df.columns[randint(0,999)]
        while x == y or (x,y) in tuples or (y,x) in tuples:
            y = df.columns[randint(0,999)]
        tuples.append((x,y))
        i+=1
    return tuples
```

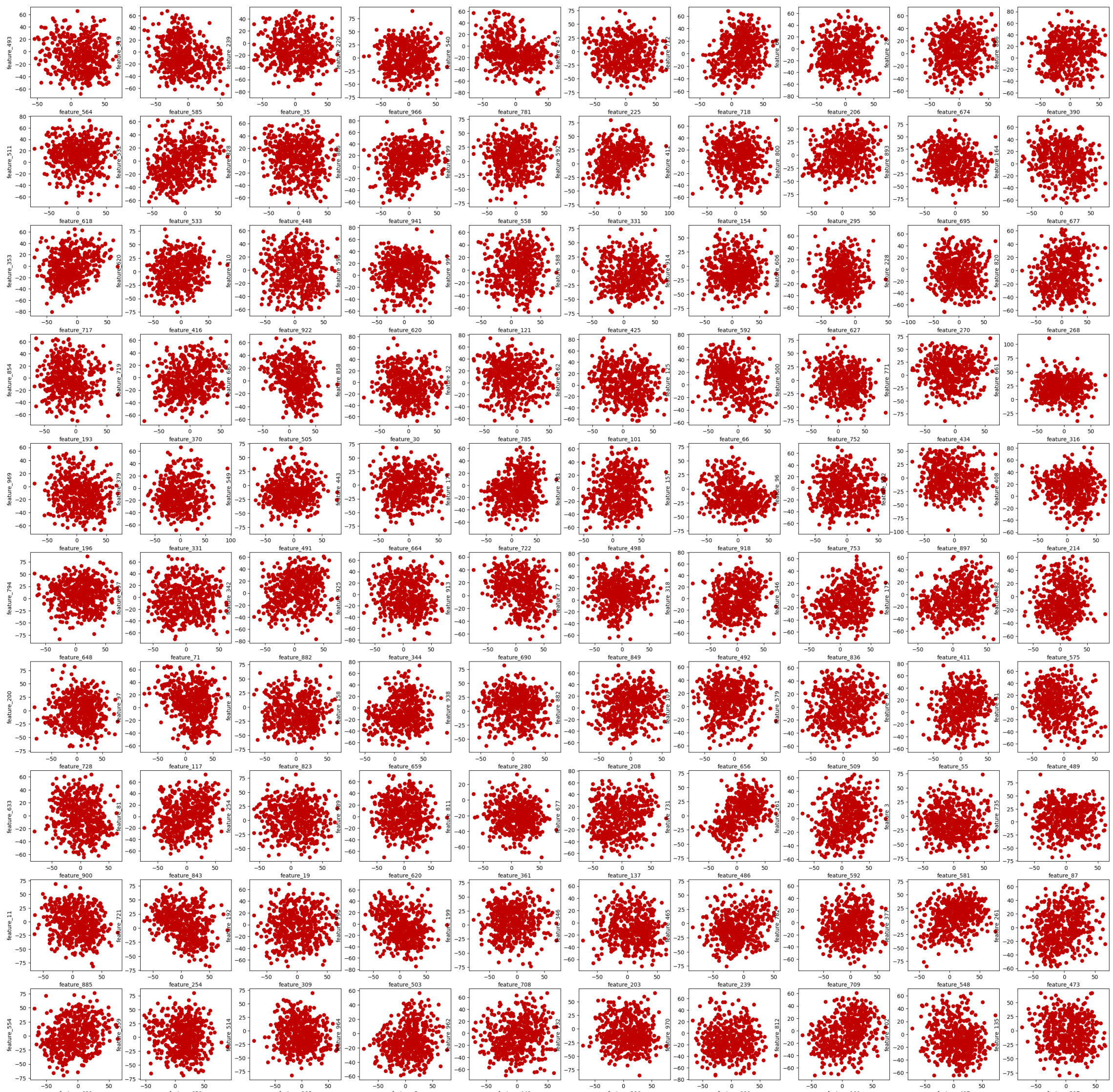
In [30]:

```
pairs = get_pairs()
```

Now let's plot them!

In [31]:

```
fig, axs = plt.subplots(10,10, figsize = (35,35))
i = 0
for rows in axs:
    for ax in rows:
        ax.scatter(df[pairs[i][0]],df[pairs[i][1]], color = "#C00000")
        ax.set_xlabel(pairs[i][0])
        ax.set_ylabel(pairs[i][1])
        i+=1
```



It looks like there is not much information hidden in pairwise features. Also, it is not possible to check every combination, due to the amount of features. Let's try to see the linear correlation between them.

In [34]:

```
# This may take 1 minute to run
corr = df.corr()
```

In [35]:
```
## This will show all the features that have correlation > 0.5 in absolute
## with correlation == 1 to remove the correlation of a feature with itself

mask = (abs(corr) > 0.5) & (abs(corr) != 1)
corr.where(mask).stack().sort_values()
```

Out[35]:
```
feature_81   feature_657   -0.631294
feature_657  feature_81    -0.631294
feature_313  feature_4     -0.615317
feature_4    feature_313   -0.615317
feature_716  feature_1     -0.609056
                              ...
feature_792  feature_547    0.620864
feature_35   feature_965    0.631424
feature_965  feature_35     0.631424
feature_395  feature_985    0.632593
feature_985  feature_395    0.632593
Length: 1870, dtype: float64
```

The maximum and minimum correlation is around 0.631 - 0.632. This does not show too much as well.

Let's try PCA decomposition to compress our data into a 2-dimensional subspace (plane) so we can plot it as scatter plot.

In [36]:
```
# Loading the PCA object
pca = PCA(n_components = 2) # Here we choose the number of components that
X_pca = pca.fit_transform(df)
df_pca = pd.DataFrame(X_pca, columns = ['principal_component_1','principal_
```

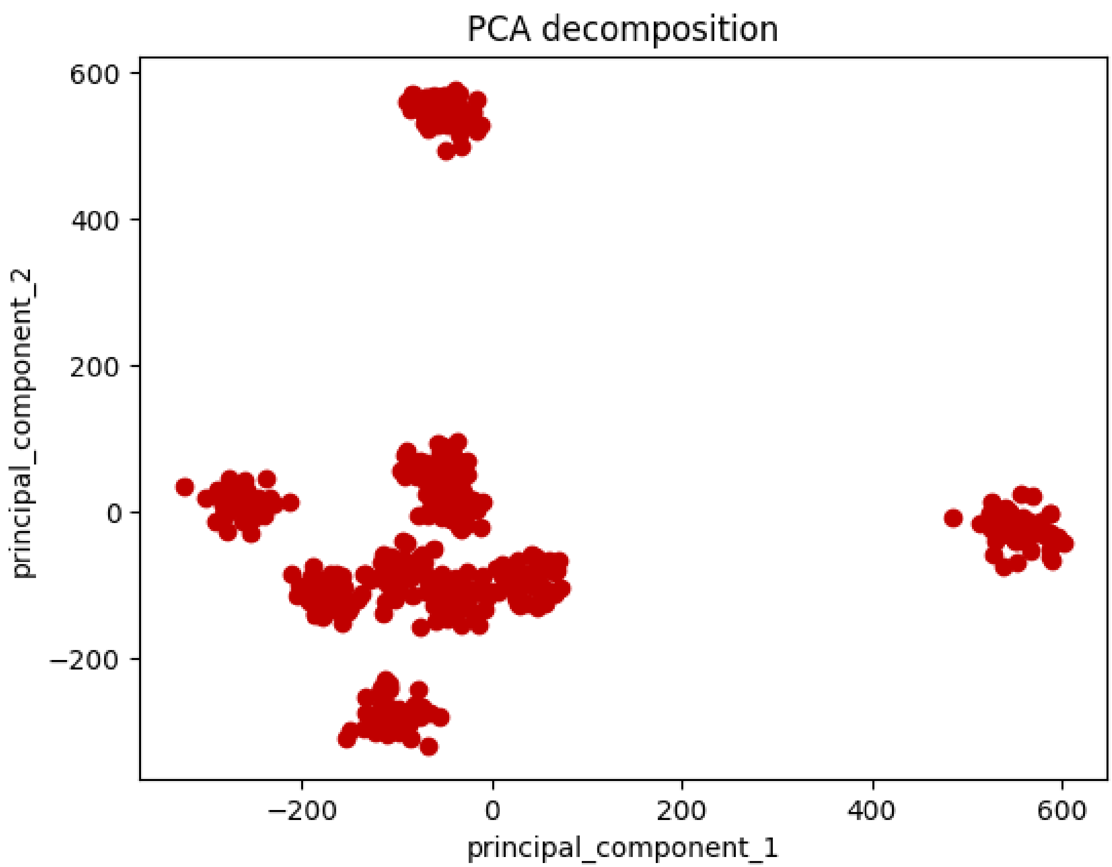
In [37]:
```
df_pca.head()
```

Out[37]:

	principal_component_1	principal_component_2
0	-46.235641	-1.672797
1	-210.208758	-84.068249
2	-26.352795	-127.895751
3	-116.106804	-269.368256
4	-110.183605	-279.657306

In [38]:
```
plt.scatter(df_pca['principal_component_1'],df_pca['principal_component_2']
plt.xlabel('principal_component_1')
plt.ylabel('principal_component_2')
plt.title('PCA decomposition')
```

Out[38]: Text(0.5, 1.0, 'PCA decomposition')



This is great! We can see well defined clusters.

In [ ]:
```
# pca.explained_variance_ration_ returns a list where it shows the amount c
sum(pca.explained_variance_ratio_)
```

And we preserved only around 14.6% of the variance!

Quite impressive! We can clearly see clusters in our data, something that we could not see before. How many clusters can you spot? 8, 10?

If we run a PCA to plot 3 dimensions, we will get more information from data.

In [ ]:
```
pca_3 = PCA(n_components = 3).fit(df)
X_t = pca_3.transform(df)
df_pca_3 = pd.DataFrame(X_t,columns = ['principal_component_1','principal_c
```

In [ ]:
```
import plotly.express as px
```

In [ ]:
```
fig = px.scatter_3d(df_pca_3, x = 'principal_component_1', y = 'principal_c
fig.show()
```

In [ ]:
```
sum(pca_3.explained_variance_ratio_)
```

Now we preserved 19% of the variance and we can clearly see 10 clusters.

Congratulations on finishing this notebook!