INF391 - Reconocimiento de Patrones en Minería de Datos

Tarea 1: Técnicas de *Clustering*

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Introducción

En esta tarea se exploran distintas técnicas de reconocimiento de patrones basadas en *clustering* vistas en cátedra. Para ello, se cuenta con tres pequeños *datasets* con distintas características, que servirán para contrastar la aptitud que cada técnica posee para cada caso.

Luego de la experimentación, se responden las dos preguntas conceptuales planteadas en el enunciado.

Parte I

Primero, se prepara la ingesta de datos.

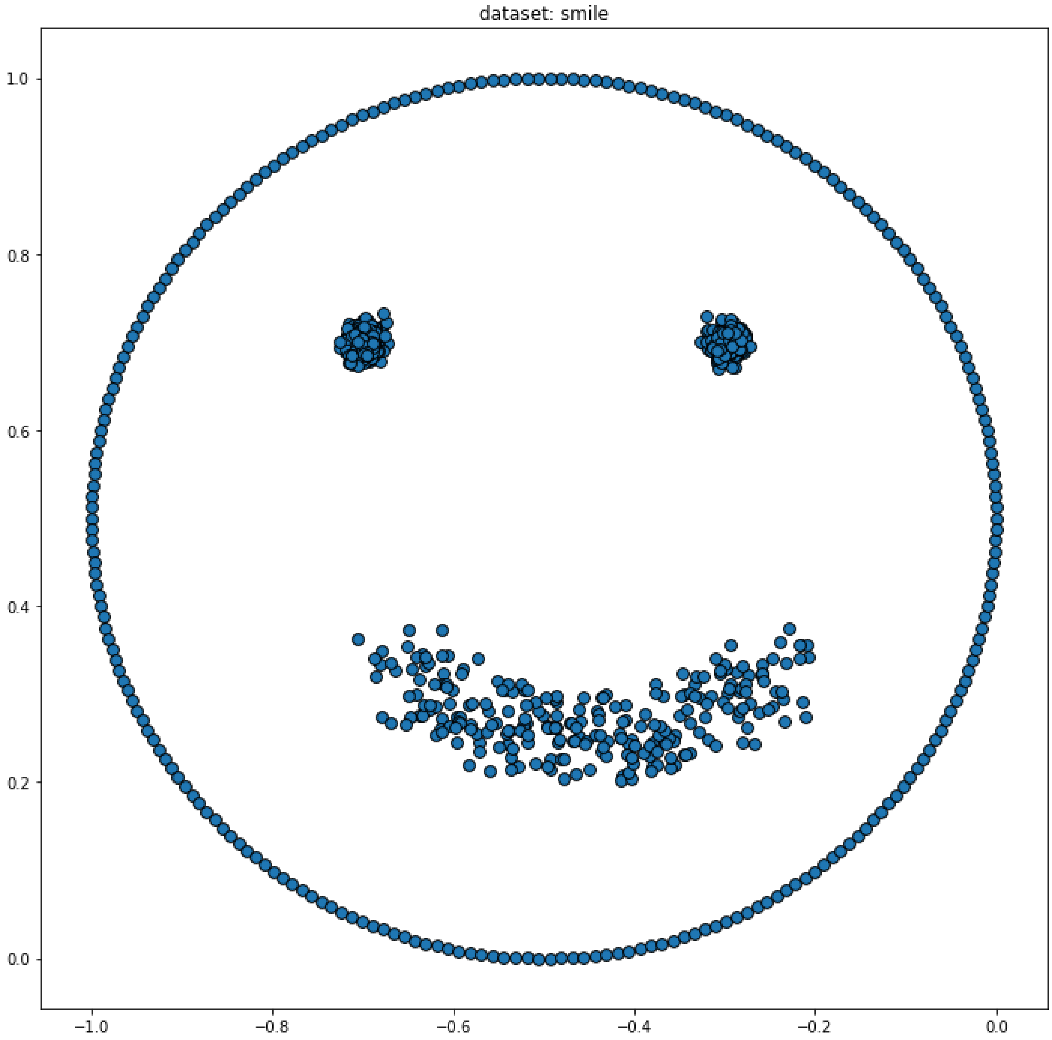
In [1]:
```python
import os.path
import numpy as np

def ingest_dataset(txt_dir):
    dataset = list()
    if os.path.exists(txt_dir):
        with open(txt_dir, 'r') as f:
            for line in f.readlines():
                data_point = line.split()
                x_coord, y_coord = float(data_point[0]), float(data_point[1])
                dataset.append([x_coord, y_coord])
    return np.array(dataset)
```

Y se instancian los tres datasets.

In [2]:
```python
smile = ingest_dataset('smile.txt')
mouse = ingest_dataset('mouse.txt')
spiral = ingest_dataset('spiral.txt')
```

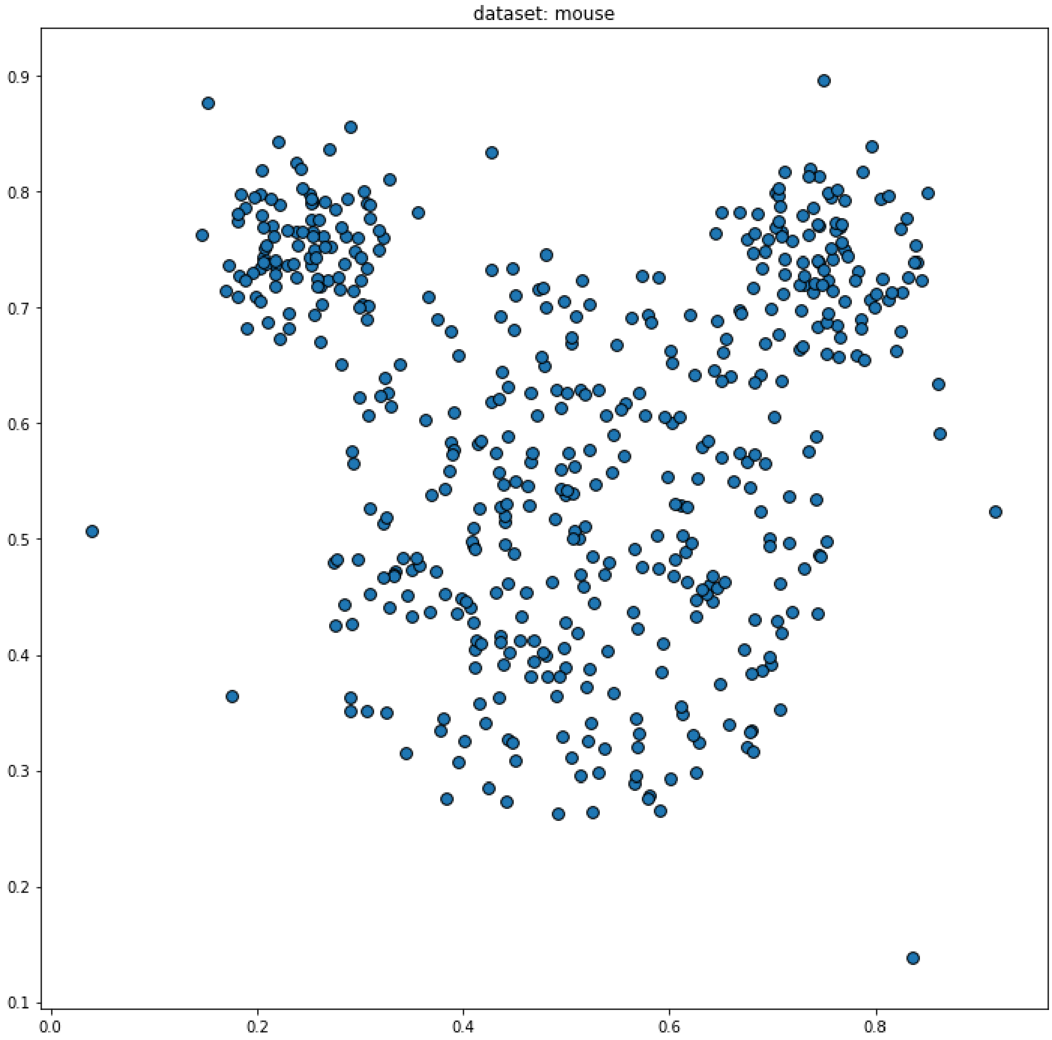
(Hacer plot y breve análisis de cada dataset: hablar sobre cantidad de datos, presencia obvia de clusters, densidad de éstos, convexidad, etc.)

In [161]:
```
# Smile
plt.figure(figsize=(12,12))
plt.scatter(smile[:, 0], smile[:, 1], marker='o',
            edgecolors='k', s=60)
plt.title('dataset: smile')
plt.show()
```

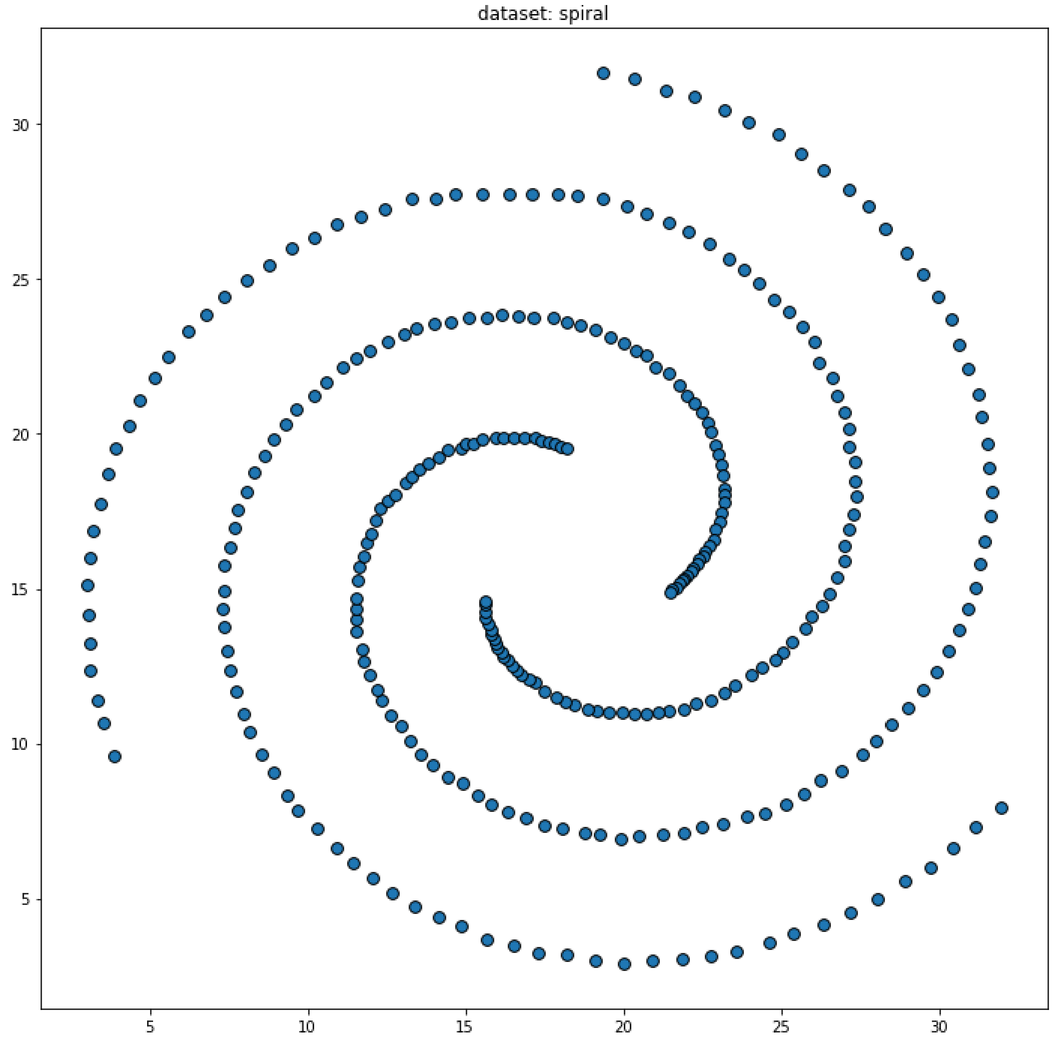


In [154]:

```python
# Mouse
plt.figure(figsize=(12,12))
plt.scatter(mouse[:, 0], mouse[:, 1], marker='o',
            edgecolors='k', s=60)
plt.title('dataset: mouse')
plt.show()
```



In [155]:
```
# Spiral
plt.figure(figsize=(12,12))
plt.scatter(spiral[:, 0], spiral[:, 1], marker='o',
            edgecolors='k', s=60)
plt.title('dataset: spiral')
plt.show()
```



A continuación, se procede a aplicar las técnicas de *clustering*.

(Info teórica sobre los algoritmos de clustering excepto Fuzzy se puede hallar acá: [https://scikit-learn.org/stable/modules/clustering.html (https://scikit-learn.org/stable/modules/clustering.html)](https://scikit-learn.org/stable/modules/clustering.html))

1. K-Means

In [92]:

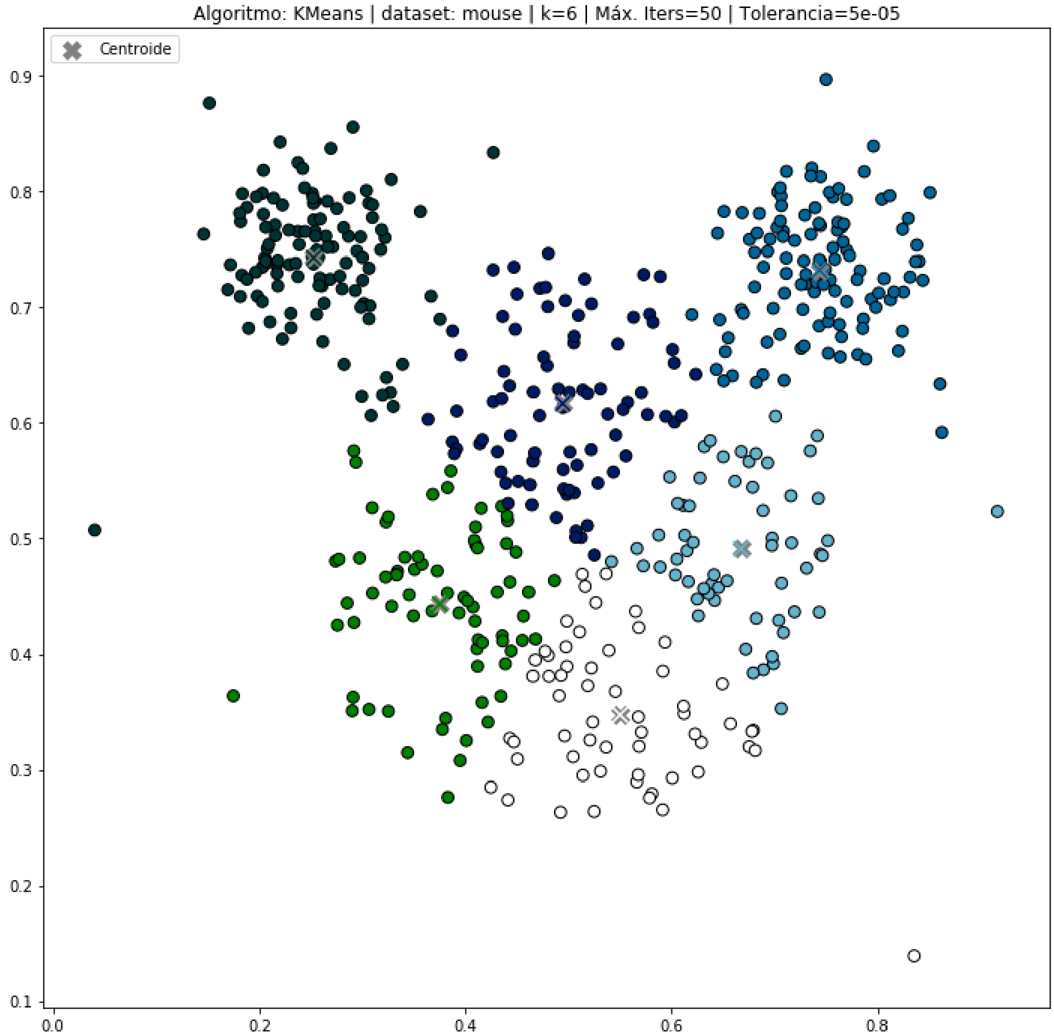
```python
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt
from ipywidgets import interact
from ipywidgets import FloatSlider

def apply_kmeans(dataset, k, max_iterations=300, tolerance=1e-4):
    kmeans = KMeans(
        n_clusters=k,
        init='random',
        n_init=1,
        max_iter=max_iterations,
        tol=tolerance,
        random_state=0,
    )
    kmeans.fit(dataset)
    return kmeans.cluster_centers_, kmeans.labels_

@interact(
    dataset_name=['smile', 'mouse', 'spiral'],
    k=(2,10, 1),
    max_iterations=(10, 100, 10),
    tolerance=FloatSlider(
        min=5e-5,
        max=5e-4,
        step=5e-5,
        continuous_update=False,
        readout=True,
        readout_format='.5f'
    ),
)
def plot_kmeans(dataset_name, k, max_iterations, tolerance):
    if dataset_name == 'smile':
        dataset = smile
    elif dataset_name == 'mouse':
        dataset = mouse
    elif dataset_name == 'spiral':
        dataset = spiral
    centroids, labels = apply_kmeans(dataset, k, max_iterations, tolerance)
    plt.figure(figsize=(12,12))
    plt.scatter(dataset[:, 0], dataset[:, 1], marker='o', c=labels,
                edgecolors='k', s=60, cmap=plt.cm.ocean)
    plt.scatter(centroids[:, 0], centroids[:, 1], marker='X', s=150,
                linewidths=.5, c='gray', cmap=plt.cm.ocean, label='Centroide')
    plt.scatter(centroids[:, 0], centroids[:, 1], marker='x', s=100,
                linewidths=2, c=list(range(len(centroids))),
                cmap=plt.cm.ocean)
    plt.title('Algoritmo: KMeans | dataset: {} | k={} | Máx. Iters={} | Tolerancia={}'.format(dataset_nam
    plt.legend(loc='upper left')
```

dataset_na… mouse

k 6

max_iterati… 50

tolerance 0.00005



Análisis K-Means

Bla...

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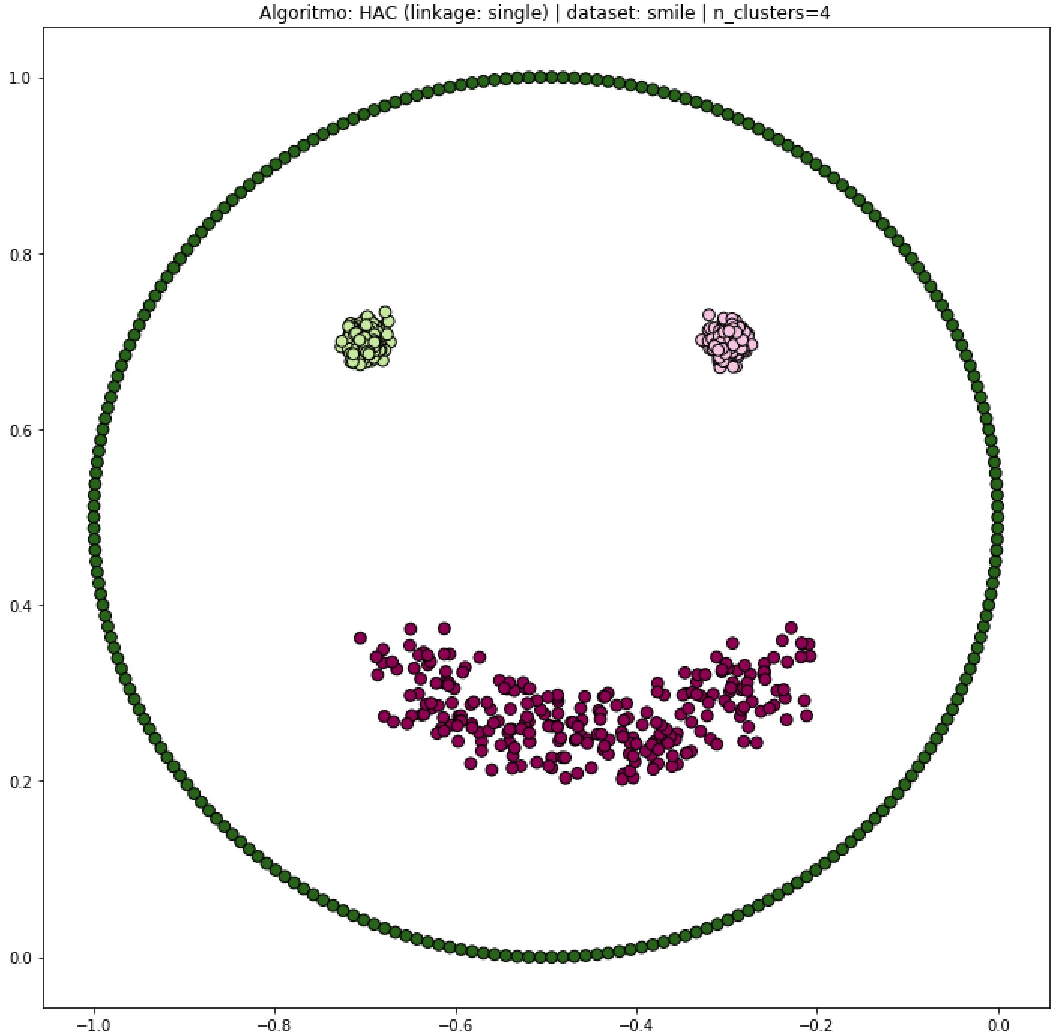
2. Agglomerative Hierarchical Clustering

In [42]:
```
from sklearn.cluster import AgglomerativeClustering

def apply_hac(dataset, linkage, n_clusters):
    hac = AgglomerativeClustering(n_clusters=n_clusters, linkage=linkage)
    hac.fit(dataset)
    return hac.labels_

@interact(
    dataset_name=['smile', 'mouse', 'spiral'],
    linkage=['single', 'complete'],
    n_clusters=(2,10, 1),
)
def plot_hac(dataset_name, linkage, n_clusters):
    if dataset_name == 'smile':
        dataset = smile
    elif dataset_name == 'mouse':
        dataset = mouse
    elif dataset_name == 'spiral':
        dataset = spiral

    labels = apply_hac(dataset, linkage, n_clusters)
    plt.figure(figsize=(12,12))
    plt.scatter(dataset[:, 0], dataset[:, 1], marker='o', c=labels,
                edgecolors='k', s=60, cmap=plt.cm.PiYG)
    plt.title('Algoritmo: HAC (linkage: {}) | dataset: {} | n_clusters={}'.format(linkage, dataset_name,

```

dataset_na... smile

linkage single

n_clusters 4



Análisis Agglomerative Hierarchical Clustering

Bla...

3. DBSCAN

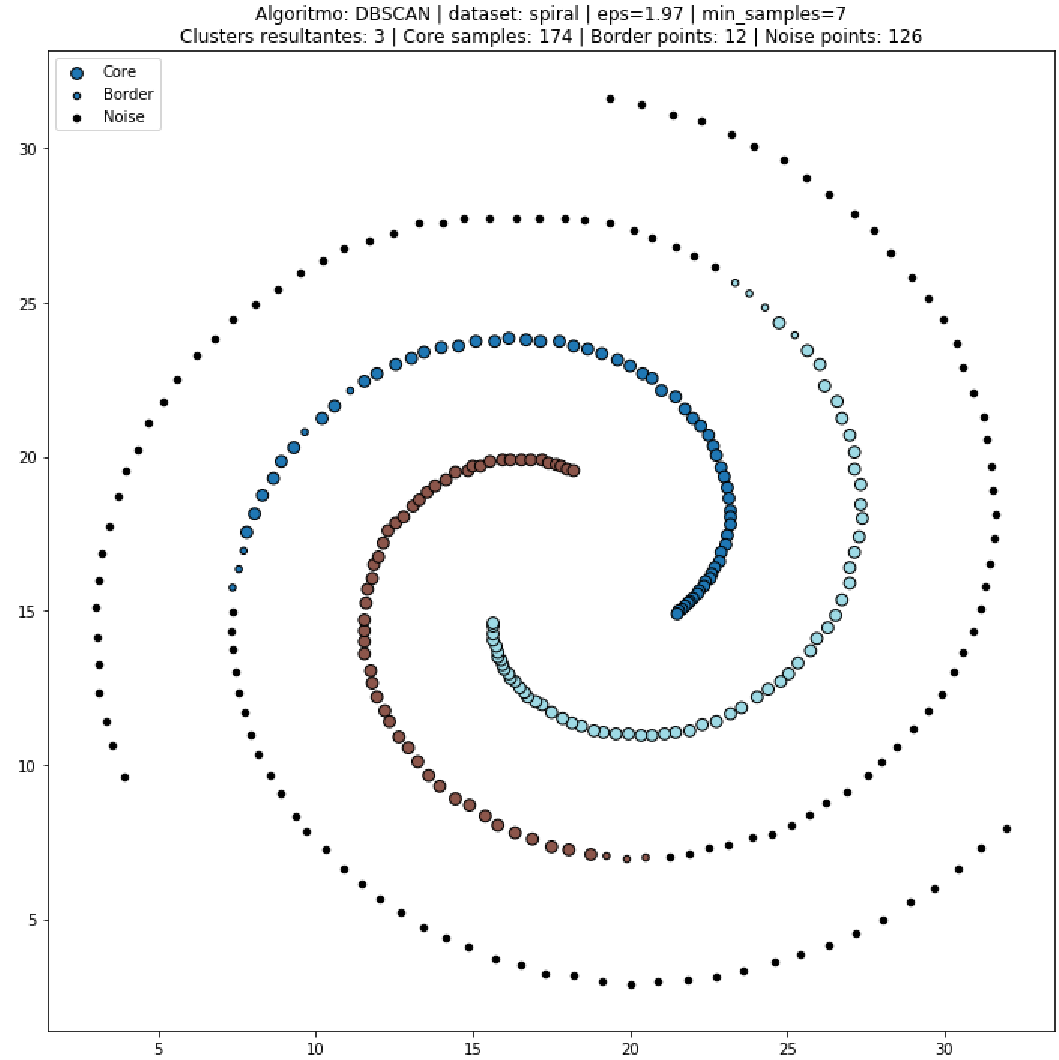
In [62]:

```
from sklearn.cluster import DBSCAN

def apply_dbscan(dataset, min_pts, eps):
    dbscan = DBSCAN(eps=eps, min_samples=min_pts)
    dbscan.fit(dataset)
    core_samples_mask = np.zeros_like(dbscan.labels_, dtype=bool)
    core_samples_mask[dbscan.core_sample_indices_] = True
    noise_points_mask = (dbscan.labels_ == -1)
    border_points_mask = np.zeros_like(dbscan.labels_, dtype=bool)
    border_points_mask[~core_samples_mask & ~noise_points_mask] = True

    # Number of clusters in labels, ignoring noise if present.
    n_clusters_ = len(set(dbscan.labels_)) - (1 if -1 in dbscan.labels_ \
                                              else 0)
    n_noise_ = list(dbscan.labels_).count(-1)
    return dbscan.labels_, n_clusters_, n_noise_, core_samples_mask, \
        border_points_mask, noise_points_mask

@interact(
    dataset_name=['smile', 'mouse', 'spiral'],
    min_pts=(1,50, 1),
    eps=(0.01, 5.0, 0.01),
)
def plot_dbscan(dataset_name, min_pts, eps):
    if dataset_name == 'smile':
        dataset = smile
    elif dataset_name == 'mouse':
        dataset = mouse
    elif dataset_name == 'spiral':
        dataset = spiral
    labels, n_clusters, n_noise, core_samples_mask, border_points_mask,\
    noise_points_mask = apply_dbscan(dataset, min_pts, eps)
    core_points = dataset[core_samples_mask]
    border_points = dataset[border_points_mask]
    noise_points = dataset[noise_points_mask]
    n_clusters = len(set(labels)) - (1 if -1 in labels else 0)
    plt.figure(figsize=(12,12))
    # Plot core samples
    plt.scatter(core_points[:, 0], core_points[:, 1], marker='o',
                c=labels[core_samples_mask], edgecolors='k', s=60,
                cmap=plt.cm.tab20, label='Core')
    # Plot border points
    plt.scatter(border_points[:, 0], border_points[:, 1], marker='o',
                c=labels[border_points_mask], edgecolors='k', s=20,
                cmap=plt.cm.tab20, label='Border')
    # Plot noise points
    plt.scatter(noise_points[:, 0], noise_points[:, 1], marker='o',
                c='black', edgecolors='k', s=20,
                cmap=plt.cm.tab20, label='Noise')
    plt.title('Algoritmo: DBSCAN | dataset: {} | eps={} | min_samples={}\n\
Clusters resultantes: {} | Core samples: {} | Border points: {} | Noise points: {}'
              .format(dataset_name, eps, min_pts, n_clusters,
                      len(core_points), len(border_points),
                      len(noise_points)))
    plt.legend(loc='upper left')

```

dataset_na… spiral

min_pts 7

eps 1.97



Análisis DBSCAN

Bla...

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4. Mean-shift

In [67]:

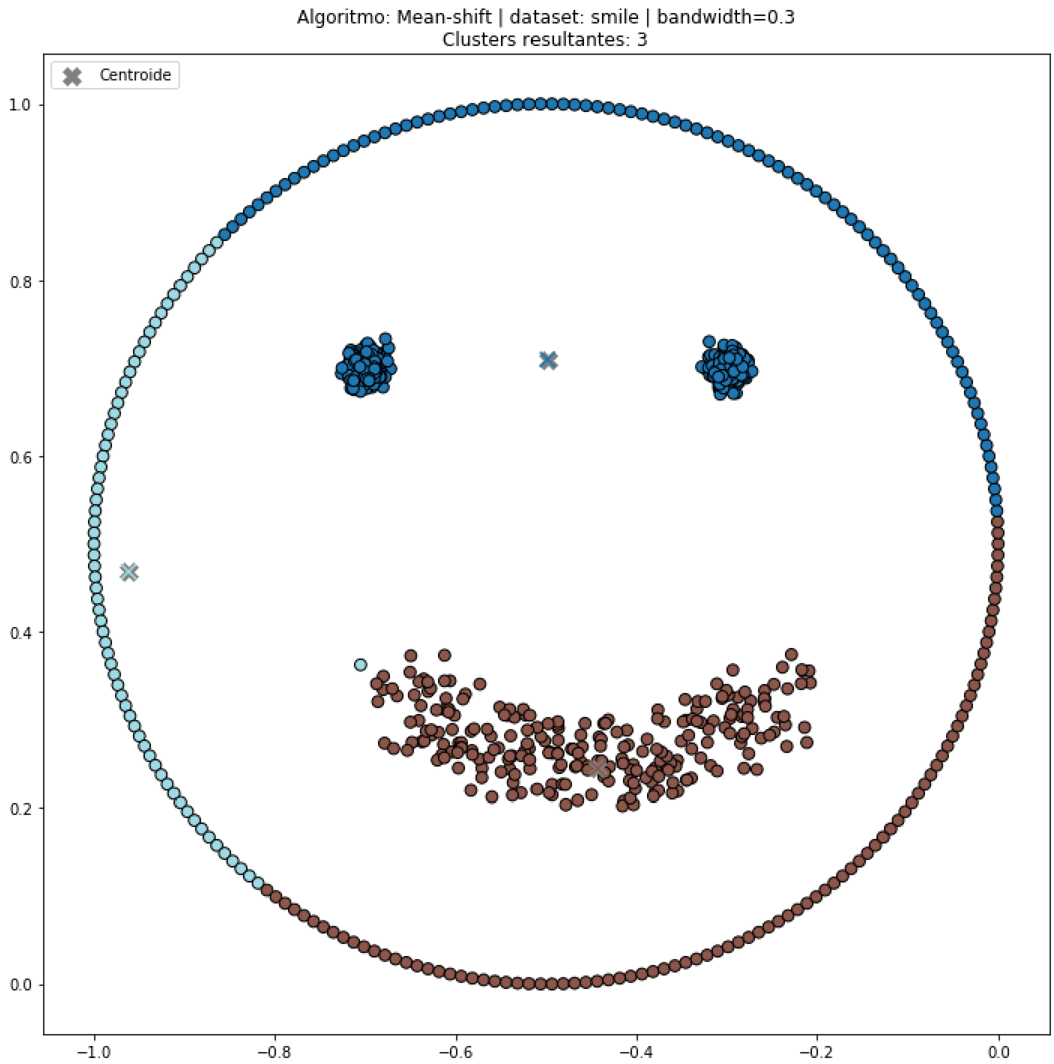
```python
from sklearn.cluster import MeanShift

def apply_meanshift(dataset, bandwidth):
    meanshift = MeanShift(bandwidth=bandwidth)
    meanshift.fit(dataset)
    return meanshift.cluster_centers_, meanshift.labels_

@interact(
    dataset_name=['smile', 'mouse', 'spiral'],
    bandwidth=(0.1, 10, 0.1),
)
def plot_kmeans(dataset_name, bandwidth):
    if dataset_name == 'smile':
        dataset = smile
    elif dataset_name == 'mouse':
        dataset = mouse
    elif dataset_name == 'spiral':
        dataset = spiral
    centroids, labels = apply_meanshift(dataset, bandwidth=bandwidth)
    plt.figure(figsize=(12,12))
    plt.scatter(dataset[:, 0], dataset[:, 1], marker='o', c=labels,
                edgecolors='k', s=60, cmap=plt.cm.tab20)
    plt.scatter(centroids[:, 0], centroids[:, 1], marker='X', s=150,
                linewidths=.5, c='gray', cmap=plt.cm.tab20, label='Centroide')
    plt.scatter(centroids[:, 0], centroids[:, 1], marker='x', s=100,
                linewidths=2, c=list(range(len(centroids))),
                cmap=plt.cm.tab20)
    plt.title('Algoritmo: Mean-shift | dataset: {} | bandwidth={}\nClusters resultantes: {}'.format(datas
    plt.legend(loc='upper left')
```

dataset_na... smile

bandwidth 0.30



Análisis Mean-shift

Bla...

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5. Spectral clustering

In [127]:

```
from sklearn.cluster import SpectralClustering

def apply_spectral_rbf(
    dataset,
    n_clusters,
    random_state=0,
    n_init=1,
    gamma=1.0,
    affinity_matrix_method='rbf',
):
    spectral = SpectralClustering(
        n_clusters=n_clusters,
        random_state=random_state,
        n_init=n_init,
        gamma=gamma,
        affinity=affinity_matrix_method,
    )
    spectral.fit(dataset)
    return spectral.labels_

def apply_spectral_nearest_neighbors(
    dataset,
    n_clusters,
    n_neighbors,
    random_state=0,
    n_init=1,
    affinity_matrix_method='nearest_neighbors',
):
    spectral = SpectralClustering(
        n_clusters=n_clusters,
        random_state=random_state,
        n_init=n_init,
        affinity=affinity_matrix_method,
        n_neighbors=n_neighbors,
    )
    spectral.fit(dataset)
    return spectral.labels_

@interact(
    dataset_name=['smile', 'mouse', 'spiral'],
    affinity=['RBF', 'K-nearest neighbors'],
    n_clusters=(2,10, 1),
    gamma=(0.1, 5.0, 0.1),
    n_neighbors=(1, 20, 1),
)
def plot_spectral(
    dataset_name,
    affinity,
    n_clusters,
    gamma,
    n_neighbors,
):
    if dataset_name == 'smile':
        dataset = smile
    elif dataset_name == 'mouse':
        dataset = mouse
    elif dataset_name == 'spiral':
        dataset = spiral
    if affinity == 'RBF':
        labels = apply_spectral_rbf(
            dataset=dataset,
            n_clusters=n_clusters,
            gamma=gamma,
            affinity_matrix_method='rbf',
        )
    elif affinity == 'K-nearest neighbors':
        labels = apply_spectral_nearest_neighbors(
            dataset=dataset,
            n_clusters=n_clusters,
            n_neighbors=n_neighbors,
            affinity_matrix_method='nearest_neighbors',
        )
    plt.figure(figsize=(12,12))
    plt.scatter(dataset[:, 0], dataset[:, 1], marker='o', c=labels,
                edgecolors='k', s=60, cmap=plt.cm.PiYG)
    if affinity == 'RBF':
        plt.title('Algoritmo: Spectral Clustering | Affinity: RBF\
 (gamma={}) | dataset: {} | n_clusters={}'.format(round(gamma, 2),
                                                  dataset_name, n_clusters))
    elif affinity == 'K-nearest neighbors':
        plt.title('Algoritmo: Spectral Clustering | Affinity: {}-nearest\
```

```
neighbors | dataset: {} | n_clusters={}'.format(n_neighbors, dataset_name,
                                                   n_clusters))

```

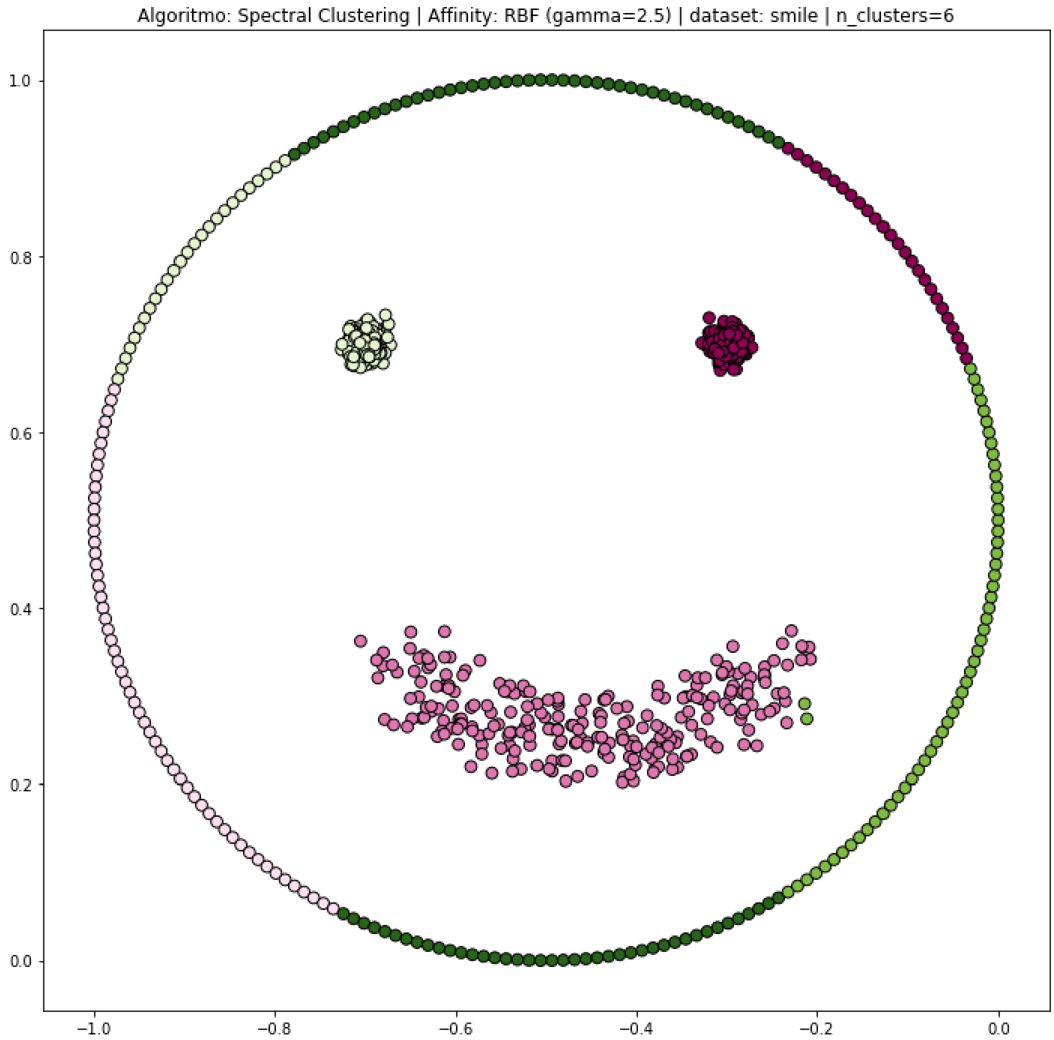
dataset_na… smile

affinity RBF

n_clusters 6

gamma 2.50

n_neighbors 10



(Se pueden agregar más métodos de construcción de matriz de afinidad)

Análisis Spectral clustering

Bla...

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6. Fuzzy C-Means

In [145]:

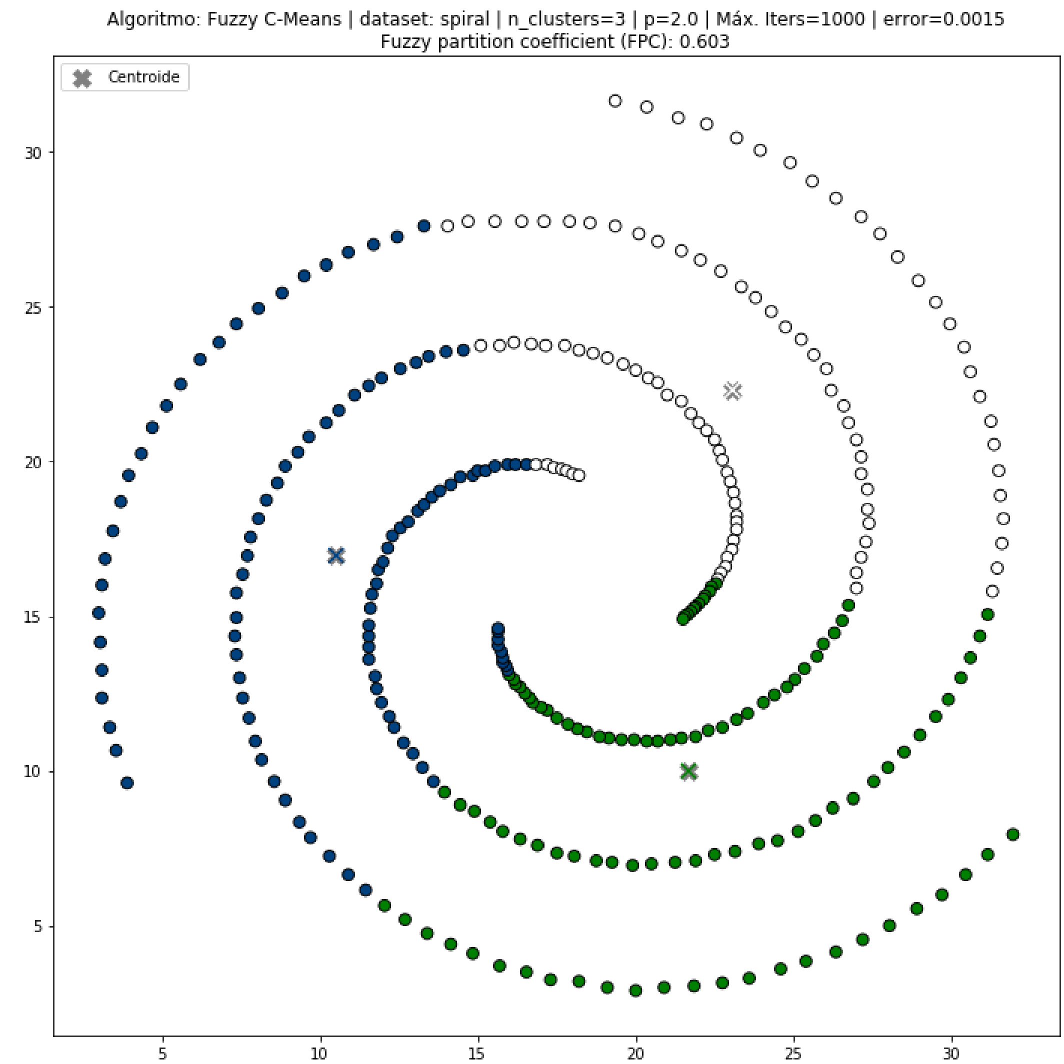
```
from skfuzzy import cluster as fuzzy
from ipywidgets import IntSlider

# Info: https://pythonhosted.org/scikit-fuzzy/auto_examples/plot_cmeans.html
def apply_cmeans(dataset, c, m, error, maxiter, seed=0):
    # El argumento 'data' de cmeans exige que el dataset venga transpuesto!
    cntr, u, u0, d, jm, p, fpc = fuzzy.cmeans(
        data=dataset.T,
        c=c,
        m=m,
        error=error,
        maxiter=maxiter,
        seed=seed,
    )
    return cntr, u, u0, d, jm, p, fpc

@interact(
    dataset_name=['smile', 'mouse', 'spiral'],
    n_clusters=(2, 10, 1),
    p_exponent=(1.1, 3.0, 0.1),
    error=FloatSlider(
        min=5e-4,
        max=5e-2,
        step=5e-4,
        continuous_update=False,
        readout=True,
        readout_format='.4f'
    ),
    max_iterations=(1, 1000, 1),
)
def plot_cmeans(
    dataset_name,
    n_clusters,
    p_exponent,
    error,
    max_iterations,
):
    if dataset_name == 'smile':
        dataset = smile
    elif dataset_name == 'mouse':
        dataset = mouse
    elif dataset_name == 'spiral':
        dataset = spiral
    cntr, u, u0, d, jm, p, fpc = apply_cmeans(
        dataset=dataset,
        c=n_clusters,
        m=p_exponent,
        error=error,
        maxiter=max_iterations,
    )
    # El color de cada punto es asignado segun el cluster al cual pertenezca
    # con mayor porcentaje
    labels = u.argmax(axis=0)
    plt.figure(figsize=(12,12))
    plt.scatter(dataset[:, 0], dataset[:, 1], marker='o', c=labels,
                edgecolors='k', s=60, cmap=plt.cm.ocean)
    plt.scatter(cntr[:, 0], cntr[:, 1], marker='X', s=150,
                linewidths=.5, c='gray', cmap=plt.cm.ocean, label='Centroide')
    plt.scatter(cntr[:, 0], cntr[:, 1], marker='x', s=100,
                linewidths=2, c=list(range(n_clusters)),
                cmap=plt.cm.ocean)
    plt.title('Algoritmo: Fuzzy C-Means | dataset: {} | n_clusters={} | \
p={} | Máx. Iters={} | error={}\nFuzzy partition coefficient (FPC): {}'.format(
        dataset_name,
        n_clusters,
        round(p_exponent, 2),
        max_iterations,
        round(error, 5),
        round(fpc, 3),
    ))
    plt.legend(loc='upper left')
```

dataset_na… spiral

n_clusters 3

p_exponent 2.00

error 0.0015



Análisis Fuzzy C-Means

(este link puede ayudar con el análisis: [https://pythonhosted.org/scikit-fuzzy/auto_examples/plot_cmeans.html (https://pythonhosted.org/scikit-fuzzy/auto_examples/plot_cmeans.html)](https://pythonhosted.org/scikit-fuzzy/auto_examples/plot_cmeans.html))

Bla...

Parte II

(a) Se tiene un conjunto de datos con 100 objetos. Se le pide realizar clustering utilizando K-means, pero para todos los valores de k, $1 \leq k \leq 100$, el algoritmo retorna que todos los clusters estan vacíos, excepto uno. ¿En que situación podría ocurrir esto? (analice los datos y no los parametros del algoritmo, i.e., iteraciones). ¿Qué resultado tendría single-link y DBSCAN para este tipo de datos?

Resp.:

(b) Considerando single-link y complete-link hierarchical clustering, ¿es posible que un objeto esté más cerca (en distancia Euclidiana) de los objetos de otros clusters en relación a los de su propio cluster? Si fuese posible, ¿en que enfoque (single y/o complete) esto podría ocurrir? Justifique con un ejemplo en cada caso.

Resp.: