Clustering

Working with Unlabeled Data – Clustering Analysis

Reference

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
```

```
from sklearn.cluster import KMeans

# https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html#sklearn.c

X = np.array([[1, 2], [1, 4], [1, 0],
              [10, 2], [10, 4], [10, 0]])
kmeans = KMeans(n_clusters=2, random_state=0, n_init="auto").fit(X)
kmeans.labels_
kmeans.predict([[0, 0], [12, 3]])
kmeans.cluster_centers_
```

```
array([[10.,  2.],
       [ 1.,  2.]])
```

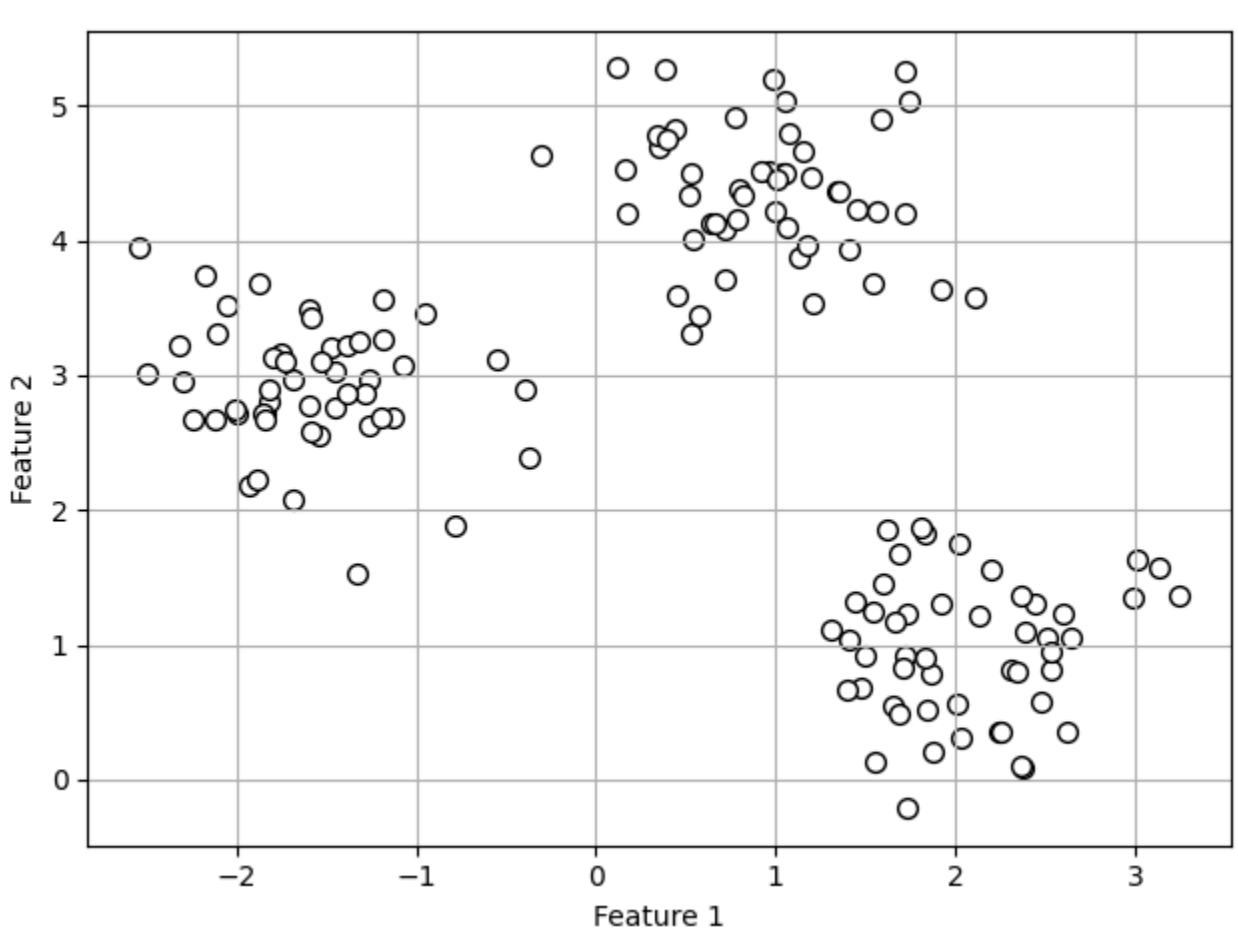
K-means clustering using scikit-learn

```
from sklearn.datasets import make_blobs

X, y = make_blobs(n_samples=150,
                  n_features=2,
                  centers=3,
                  cluster_std=0.5,
                  shuffle=True,
                  random_state=0)
```

```
plt.scatter(X[:, 0], X[:, 1],
            c='white', marker='o', edgecolor='black', s=50)
plt.xlabel('Feature 1')
plt.ylabel('Feature 2')

plt.grid()
plt.tight_layout()
#plt.savefig('figures/10_01.png', dpi=300)
plt.show()
```




```
from sklearn.cluster import KMeans

km = KMeans(n_clusters=3,
            init='random',
            n_init=10,
            max_iter=300,
            tol=1e-04,
            random_state=0)

y_km = km.fit_predict(X)
```

```
plt.scatter(X[y_km == 0, 0],
            X[y_km == 0, 1],
            s=50, c='lightgreen',
            marker='s', edgecolor='black',
            label='Cluster 1')
plt.scatter(X[y_km == 1, 0],
            X[y_km == 1, 1],
            s=50, c='orange',
            marker='o', edgecolor='black',
            label='Cluster 2')
plt.scatter(X[y_km == 2, 0],
            X[y_km == 2, 1],
```

```
            X[y_km == 2, 1],
            s=50, c='lightblue',
            marker='v', edgecolor='black',
            label='Cluster 3')
plt.scatter(km.cluster_centers_[:, 0],
            km.cluster_centers_[:, 1],
            s=250, marker='*',
            c='red', edgecolor='black',
            label='Centroids')

plt.xlabel('Feature 1')
plt.ylabel('Feature 2')

plt.legend(scatterpoints=1)
plt.grid()
plt.tight_layout()
#plt.savefig('figures/10_02.png', dpi=300)
plt.show()
```

More research to do with:

- A smarter way of placing the initial cluster centroids using k-means++
- Hard versus soft clustering

Using the elbow method to find the optimal number of clusters

- Distortion is the average of the euclidean squared distance from the centroid of the respective clusters.
- Inertia is the sum of squared distances of samples to their closest cluster centre.

```
# What is the 'distortion'?
print(f'Distortion: {km.inertia_:.2f}')
```

```
Distortion: 72.48
```

```
distortions = []
for i in range(1, 11):
    km = KMeans(n_clusters=i,
                init='k-means++',
                n_init=10,
                max_iter=300,
                random_state=0)
    km.fit(X)
    distortions.append(km.inertia_)
plt.plot(range(1, 11), distortions, marker='o')
plt.xlabel('Number of clusters')
plt.ylabel('Distortion')
plt.tight_layout()
plt.show()
```

Quantifying the quality of clustering via silhouette plots

The Silhouette method evaluates clustering quality by considering how well each data point fits within its assigned cluster compared to other clusters.

Silhouette Coefficient:

For each data point:

- ○ Calculate (ai): the average distance to all other points in its own cluster (cohesion).

Calculate (bi): the average distance to all points in the nearest neighboring cluster (separation).

- The Silhouette Coefficient for that point is:

$$\frac{b_i - a_i}{\max(a_i, b_i)}$$

Close to 1: Point is well-clustered. Close to 0: Point is near the decision boundary between clusters. Close to -1: Point might be in the wrong cluster.

Global Silhouette Coefficient:

The average of all individual Silhouette Coefficients provides an overall measure of clustering quality:

Close to 1: Good clustering (well-separated and cohesive clusters). Close to -1: Poor clustering (significant overlap or misclassification). Close to 0: Overlapping clusters or unclear clustering.

```
from matplotlib import cm
from sklearn.metrics import silhouette_samples

km = KMeans(n_clusters=3,
            init='k-means++',
            n_init=10,
            max_iter=300,
            tol=1e-04,
            random_state=0)
y_km = km.fit_predict(X)

cluster_labels = np.unique(y_km)
n_clusters = cluster_labels.shape[0]
silhouette_vals = silhouette_samples(X, y_km, metric='euclidean')
y_ax_lower, y_ax_upper = 0, 0
```

```
yticks = []
for i, c in enumerate(cluster_labels):
    c_silhouette_vals = silhouette_vals[y_km == c]
    c_silhouette_vals.sort()
    y_ax_upper += len(c_silhouette_vals)
    color = cm.jet(float(i) / n_clusters)
    plt.barh(range(y_ax_lower, y_ax_upper), c_silhouette_vals, height=1.0,
             edgecolor='none', color=color)

    yticks.append((y_ax_lower + y_ax_upper) / 2.)
    y_ax_lower += len(c_silhouette_vals)

silhouette_avg = np.mean(silhouette_vals)
plt.axvline(silhouette_avg, color="red", linestyle="--")

plt.yticks(yticks, cluster_labels + 1)
plt.ylabel('Cluster')
plt.xlabel('Silhouette coefficient')

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

Organizing clusters as a hierarchical tree

- Grouping clusters in bottom-up fashion

```
np.random.seed(123)

variables = ['X', 'Y', 'Z']
labels = ['ID_0', 'ID_1', 'ID_2', 'ID_3', 'ID_4']

X = np.random.random_sample([5, 3])*10
df = pd.DataFrame(X, columns=variables, index=labels)
df
```

Next steps: Generate code with df | View recommended plots | New interactive sheet

```
# Performing hierarchical clustering on a distance matrix
from scipy.spatial.distance import pdist, squareform


row_dist = pd.DataFrame(squareform(pdist(df, metric='euclidean')),
                        columns=labels,
                        index=labels)
row_dist
```

Next steps: Generate code with row_dist | View recommended plots | New interactive sheet

```
from scipy.cluster.hierarchy import linkage
```

```
row_clusters = linkage(df.values, method='complete', metric='euclidean')
pd.DataFrame(row_clusters,
             columns=['row label 1', 'row label 2',
                      'distance', 'no. of items in clust.'],
             index=[f'cluster {(i + 1)}'
                    for i in range(row_clusters.shape[0])])
```

```
from scipy.cluster.hierarchy import dendrogram

row_dendr = dendrogram(row_clusters,
                       labels=labels,
                       )
plt.tight_layout()
plt.ylabel('Euclidean distance')
plt.show()
```

Locating regions of high density via DBSCAN

```
from sklearn.datasets import make_moons


X, y = make_moons(n_samples=200, noise=0.05, random_state=0)
plt.scatter(X[:, 0], X[:, 1])

plt.xlabel('Feature 1')
plt.ylabel('Feature 2')

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

```
from sklearn.cluster import AgglomerativeClustering

f, (ax1, ax2) = plt.subplots(1, 2, figsize=(8, 3))

km = KMeans(n_clusters=2, random_state=0)
y_km = km.fit_predict(X)
```

```
ax1.scatter(X[y_km == 0, 0], X[y_km == 0, 1],
            edgecolor='black',
            c='lightblue', marker='o', s=40, label='cluster 1')
ax1.scatter(X[y_km == 1, 0], X[y_km == 1, 1],
            edgecolor='black',
            c='red', marker='s', s=40, label='cluster 2')
ax1.set_title('K-means clustering')

ax1.set_xlabel('Feature 1')
ax1.set_ylabel('Feature 2')

ac = AgglomerativeClustering(n_clusters=2, linkage='complete')
y_ac = ac.fit_predict(X)
ax2.scatter(X[y_ac == 0, 0], X[y_ac == 0, 1], c='lightblue',
            edgecolor='black',
            marker='o', s=40, label='Cluster 1')
ax2.scatter(X[y_ac == 1, 0], X[y_ac == 1, 1], c='red',
            edgecolor='black',
            marker='s', s=40, label='Cluster 2')
ax2.set_title('Agglomerative clustering')

ax2.set_xlabel('Feature 1')
ax2.set_ylabel('Feature 2')

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

```
# Density-based clustering
from sklearn.cluster import DBSCAN

db = DBSCAN(eps=0.2, min_samples=5, metric='euclidean')
y_db = db.fit_predict(X)
plt.scatter(X[y_db == 0, 0], X[y_db == 0, 1]
```

```
            c='lightblue', marker='o', s=40,
            edgecolor='black',
            label='Cluster 1')
plt.scatter(X[y_db == 1, 0], X[y_db == 1, 1],
            c='red', marker='s', s=40,
            edgecolor='black',
            label='Cluster 2')

plt.xlabel('Feature 1')
plt.ylabel('Feature 2')

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

Your work

Task 1: Execute the provided code in your notebook to observe how the silhouette score aids in selecting the optimal number of clusters in K-means.

https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html

Task 2: Execute the provided code in your notebook to observe which clustering algorithms are

Task 2: Execute the provided code in your notebook to observe which clustering algorithms are suitable for different data structures.

https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html#sphx-glr-auto-examples-cluster-plot-cluster-comparison-py

Submit your notebook in PDF format to BrightSpace by 5/4/2025 11:50 pm.

```
# Authors: The scikit-learn developers
# SPDX-License-Identifier: BSD-3-Clause

import matplotlib.cm as cm
import matplotlib.pyplot as plt
import numpy as np

from sklearn.cluster import KMeans
from sklearn.datasets import make_blobs
from sklearn.metrics import silhouette_samples, silhouette_score

# Generating the sample data from make_blobs
# This particular setting has one distinct cluster and 3 clusters placed close
# together.
X, y = make_blobs(
    n_samples=500,
    n_features=2,
    centers=4,
    cluster_std=1,
    center_box=(-10.0, 10.0),
    shuffle=True,
    random_state=1,
)  # For reproducibility

range_n_clusters = [2, 3, 4, 5, 6]

for n_clusters in range_n_clusters:
    # Create a subplot with 1 row and 2 columns
    fig, (ax1, ax2) = plt.subplots(1, 2)
    fig.set_size_inches(18, 7)

    # The 1st subplot is the silhouette plot
    # The silhouette coefficient can range from -1, 1 but in this example all
    # lie within [-0.1, 1]
    ax1.set_xlim([-0.1, 1])
    # The (n_clusters+1)*10 is for inserting blank space between silhouette
    # plots of individual clusters, to demarcate them clearly.
    ax1.set_ylim([0, len(X) + (n_clusters + 1) * 10])

    # Initialize the clusterer with n_clusters value and a random generator
    # seed of 10 for reproducibility.
    clusterer = KMeans(n_clusters=n_clusters, random_state=10)
```

```
    cluster_labels = clusterer.fit_predict(X)

    # The silhouette_score gives the average value for all the samples.
    # This gives a perspective into the density and separation of the formed
    # clusters
    silhouette_avg = silhouette_score(X, cluster_labels)
    print(
        "For n_clusters =",
        n_clusters,
        "The average silhouette_score is :",
        silhouette_avg,
    )

    # Compute the silhouette scores for each sample
    sample_silhouette_values = silhouette_samples(X, cluster_labels)

    y_lower = 10
    for i in range(n_clusters):
        # Aggregate the silhouette scores for samples belonging to
        # cluster i, and sort them
        ith_cluster_silhouette_values = sample_silhouette_values[cluster_labels == i]

        ith_cluster_silhouette_values.sort()

        size_cluster_i = ith_cluster_silhouette_values.shape[0]
        y_upper = y_lower + size_cluster_i

        color = cm.nipy_spectral(float(i) / n_clusters)
        ax1.fill_betweenx(
            np.arange(y_lower, y_upper),
            0,
            ith_cluster_silhouette_values,
            facecolor=color,
            edgecolor=color,
            alpha=0.7,
        )

        # Label the silhouette plots with their cluster numbers at the middle
        ax1.text(-0.05, y_lower + 0.5 * size_cluster_i, str(i))

        # Compute the new y_lower for next plot
        y_lower = y_upper + 10  # 10 for the 0 samples

    ax1.set_title("The silhouette plot for the various clusters.")
    ax1.set_xlabel("The silhouette coefficient values")
    ax1.set_ylabel("Cluster label")

    # The vertical line for average silhouette score of all the values
    ax1.axvline(x=silhouette_avg, color="red", linestyle="--")

    ax1.set_yticks([])  # Clear the yaxis labels / ticks
```

```
    ax1.set_xticks([-0.1, 0, 0.2, 0.4, 0.6, 0.8, 1])

    # 2nd Plot showing the actual clusters formed
    colors = cm.nipy_spectral(cluster_labels.astype(float) / n_clusters)
    ax2.scatter(
        X[:, 0], X[:, 1], marker=".", s=30, lw=0, alpha=0.7, c=colors, edgecolor="k"
    )

    # Labeling the clusters
    centers = clusterer.cluster_centers_
    # Draw white circles at cluster centers
    ax2.scatter(
        centers[:, 0],
        centers[:, 1],
        marker="o",
        c="white",
        alpha=1,
        s=200,
        edgecolor="k",
    )

    for i, c in enumerate(centers):
        ax2.scatter(c[0], c[1], marker="$%d$" % i, alpha=1, s=50, edgecolor="k")

    ax2.set_title("The visualization of the clustered data.")
    ax2.set_xlabel("Feature space for the 1st feature")
    ax2.set_ylabel("Feature space for the 2nd feature")

    plt.suptitle(
        "Silhouette analysis for KMeans clustering on sample data with n_clusters = %d"
        % n_clusters,
        fontsize=14,
        fontweight="bold",
    )

plt.show()
```

```
# Authors: The scikit-learn developers
# SPDX-License-Identifier: BSD-3-Clause

import time
import warnings
from itertools import cycle, islice

import matplotlib.pyplot as plt
import numpy as np

from sklearn import cluster, datasets, mixture
from sklearn.neighbors import kneighbors_graph
from sklearn.preprocessing import StandardScaler

# ============
```

```
# Generate datasets. We choose the size big enough to see the scalability
# of the algorithms, but not too big to avoid too long running times
# ============
n_samples = 500
seed = 30
noisy_circles = datasets.make_circles(
    n_samples=n_samples, factor=0.5, noise=0.05, random_state=seed
)
noisy_moons = datasets.make_moons(n_samples=n_samples, noise=0.05, random_state=seed)
blobs = datasets.make_blobs(n_samples=n_samples, random_state=seed)
rng = np.random.RandomState(seed)
no_structure = rng.rand(n_samples, 2), None

# Anisotropicly distributed data
random_state = 170
X, y = datasets.make_blobs(n_samples=n_samples, random_state=random_state)
transformation = [[0.6, -0.6], [-0.4, 0.8]]
X_aniso = np.dot(X, transformation)
aniso = (X_aniso, y)

# blobs with varied variances
varied = datasets.make_blobs(
    n_samples=n_samples, cluster_std=[1.0, 2.5, 0.5], random_state=random_state
)

# ============
# Set up cluster parameters
# ============
plt.figure(figsize=(9 * 2 + 3, 13))
plt.subplots_adjust(
    left=0.02, right=0.98, bottom=0.001, top=0.95, wspace=0.05, hspace=0.01
)

plot_num = 1

default_base = {
    "quantile": 0.3,
    "eps": 0.3,
    "damping": 0.9,
    "preference": -200,
    "n_neighbors": 3,
    "n_clusters": 3,
    "min_samples": 7,
    "xi": 0.05,
    "min_cluster_size": 0.1,
    "allow_single_cluster": True,
    "hdbscan_min_cluster_size": 15,
    "hdbscan_min_samples": 3,
    "random_state": 42,
}
```

```
datasets = [
    (
        noisy_circles,
        {
            "damping": 0.77,
            "preference": -240,
            "quantile": 0.2,
            "n_clusters": 2,
            "min_samples": 7,
            "xi": 0.08,
        },
    ),
    (
        noisy_moons,
        {
            "damping": 0.75,
            "preference": -220,
            "n_clusters": 2,
            "min_samples": 7,
            "xi": 0.1,
        },
    ),
    (
        varied,
        {
            "eps": 0.18,
            "n_neighbors": 2,
            "min_samples": 7,
            "xi": 0.01,
            "min_cluster_size": 0.2,
        },
    ),
    (
        aniso,
        {
            "eps": 0.15,
            "n_neighbors": 2,
            "min_samples": 7,
            "xi": 0.1,
            "min_cluster_size": 0.2,
        },
    ),
    (blobs, {"min_samples": 7, "xi": 0.1, "min_cluster_size": 0.2}),
    (no_structure, {}),
]

for i_dataset, (dataset, algo_params) in enumerate(datasets):
    # update parameters with dataset-specific values
    params = default_base.copy()
    params.update(algo_params)
```

```
    X, y = dataset

    # normalize dataset for easier parameter selection
    X = StandardScaler().fit_transform(X)

    # estimate bandwidth for mean shift
    bandwidth = cluster.estimate_bandwidth(X, quantile=params["quantile"])

    # connectivity matrix for structured Ward
    connectivity = kneighbors_graph(
        X, n_neighbors=params["n_neighbors"], include_self=False
    )
    # make connectivity symmetric
    connectivity = 0.5 * (connectivity + connectivity.T)

    # ============
    # Create cluster objects
    # ============
    ms = cluster.MeanShift(bandwidth=bandwidth, bin_seeding=True)
    two_means = cluster.MiniBatchKMeans(
        n_clusters=params["n_clusters"],
        random_state=params["random_state"],
    )
    ward = cluster.AgglomerativeClustering(
        n_clusters=params["n_clusters"], linkage="ward", connectivity=connectivity
    )
    spectral = cluster.SpectralClustering(
        n_clusters=params["n_clusters"],
        eigen_solver="arpack",
        affinity="nearest_neighbors",
        random_state=params["random_state"],
    )
    dbscan = cluster.DBSCAN(eps=params["eps"])
    hdbscan = cluster.HDBSCAN(
        min_samples=params["hdbscan_min_samples"],
        min_cluster_size=params["hdbscan_min_cluster_size"],
        allow_single_cluster=params["allow_single_cluster"],
    )
    optics = cluster.OPTICS(
        min_samples=params["min_samples"],
        xi=params["xi"],
        min_cluster_size=params["min_cluster_size"],
    )
    affinity_propagation = cluster.AffinityPropagation(
        damping=params["damping"],
        preference=params["preference"],
        random_state=params["random_state"],
    )
    average_linkage = cluster.AgglomerativeClustering(
```

```
        linkage="average",
        metric="cityblock",
        n_clusters=params["n_clusters"],
        connectivity=connectivity,
    )
    birch = cluster.Birch(n_clusters=params["n_clusters"])
    gmm = mixture.GaussianMixture(
        n_components=params["n_clusters"],
        covariance_type="full",
        random_state=params["random_state"],
    )

    clustering_algorithms = (
        ("MiniBatch\nKMeans", two_means),
        ("Affinity\nPropagation", affinity_propagation),
        ("MeanShift", ms),
        ("Spectral\nClustering", spectral),
        ("Ward", ward),
        ("Agglomerative\nClustering", average_linkage),
        ("DBSCAN", dbscan),
        ("HDBSCAN", hdbscan),
        ("OPTICS", optics),
        ("BIRCH", birch),
        ("Gaussian\nMixture", gmm),
    )

    for name, algorithm in clustering_algorithms:
        t0 = time.time()

        # catch warnings related to kneighbors_graph
        with warnings.catch_warnings():
            warnings.filterwarnings(
                "ignore",
                message="the number of connected components of the "
                + "connectivity matrix is [0-9]{1,2}"
                + " > 1. Completing it to avoid stopping the tree early.",
                category=UserWarning,
            )
            warnings.filterwarnings(
                "ignore",
                message="Graph is not fully connected, spectral embedding"
                + " may not work as expected.",
                category=UserWarning,
            )
            algorithm.fit(X)

        t1 = time.time()
        if hasattr(algorithm, "labels_"):
            y_pred = algorithm.labels_.astype(int)
        else:
            y_pred = algorithm.predict(X)
```

```
        plt.subplot(len(datasets), len(clustering_algorithms), plot_num)
        if i_dataset == 0:
            plt.title(name, size=18)

        colors = np.array(
            list(
                islice(
                    cycle(
                        [
                            "#377eb8",
                            "#ff7f00",
                            "#4daf4a",
                            "#f781bf",
                            "#a65628",
                            "#984ea3",
                            "#999999",
                            "#e41a1c",
                            "#dede00",
                        ]
                    ),
                    int(max(y_pred) + 1),
                )
            )
        )
        # add black color for outliers (if any)
        colors = np.append(colors, ["#000000"])
        plt.scatter(X[:, 0], X[:, 1], s=10, color=colors[y_pred])

        plt.xlim(-2.5, 2.5)
        plt.ylim(-2.5, 2.5)
        plt.xticks(())
        plt.yticks(())
        plt.text(
            0.99,
            0.01,
            ("%.2fs" % (t1 - t0)).lstrip("0"),
            transform=plt.gca().transAxes,
            size=15,
            horizontalalignment="right",
        )
        plot_num += 1

plt.show()
```