Machine Learning: Examen 1

Clustering methods and principal component analysis

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In [1]:
```
import importlib

from itertools import permutations

import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt

from sklearn.model_selection import KFold
from sklearn.preprocessing import StandardScaler, MinMaxScaler

from utils import eda, dimensionality_reduction, clustering, visualization

pd.set_option('display.max_columns', None)
sns.set_theme(style="darkgrid")
```

Paths

In [2]:
```
DATA_PATH = "../data/"
FIGURES_PATH = "./figures/"
```

Data loading

In [3]:
```
data = pd.read_csv(DATA_PATH + "bodyPerformance.csv")
print(f"Total instances: {data.shape[0]}")
print(f"Total features: {data.shape[1]}")
data.head(10)
```

```
Total instances: 13393
Total features: 12
```

Out[3]:

	age	gender	height_cm	weight_kg	body fat_%	diastolic	systolic	gripForce	sit and bend forward_cm
0	27.0	M	172.3	75.24	21.3	80.0	130.0	54.9	18.4
1	25.0	M	165.0	55.80	15.7	77.0	126.0	36.4	16.3
2	31.0	M	179.6	78.00	20.1	92.0	152.0	44.8	12.0
3	32.0	M	174.5	71.10	18.4	76.0	147.0	41.4	15.2
4	28.0	M	173.8	67.70	17.1	70.0	127.0	43.5	27.1
5	36.0	F	165.4	55.40	22.0	64.0	119.0	23.8	21.0
6	42.0	F	164.5	63.70	32.2	72.0	135.0	22.7	0.8
7	33.0	M	174.9	77.20	36.9	84.0	137.0	45.9	12.3
8	54.0	M	166.8	67.50	27.6	85.0	165.0	40.4	18.6
9	28.0	M	185.0	84.60	14.4	81.0	156.0	57.9	12.1

Rename some columns for easier access

In [4]:
```
data = data.rename(columns={
    "body fat_%": "body_fat_pct",
    "gripForce": "grip_force",
    "sit and bend forward_cm": "sit_and_bend_forward_cm",
    "sit-ups counts": "sit_ups_counts",
    "broad jump_cm": "broad_jump_cm",
})
data.head(10)
```

Out[4]:

	age	gender	height_cm	weight_kg	body_fat_pct	diastolic	systolic	grip_force	sit_
0	27.0	M	172.3	75.24	21.3	80.0	130.0	54.9	
1	25.0	M	165.0	55.80	15.7	77.0	126.0	36.4	
2	31.0	M	179.6	78.00	20.1	92.0	152.0	44.8	
3	32.0	M	174.5	71.10	18.4	76.0	147.0	41.4	
4	28.0	M	173.8	67.70	17.1	70.0	127.0	43.5	
5	36.0	F	165.4	55.40	22.0	64.0	119.0	23.8	
6	42.0	F	164.5	63.70	32.2	72.0	135.0	22.7	
7	33.0	M	174.9	77.20	36.9	84.0	137.0	45.9	
8	54.0	M	166.8	67.50	27.6	85.0	165.0	40.4	
9	28.0	M	185.0	84.60	14.4	81.0	156.0	57.9	

Exploratory Data Analysis

The dataset has NaN values?

In [5]:
```
eda.get_nan_count(data)
```

Out[5]:

	nan_count	nan_percentage
age	0	0.0
gender	0	0.0
height_cm	0	0.0
weight_kg	0	0.0
body_fat_pct	0	0.0
diastolic	0	0.0
systolic	0	0.0
grip_force	0	0.0
sit_and_bend_forward_cm	0	0.0
sit_ups_counts	0	0.0
broad_jump_cm	0	0.0
class	0	0.0

R: No, the dataset is complete

What about the data types?

In [6]:
```
data.dtypes
```

Out[6]:
```
age                         float64
gender                       object
height_cm                   float64
weight_kg                   float64
body_fat_pct                float64
diastolic                   float64
systolic                    float64
grip_force                  float64
sit_and_bend_forward_cm     float64
sit_ups_counts              float64
broad_jump_cm               float64
class                        object
dtype: object
```

R: It's needed to code the columns 'gender' and 'class'

In [7]:
```
eda.code_categorical(data, "gender")
eda.code_categorical(data, "class")
data.head(10)
```

Out[7]:

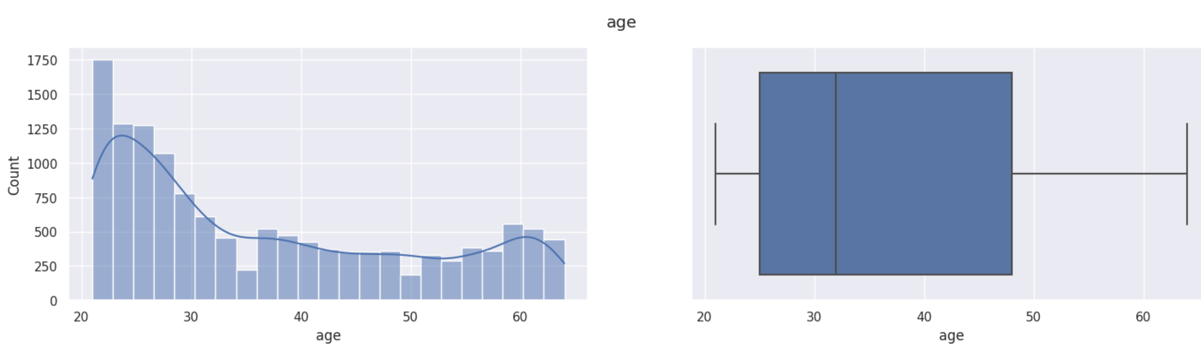
	age	gender	height_cm	weight_kg	body_fat_pct	diastolic	systolic	grip_force	sit_
0	27.0	1	172.3	75.24	21.3	80.0	130.0	54.9	
1	25.0	1	165.0	55.80	15.7	77.0	126.0	36.4	
2	31.0	1	179.6	78.00	20.1	92.0	152.0	44.8	
3	32.0	1	174.5	71.10	18.4	76.0	147.0	41.4	
4	28.0	1	173.8	67.70	17.1	70.0	127.0	43.5	
5	36.0	0	165.4	55.40	22.0	64.0	119.0	23.8	
6	42.0	0	164.5	63.70	32.2	72.0	135.0	22.7	
7	33.0	1	174.9	77.20	36.9	84.0	137.0	45.9	
8	54.0	1	166.8	67.50	27.6	85.0	165.0	40.4	
9	28.0	1	185.0	84.60	14.4	81.0	156.0	57.9	

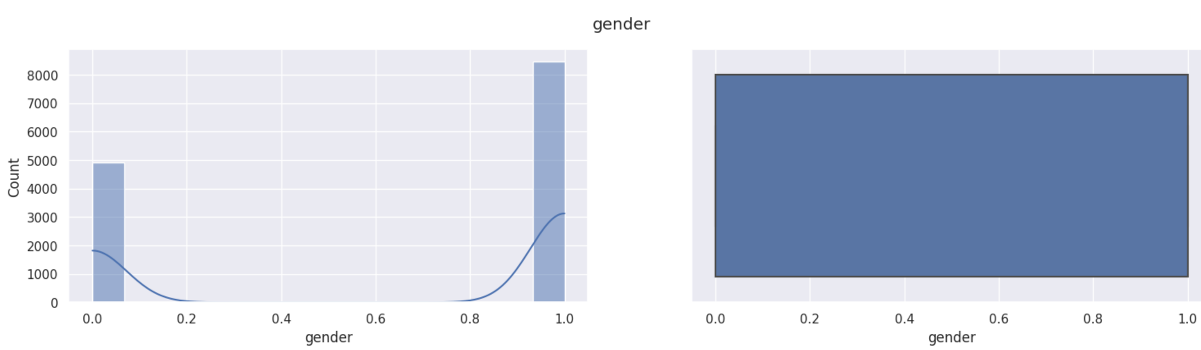
What about the distribution of the data?

Original distributions

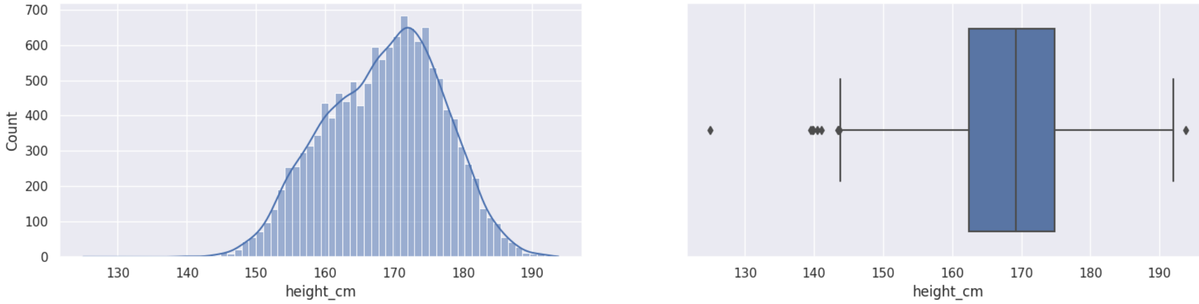
In [8]:

```
for column in data.columns.tolist():
    eda.plot_distribution(data, column, figures_path=FIGURES_PATH)
```

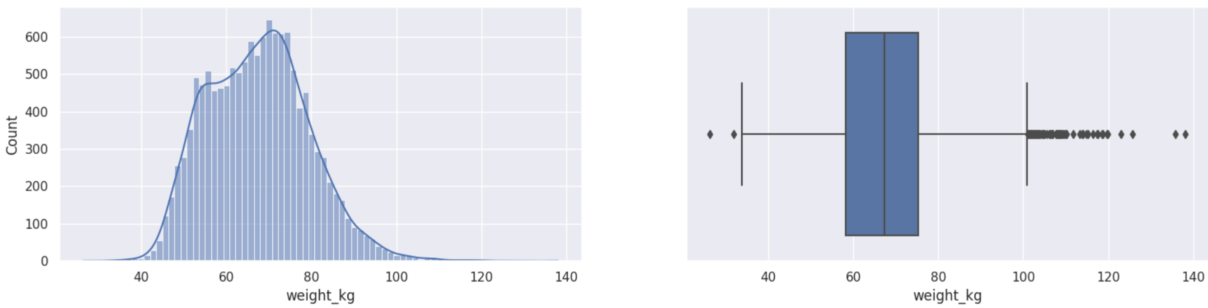




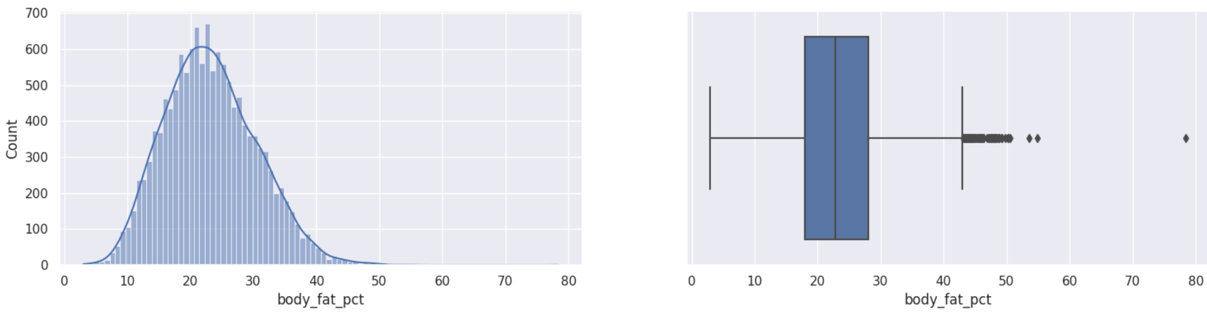
height_cm



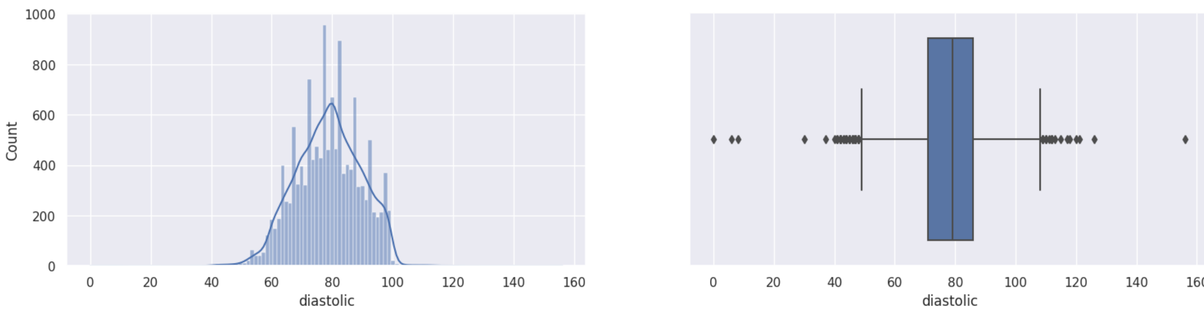
weight_kg



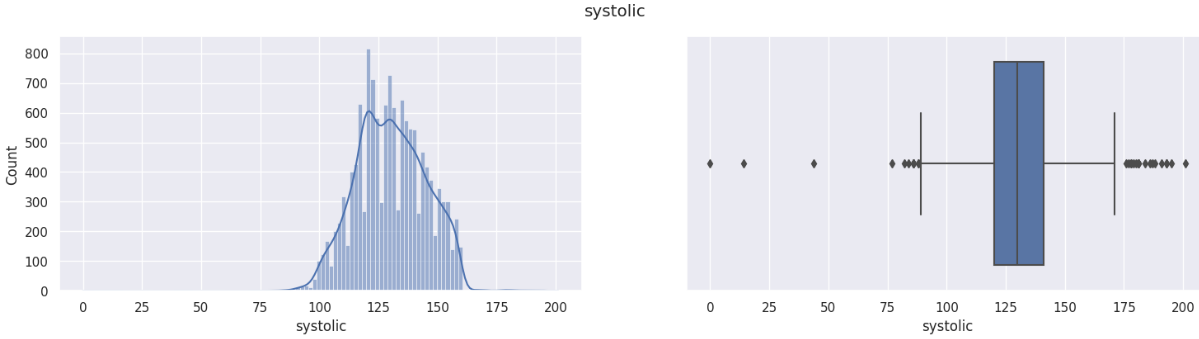
body_fat_pct



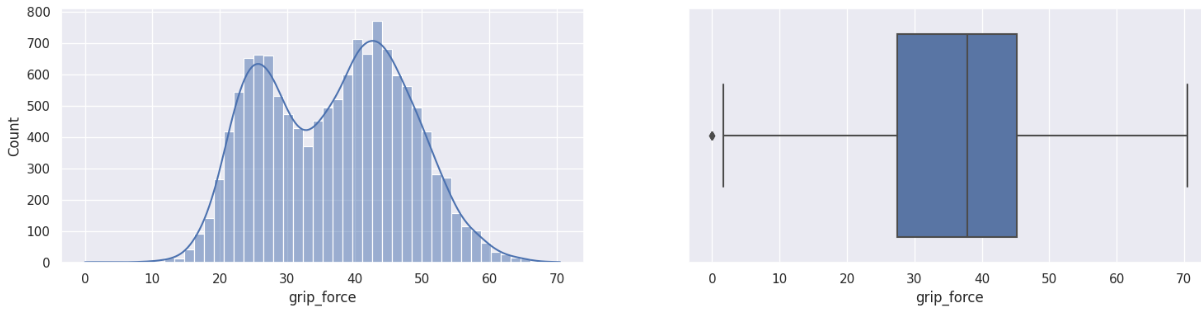
diastolic



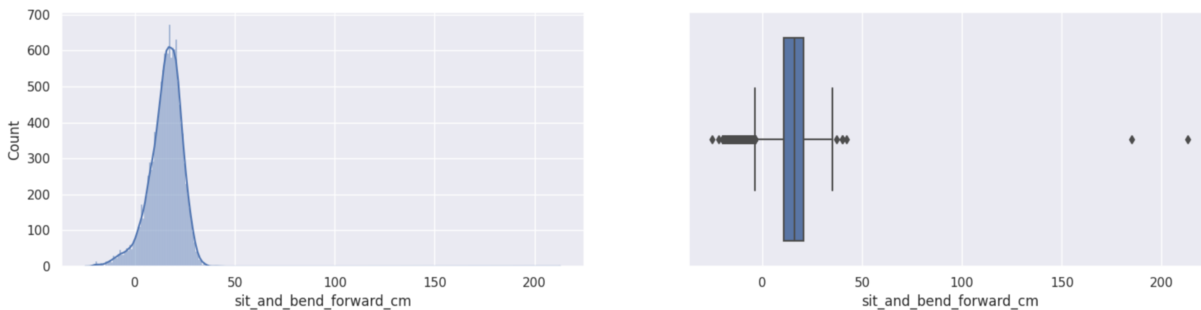
systolic



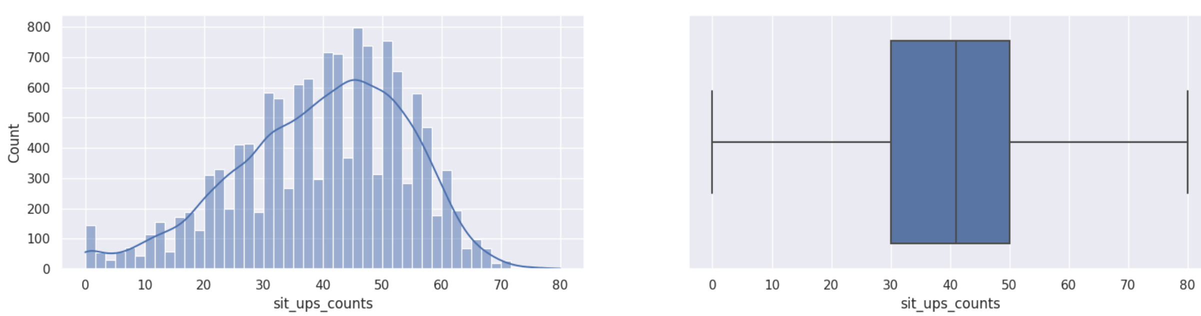
grip_force



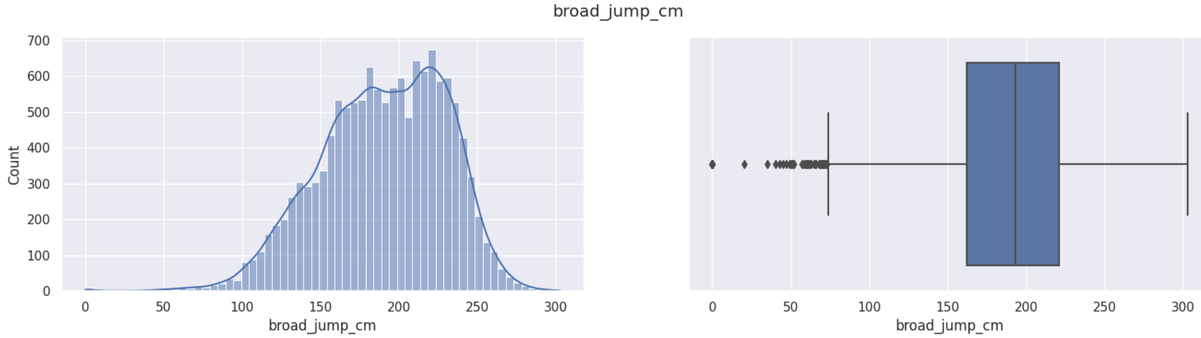
sit_and_bend_forward_cm



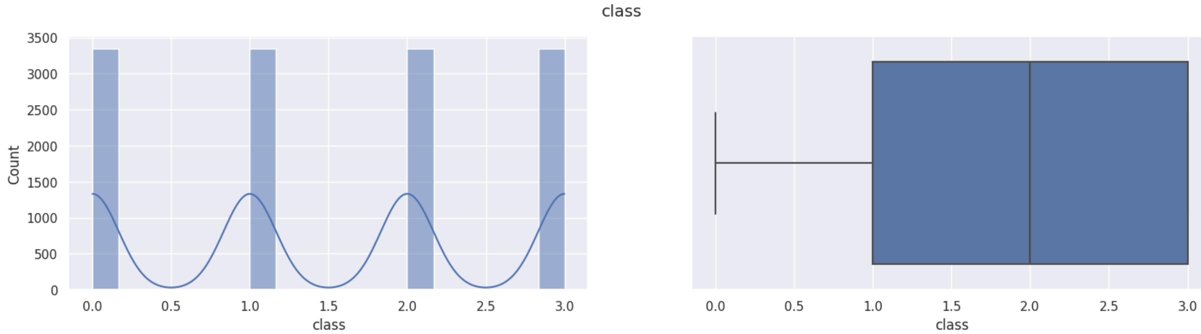
sit_ups_counts



broad_jump_cm



class



R: Most of the features present a distribution close to the normal distribution. Standard scaler will be used for these features

```
In [9]: data_norm = data.copy()
```

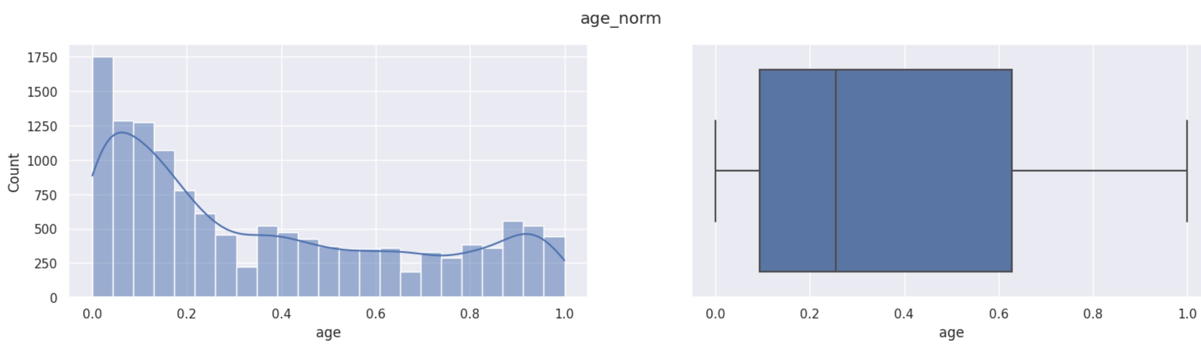
```
In [10]: features = ["height_cm", "weight_kg", "body_fat_pct", "diastolic", "systolic
                     "grip_force", "sit_and_bend_forward_cm", "sit_ups_counts","broac
         for feature in features:
             data_norm[feature] = StandardScaler().fit_transform(data_norm[[feature]]
```

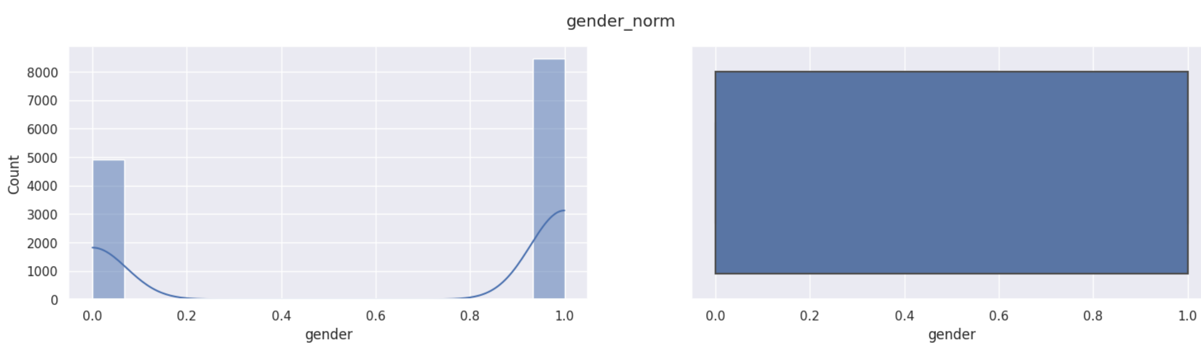
R: Age will be scaled using the min max method, this to ensure that the clustering algorithm has comparable ranges between all attributes

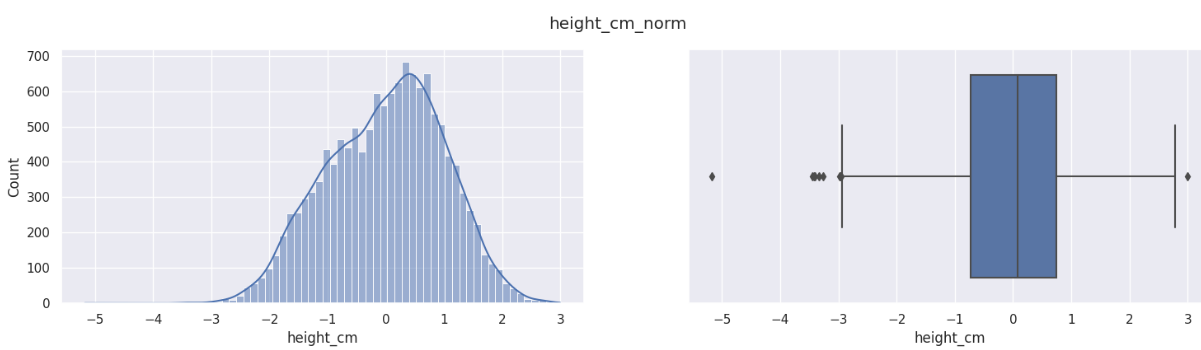
```
In [11]: data_norm["age"] = MinMaxScaler().fit_transform(data_norm[["age"]])
```

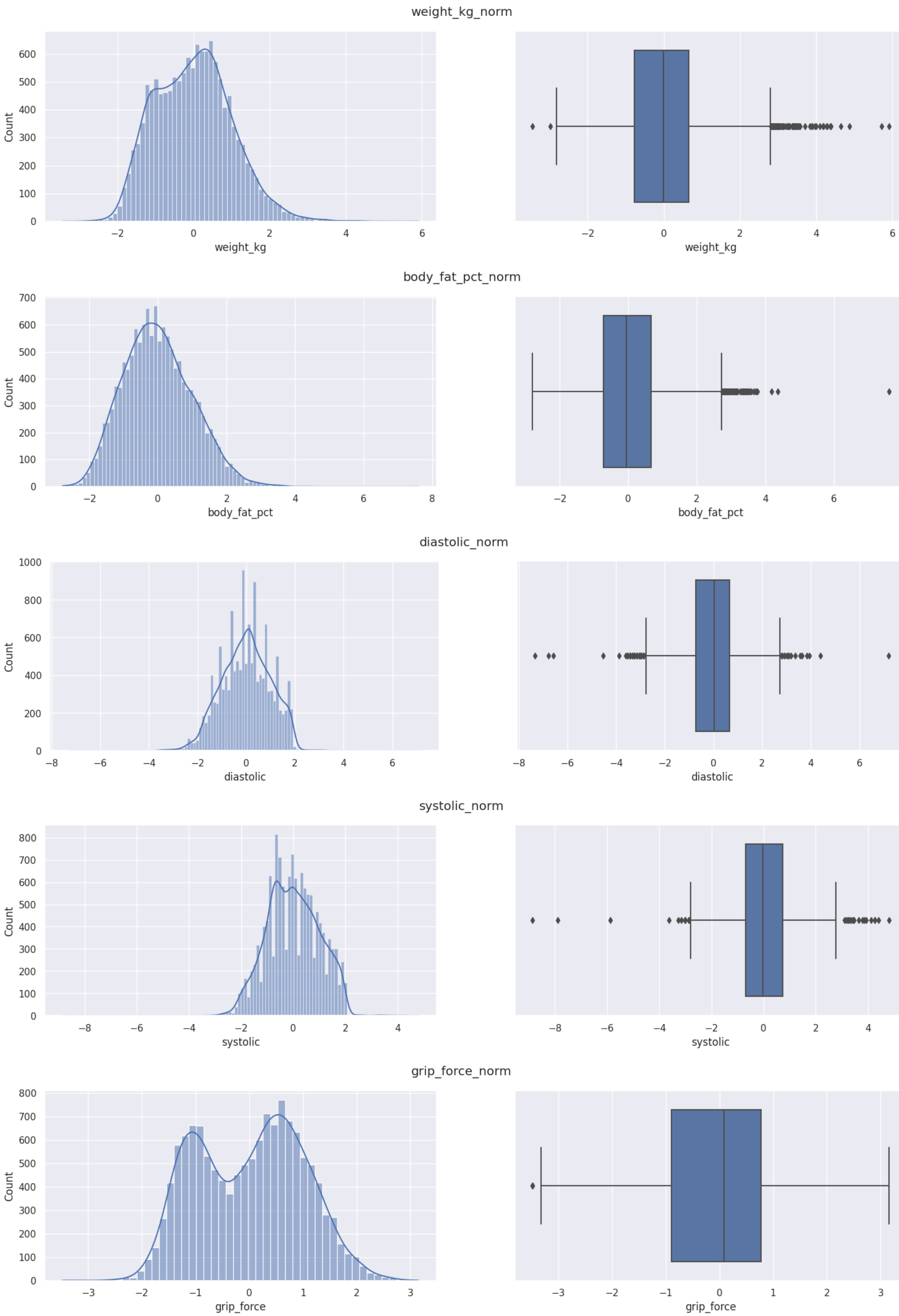
Scaled distributions

```
In [12]: for column in data_norm.columns.tolist():
             eda.plot_distribution(data_norm, column, figures_path=FIGURES_PATH, sufi
```









weight_kg_norm
Count
weight_kg
weight_kg
body_fat_pct_norm
Count
body_fat_pct
body_fat_pct
diastolic_norm
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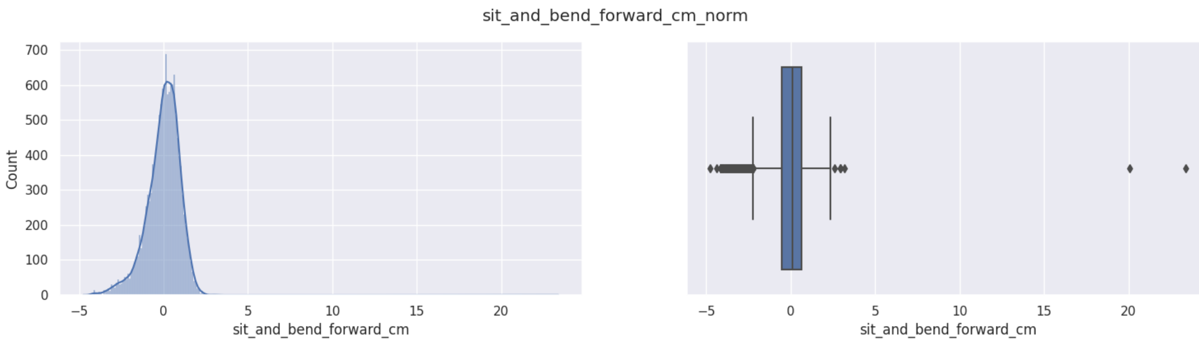
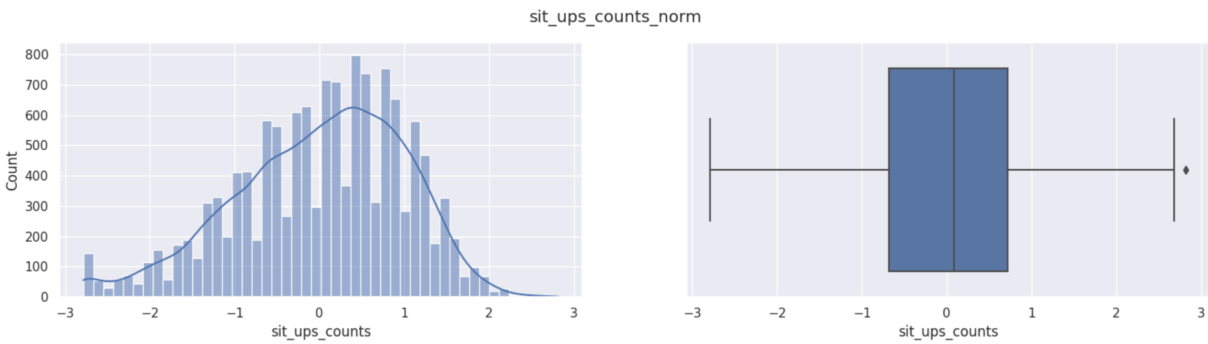
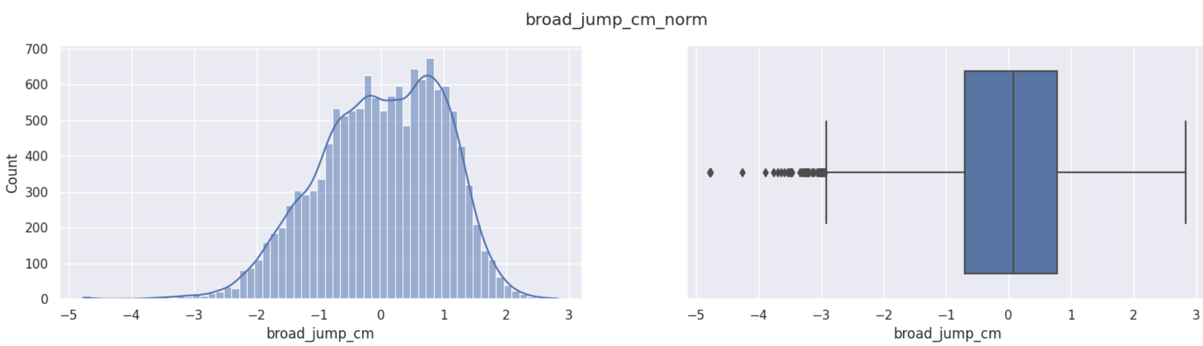
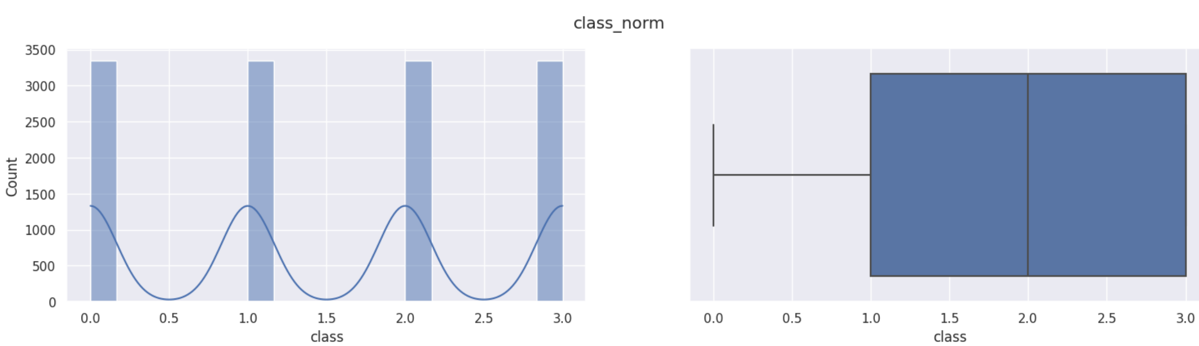
systolic_norm
Count
systolic
systolic
grip_force_norm
Count
grip_force
grip_force



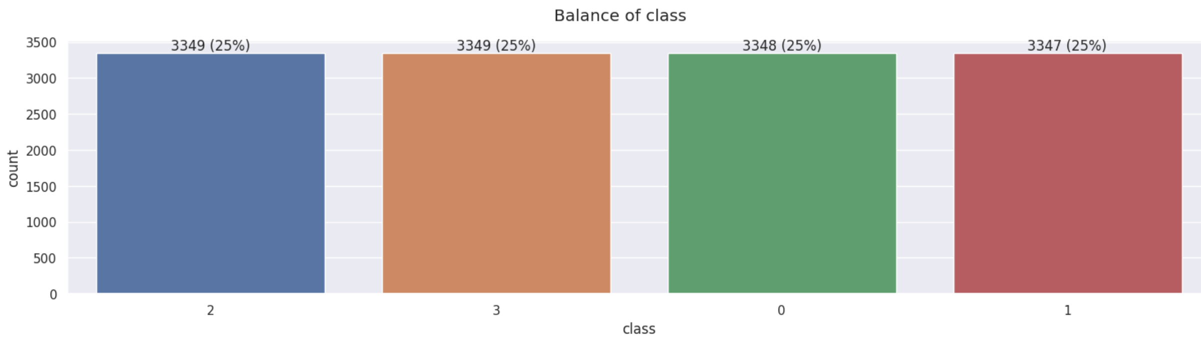






What do we know about the classes? are they balanced?

In [13]:
```
eda.plot_count(data, "class", figures_path=FIGURES_PATH)
```



R: The total number of instances per class varies by 1 or 2 instances, so it could be considered that they are balanced

Dimensionality reduction: Principal component analysis (PCA)

The attributes and the objective variable must be segmented

In [14]:
```
X = data_norm.drop(columns=["class"])
Y = data_norm['class'].to_numpy()
```

Obtaining the most relevant attributes

In [15]:
```
pca_features = dimensionality_reduction.pca_features(X, normalize_data=False
pca_features
```

Out[15]:

	relevance
age	45.201545
gender	19.945752
height_cm	13.057954
weight_kg	7.159068
body_fat_pct	4.281306
broad_jump_cm	3.398194
sit_ups_counts	2.788807
sit_and_bend_forward_cm	2.012700
grip_force	1.147991
systolic	0.639009
diastolic	0.367673

In [16]:
```
relevant_features = pca_features.iloc[:4].index.tolist()
X_relevant = X[relevant_features]
```

```
print(f"Total gain: {pca_features.loc[relevant_features].sum(axis=0)[0]:.2f}
X_relevant.head(10)
```

```
Total gain: 85.36%
```

Out[16]:

	age	gender	height_cm	weight_kg
0	0.139535	1	0.443873	0.652150
1	0.093023	1	-0.422465	-0.974734
2	0.232558	1	1.310211	0.883127
3	0.255814	1	0.704961	0.305684
4	0.162791	1	0.621888	0.021147
5	0.348837	0	-0.374995	-1.008209
6	0.488372	0	-0.481804	-0.313603
7	0.279070	1	0.752432	0.816177
8	0.767442	1	-0.208848	0.004409
9	0.162791	1	1.951065	1.435465

Using the 'age', 'gender', 'height_cm' and 'weight_cm' features yields a gain of 85%

Obtaining subspace of principal components

In [17]:

```
X_pca = dimensionality_reduction.pca(X, 2, normalize_data=False)
X_pca.head(10)
```

Out[17]:

	PC1	PC2
0	2.216666	0.437671
1	0.653010	1.348408
2	2.081523	-1.615139
3	1.790092	0.014114
4	1.191661	1.429019
5	-2.085863	1.242047
6	-2.259175	-1.384257
7	1.240391	-1.332304
8	-0.119634	-2.072823
9	3.752017	-0.844322

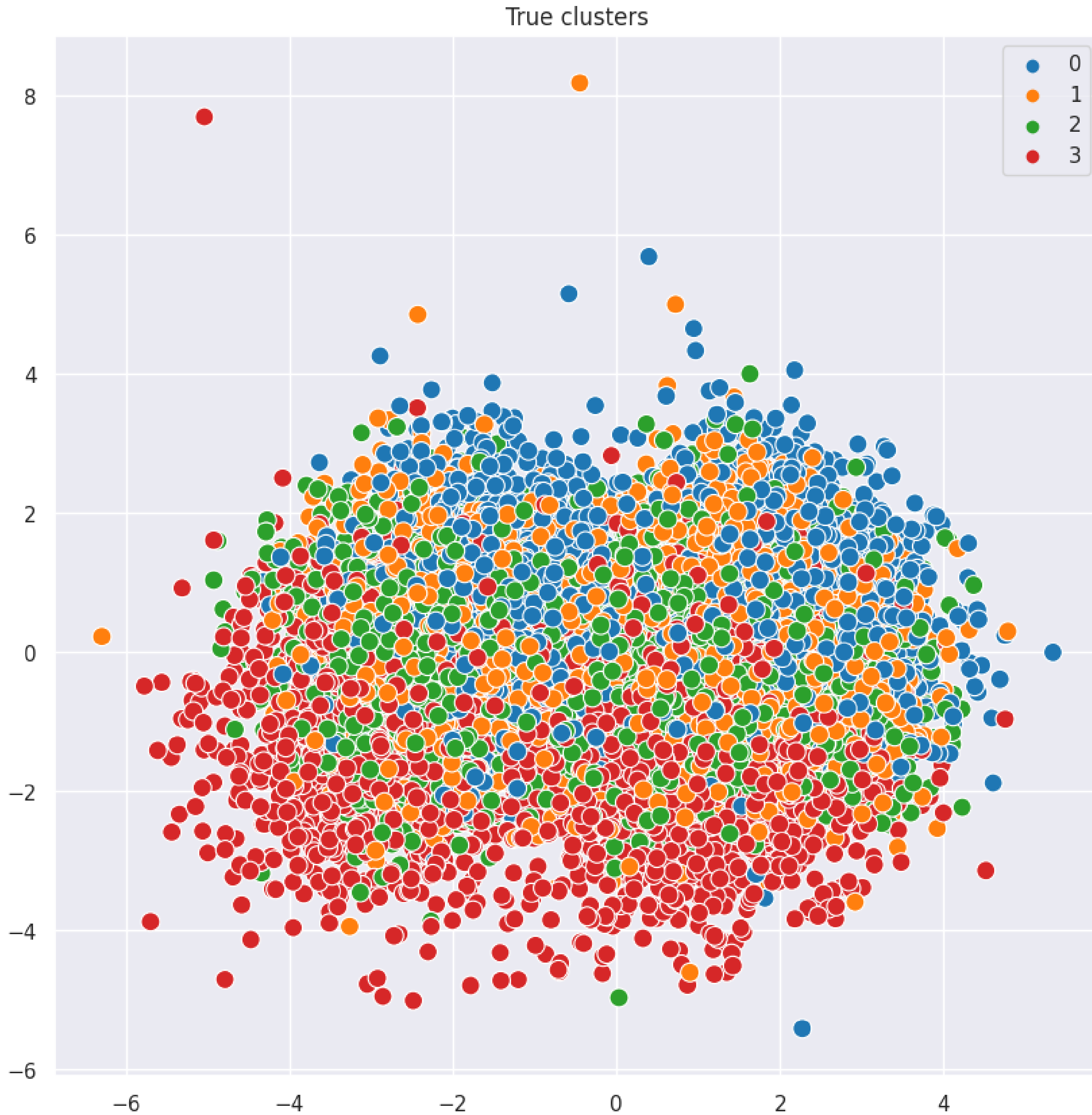
Convert X variables to numpy arrays

In [18]:

```
X = X.to_numpy()
X_relevant = X_relevant.to_numpy()
X_pca = X_pca.to_numpy()
```

Target variable visualization

In [19]:
```
visualization.plot_clustering_result(X_pca, Y, title="True clusters", filena
```

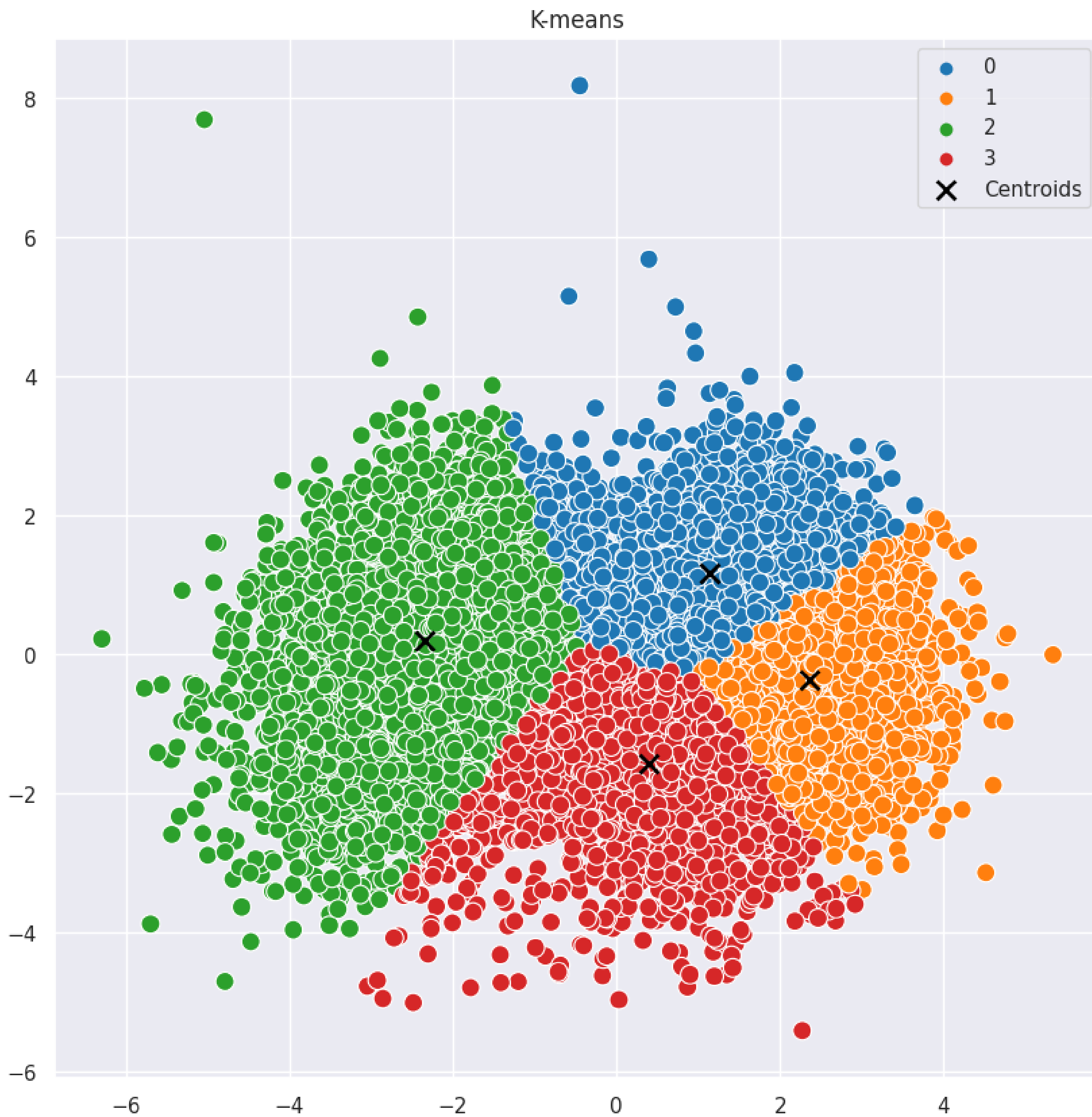


Clustering

K-means example

In [20]:
```
Y_predict, centroids = clustering.k_means(X_pca, 4, max_iter=50, tol=1e-3)
visualization.plot_clustering_result(X_pca, Y_predict, centroids=centroids,
```

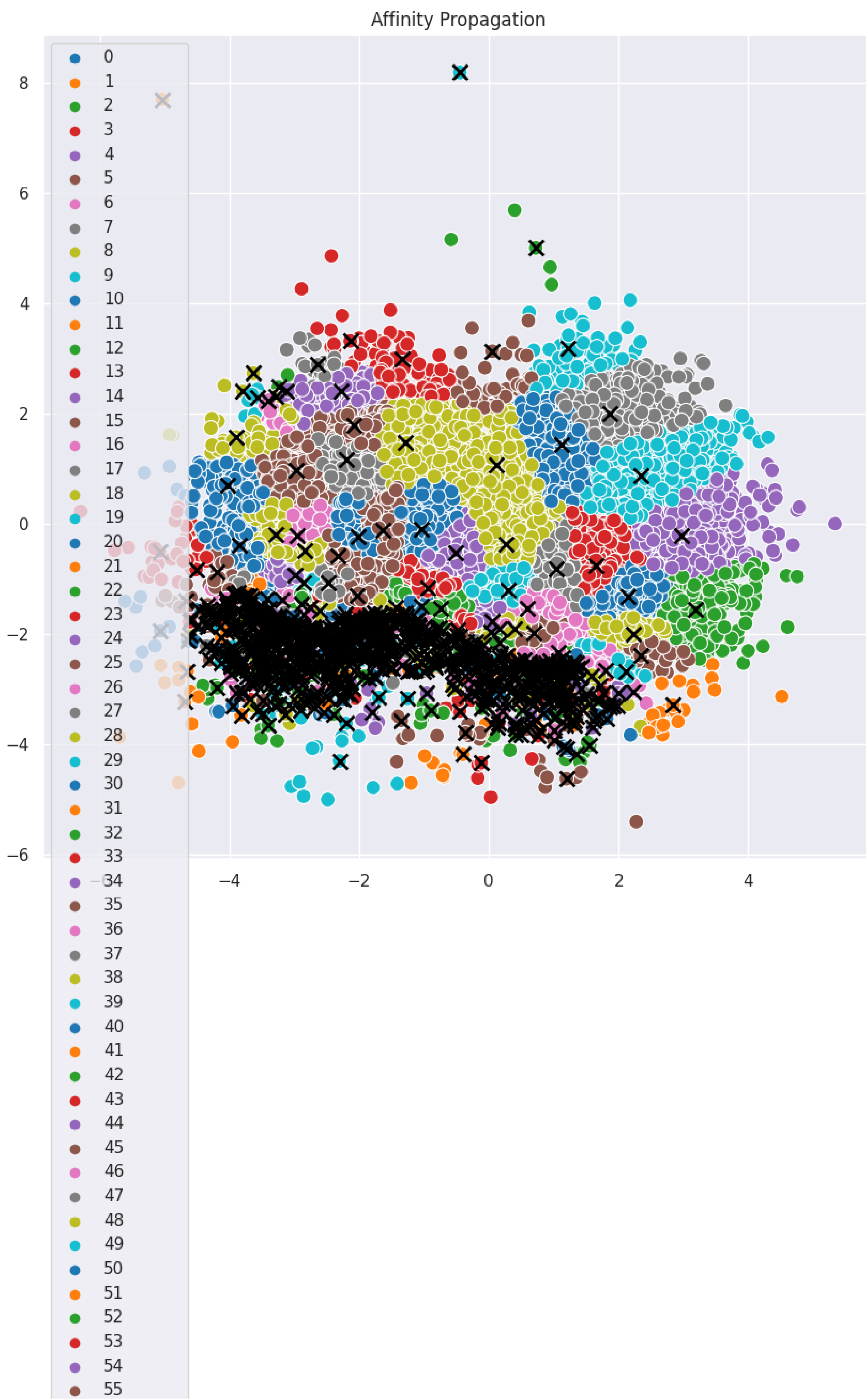
```
34%|███          | 17/50 [00:00<00:00, 477.41it/s]
```



Affinity propagation example

In [21]:
```
Y_predict, centroids = clustering.affinity_propagation(X_pca, damping=0.5, m
visualization.plot_clustering_result(X_pca, Y_predict, centroids=centroids,
```

```
/mnt/Datos/.enviroments/ubu20/ML-E1/lib/python3.8/site-packages/sklearn/clust
er/_affinity_propagation.py:143: ConvergenceWarning: Affinity propagation did
not converge, this model may return degenerate cluster centers and labels.
  warnings.warn(
```



Affinity Propagation
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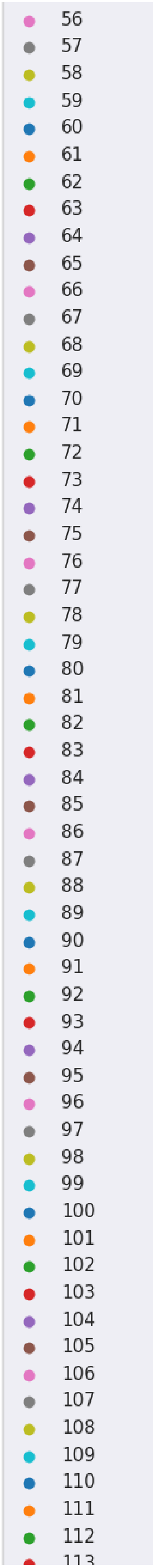
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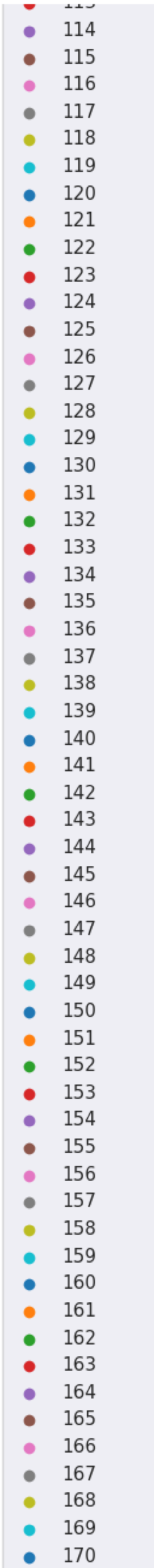
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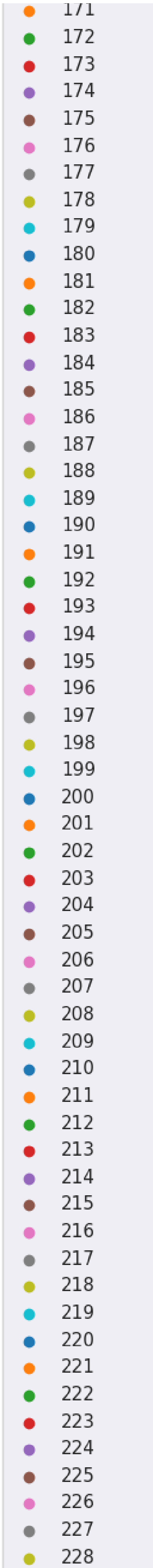
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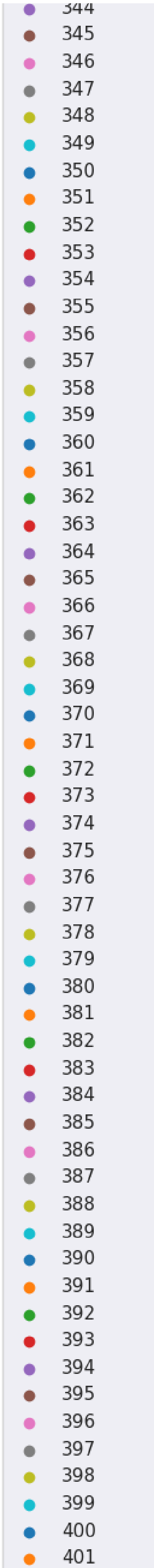
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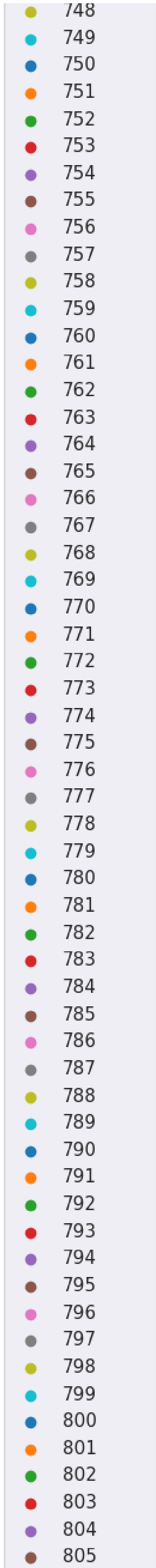
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Centroids

Evaluation

In [22]:
```
def get_accuracy(y, predictions):
    allPermutations=np.array(list(permutations(np.unique(y))))
    acc=[]
    for perm in allPermutations:
        classes=np.arange(0,y.shape[0])
        for index in range(classes.shape[0]):
            classes[index]=np.where(y[index]==perm)[0][0]
        acc.append(np.sum(classes==predictions))
    acc=np.array(acc)
    bestAccIndex=np.where(max(acc)==acc)[0][0]
    return dict(zip(np.arange(0,allPermutations.shape[1]),allPermutations[be
```

In [23]:
```
def k_means_k_fold(X, Y, k, max_iter=100, tol=1e-3, splits=5):
    """Implementation of the k-means algorithm with k-fold cross validation.

    :param np.ndarray X: Data to cluster.
    :param np.ndarray Y: Labels.
    :param int k: Number of clusters.
    :param int max_iter: Maximum number of iterations. Defaults to 100.
    :param float tol: Tolerance. Defaults to 1e-3.
    :param int splits: Number of splits for k-fold cross validation. Default
    """
    kf = KFold(n_splits=splits)
    accuracies = []

    for train_index, test_index in kf.split(X):
        X_train, X_test = X[train_index], X[test_index]
        Y_train, Y_test = Y[train_index], Y[test_index]

        _, centroids = clustering.k_means(X_train, k, max_iter=max_iter, tol

        Y_predict = clustering.k_means_predict(X_test, centroids)
        _, accuracy = get_accuracy(Y_test, Y_predict)
        accuracies.append((accuracy/Y_test.shape[0])*100)

    return np.array(accuracies)
```

In [24]:
```
def boxplot(data: pd.DataFrame, title: str, filename: str):
    """Plots a nice boxplot.

    :param pd.DataFrame data: Data to plot.
    :param str title: Title of the plot.
    :param str filename: Filename to save the plot.
    """
    fig, ax = plt.subplots(figsize=(9, 4))
    ax.set_title(title)
    ax.set_ylabel("Accuracy [%]")
    sns.boxplot(data=data, ax=ax)

    decribed_data = data.describe().T
    for x, wt in enumerate(ax.get_xticklabels()):
        median_ = decribed_data.loc[wt.get_text(), '50%']
```

```
        min_ = decribed_data.loc[wt.get_text(), 'min']
        max_ = decribed_data.loc[wt.get_text(), 'max']
        q1_ = decribed_data.loc[wt.get_text(), '25%']
        q3_ = decribed_data.loc[wt.get_text(), '75%']

        ax.text(x, median_, f'{median_:.4f}', horizontalalignment='center',
                color='w', backgroundcolor='k', weight='semibold', fontsize=
        ax.text(x, min_, f'{min_:.4f}', horizontalalignment='center',
                color='w', backgroundcolor='k', weight='semibold', fontsize=
        ax.text(x, max_, f'{max_:.4f}', horizontalalignment='center',
                color='w', backgroundcolor='k', weight='semibold', fontsize=
        ax.text(x, q1_, f'{q1_:.4f}', horizontalalignment='center',
                color='w', backgroundcolor='k', weight='semibold', fontsize=
        ax.text(x, q3_, f'{q3_:.4f}', horizontalalignment='center',
                color='w', backgroundcolor='k', weight='semibold', fontsize=

    plt.savefig(f"{filename}.png")
    plt.show()
```

K-Means with all features

In [25]:
```
all_features_accuracies = k_means_k_fold(X, Y, 4, max_iter=100, tol=1e-3, sp
print(f"Mean accuracy: {all_features_accuracies.mean():.2f}%")
```

```
 46%|████▌     | 46/100 [00:00<00:00, 429.32it/s]
 36%|███▌      | 36/100 [00:00<00:00, 487.41it/s]
 42%|████▏     | 42/100 [00:00<00:00, 487.94it/s]
 30%|███       | 30/100 [00:00<00:00, 481.39it/s]
 70%|███████   | 70/100 [00:00<00:00, 481.42it/s]
 55%|█████▌    | 55/100 [00:00<00:00, 470.20it/s]
 46%|████▌     | 46/100 [00:00<00:00, 481.56it/s]
 32%|███▏      | 32/100 [00:00<00:00, 480.52it/s]
 34%|███▍      | 34/100 [00:00<00:00, 485.09it/s]
 23%|██▎       | 23/100 [00:00<00:00, 479.39it/s]
Mean accuracy: 36.42%
```

K-Means with relevant features

In [26]:
```
relevant_features_accuracies = k_means_k_fold(X_relevant, Y, 4, max_iter=100
print(f"Mean accuracy: {relevant_features_accuracies.mean():.2f}%")
```

```
 77%|███████▋  | 77/100 [00:00<00:00, 667.78it/s]
 13%|█▎        | 13/100 [00:00<00:00, 432.60it/s]
 68%|██████▊   | 68/100 [00:00<00:00, 654.50it/s]
100%|██████████| 100/100 [00:00<00:00, 675.35it/s]
 63%|██████▎   | 63/100 [00:00<00:00, 671.95it/s]
100%|██████████| 100/100 [00:00<00:00, 686.43it/s]
100%|██████████| 100/100 [00:00<00:00, 665.78it/s]
100%|██████████| 100/100 [00:00<00:00, 690.27it/s]
 74%|███████▍  | 74/100 [00:00<00:00, 685.27it/s]
 15%|█▌        | 15/100 [00:00<00:00, 638.85it/s]
Mean accuracy: 30.55%
```

K-Means with PCA features

In [27]:
```
pca_features_accuracies = k_means_k_fold(X_pca, Y, 4, max_iter=100, tol=1e-3
print(f"Mean accuracy: {pca_features_accuracies.mean():.2f}%")
```

```
 22%|██▏        | 22/100 [00:00<00:00, 602.22it/s]
 31%|███        | 31/100 [00:00<00:00, 681.11it/s]
 19%|█▉         | 19/100 [00:00<00:00, 666.91it/s]
 36%|███▌       | 36/100 [00:00<00:00, 687.26it/s]
 19%|█▉         | 19/100 [00:00<00:00, 664.97it/s]
 31%|███        | 31/100 [00:00<00:00, 684.78it/s]
 53%|█████▎     | 53/100 [00:00<00:00, 698.08it/s]
 34%|███▍       | 34/100 [00:00<00:00, 689.15it/s]
 22%|██▏        | 22/100 [00:00<00:00, 672.66it/s]
 24%|██▍        | 24/100 [00:00<00:00, 674.43it/s]
Mean accuracy: 34.35%
```

Comparsion

In [28]:
```
results = pd.DataFrame(
    np.array([all_features_accuracies, relevant_features_accuracies, pca_fea
    columns=["all_features", "relevant_features", "pca_features"]
)
results.head(10)

boxplot(results, "Accuracy of each K-Means method", FIGURES_PATH + "k_means_
```