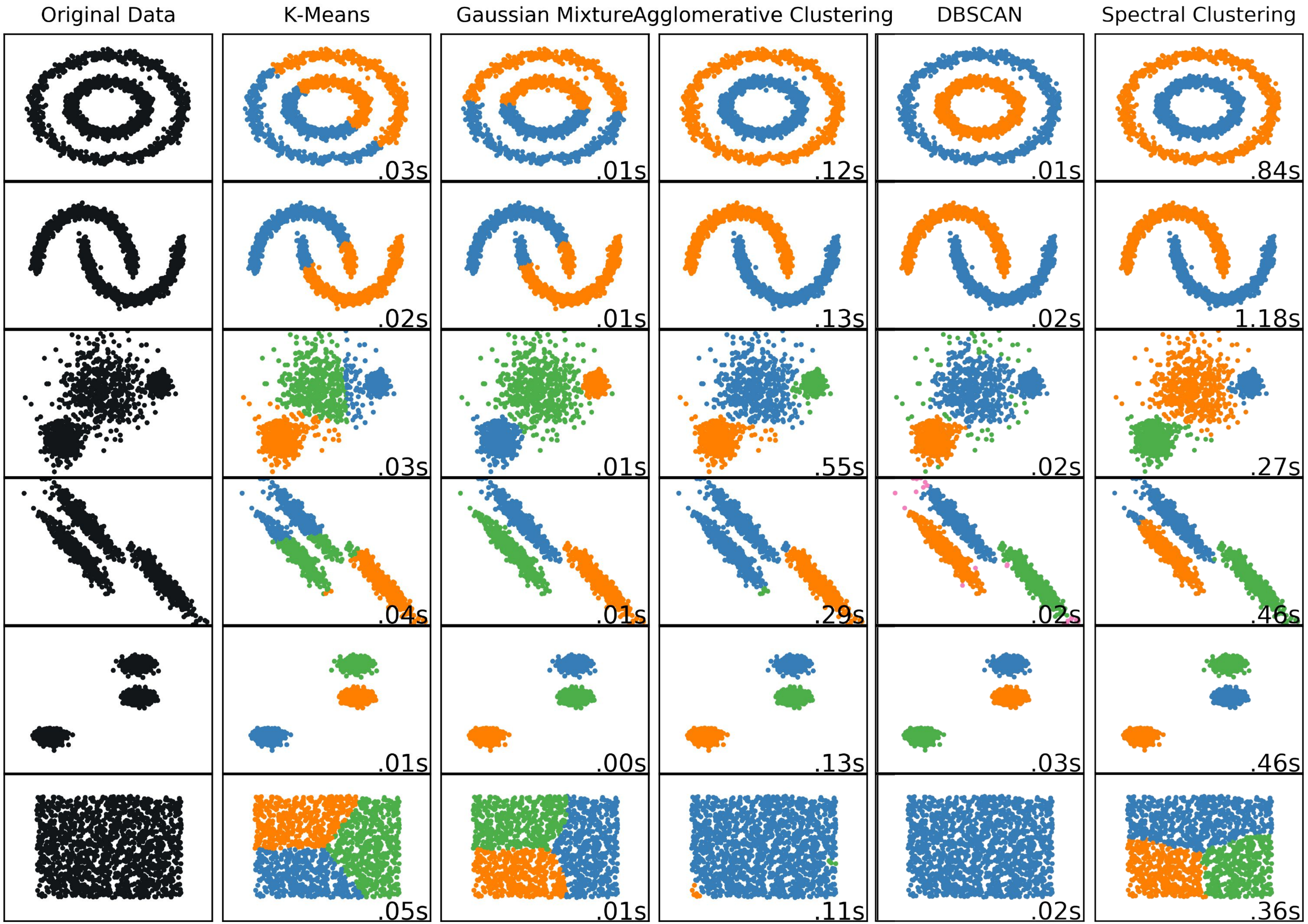
# Clustering II

# Agglomerative Clustering

# DBSCAN

# Spectral Clustering



# Hierarchical Clustering

agglomerative (bottom-up) clustering

divisive (top-down) clustering

# Agglomerative clustering components

## Distance metric

How we measure distance/dissimilarity

Euclidean distance ($L_2$ norm): $D(\boldsymbol{a}, \boldsymbol{b}) = \|\boldsymbol{a} - \boldsymbol{b}\|_2$

Squared Euclidean distance: $D(\boldsymbol{a}, \boldsymbol{b}) = \|\boldsymbol{a} - \boldsymbol{b}\|_2^2$

Manhattan distance ($L_1$ norm): $D(\boldsymbol{a}, \boldsymbol{b}) = \|\boldsymbol{a} - \boldsymbol{b}\|_1$

Maximum distance:

$$D(\boldsymbol{a}, \boldsymbol{b}) = \|\boldsymbol{a} - \boldsymbol{b}\|_\infty = \max_i |a_i - b_i|$$

## Linkage criterion

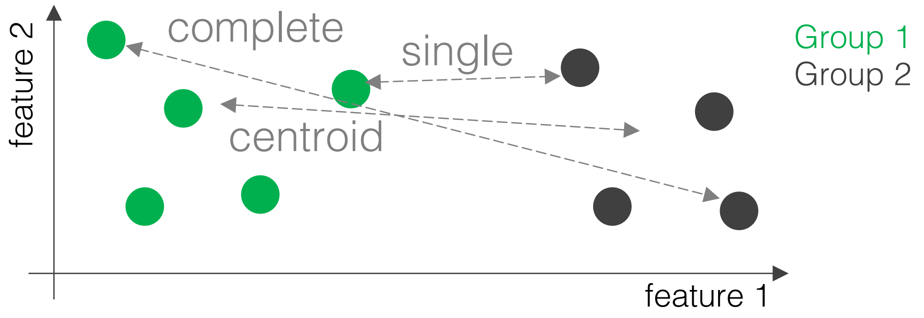
How to measure distance/dissimilarity between groups or sets

**Complete** = maximum intercluster dissimilarity

**Single** = minimum intercluster dissimilarity

**Average** = average intercluster dissimilarity (calculate the dissimilarity between all pairs of points, take the average)

**Centroid** = dissimilarity between cluster centroids

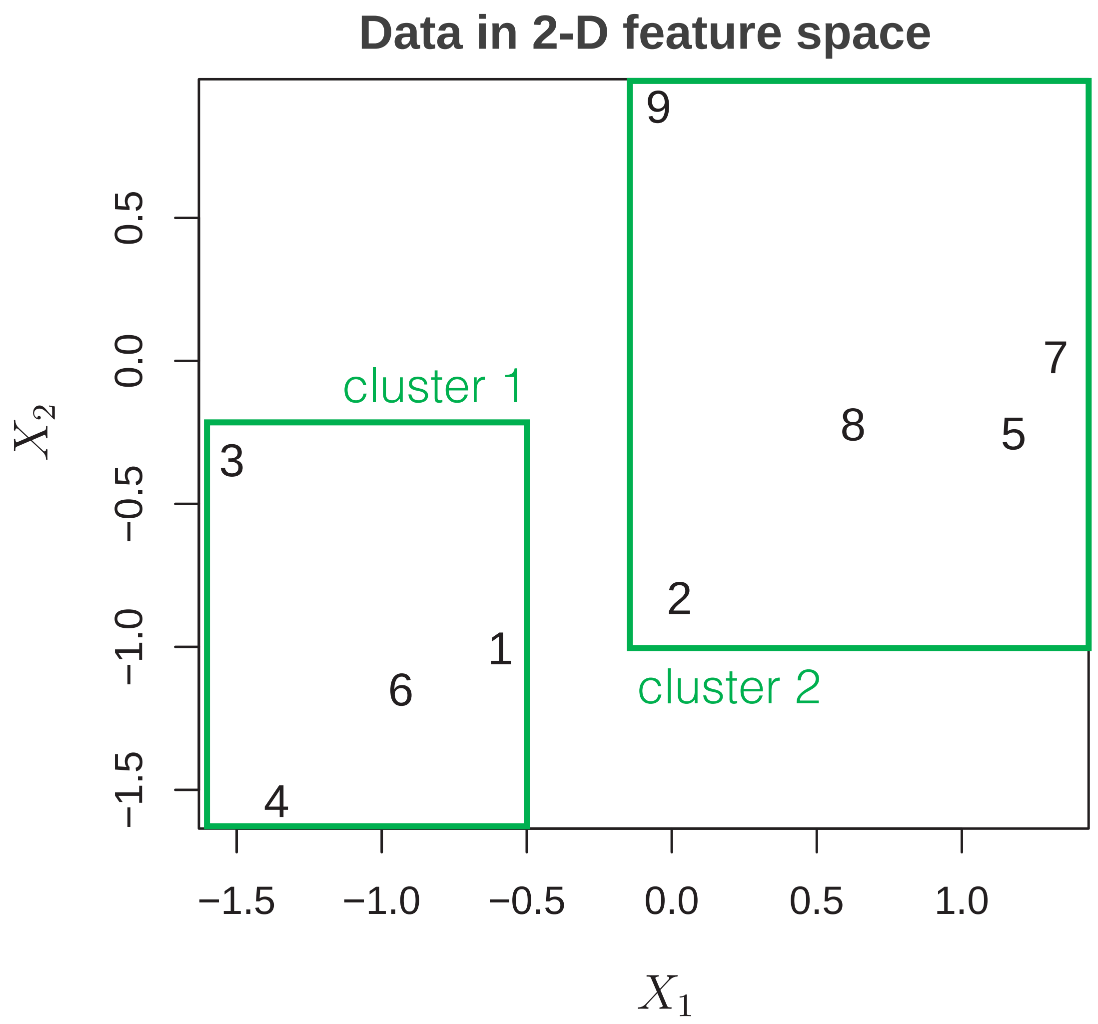


# Agglomerative clustering

With complete linkage and Euclidean distance

**Algorithm**:

1. Select a measure of dissimilarity and linkage
2. Set each observation as a unique cluster
3. Group the two closest clusters together
4. Repeat until there is only one cluster



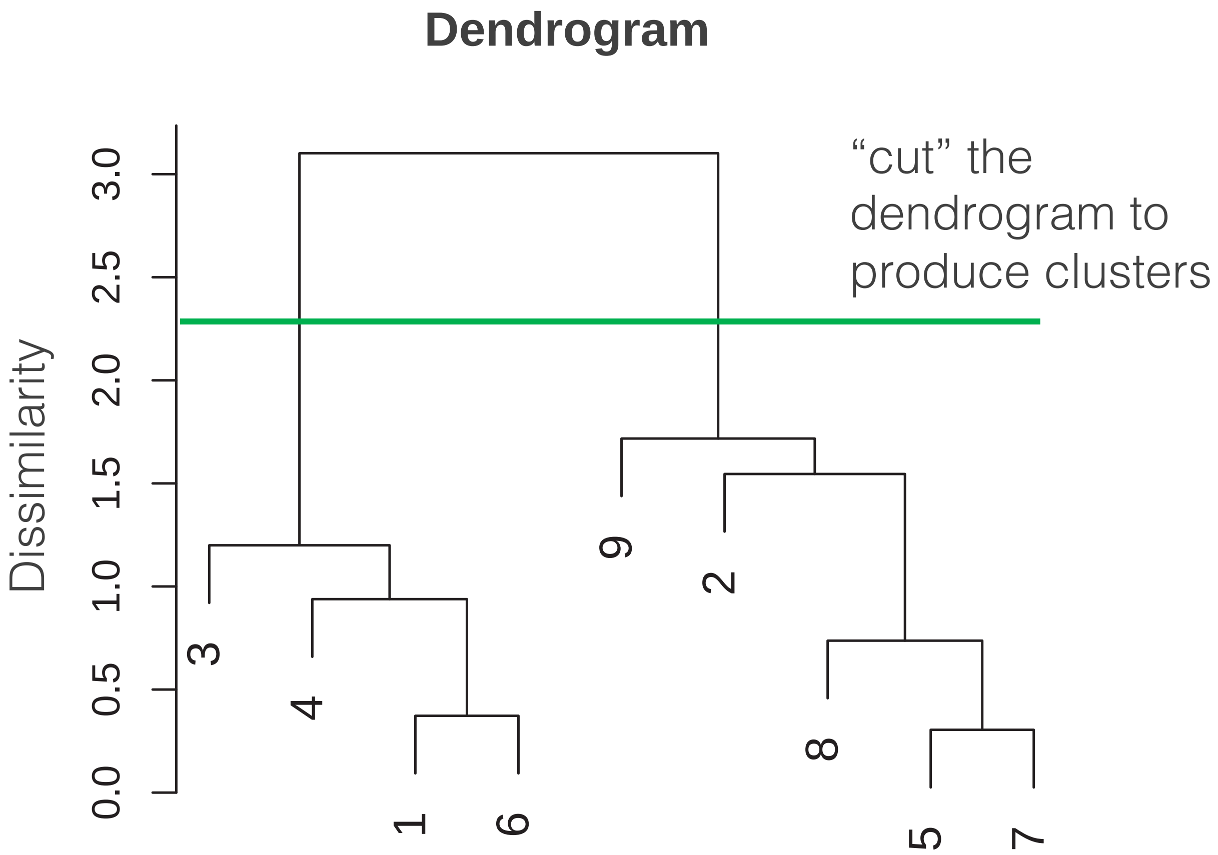




Image from James et al., Introduction to Statistical Learning, 2013

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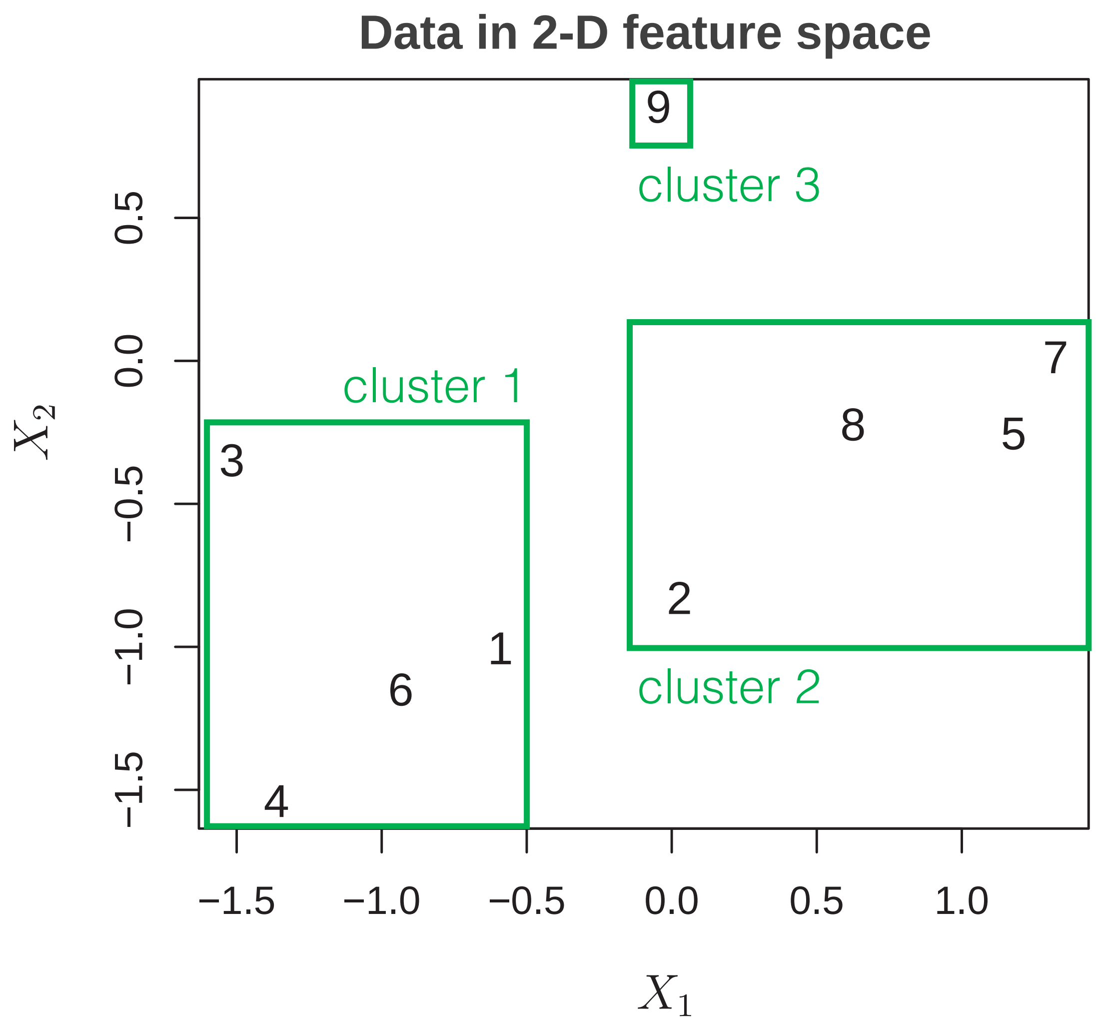


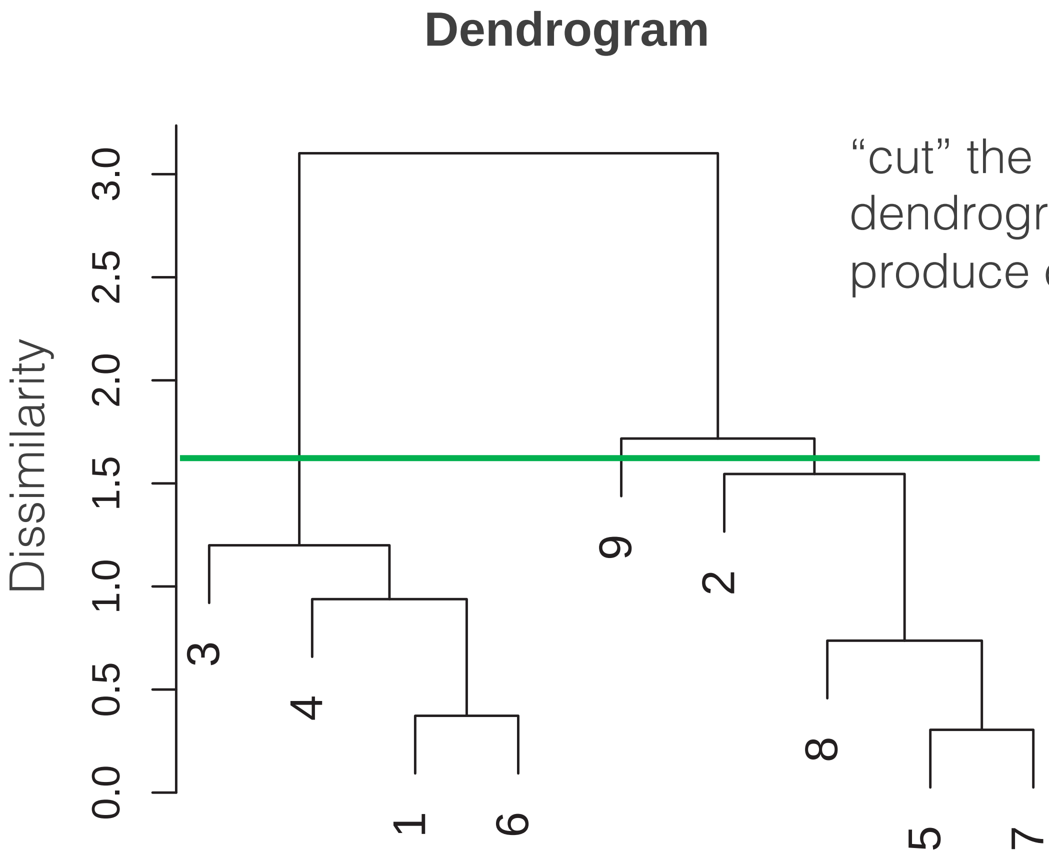


"cut" the dendrogram to produce clusters

Image from James et al., Introduction to Statistical Learning, 2013

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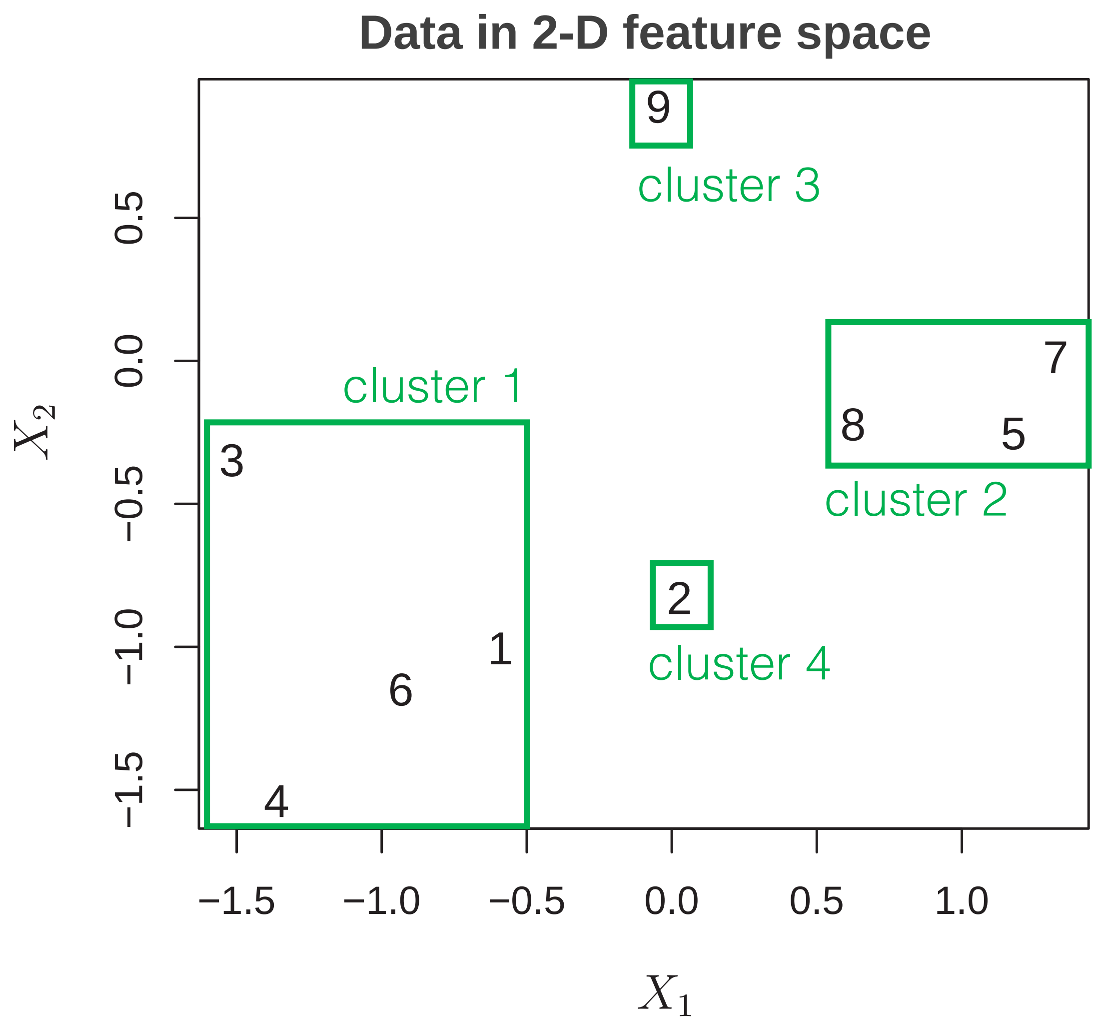
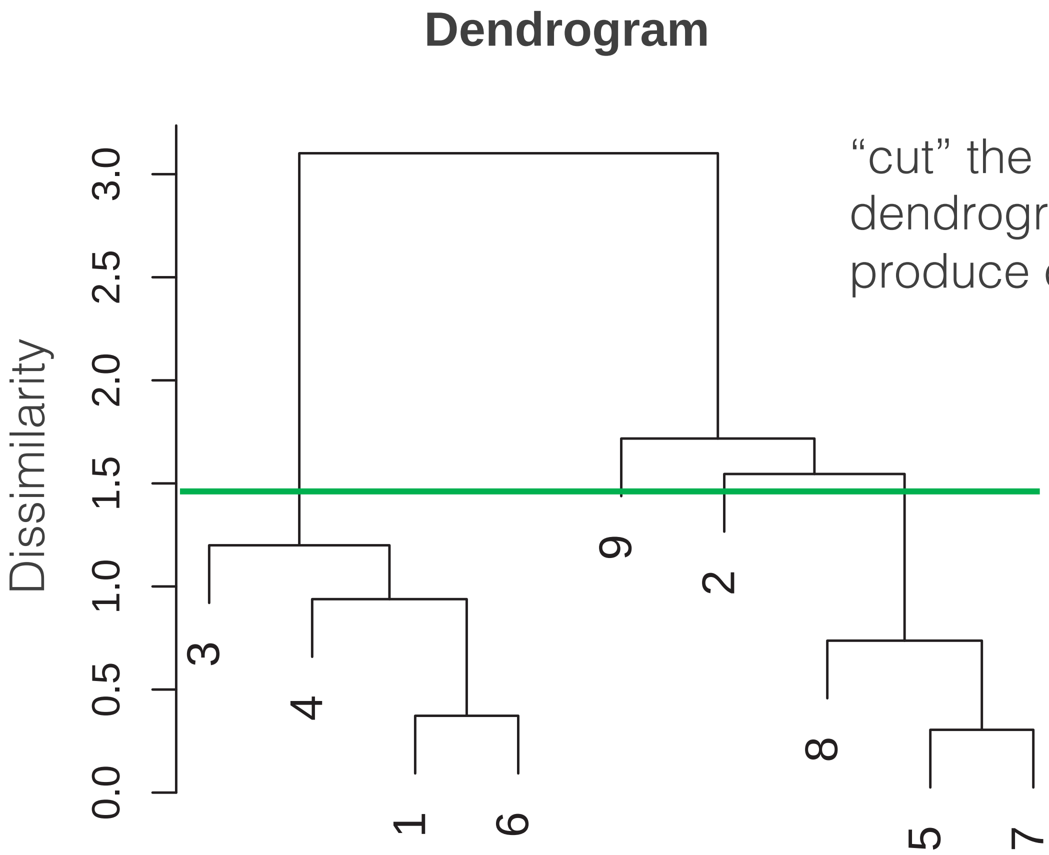


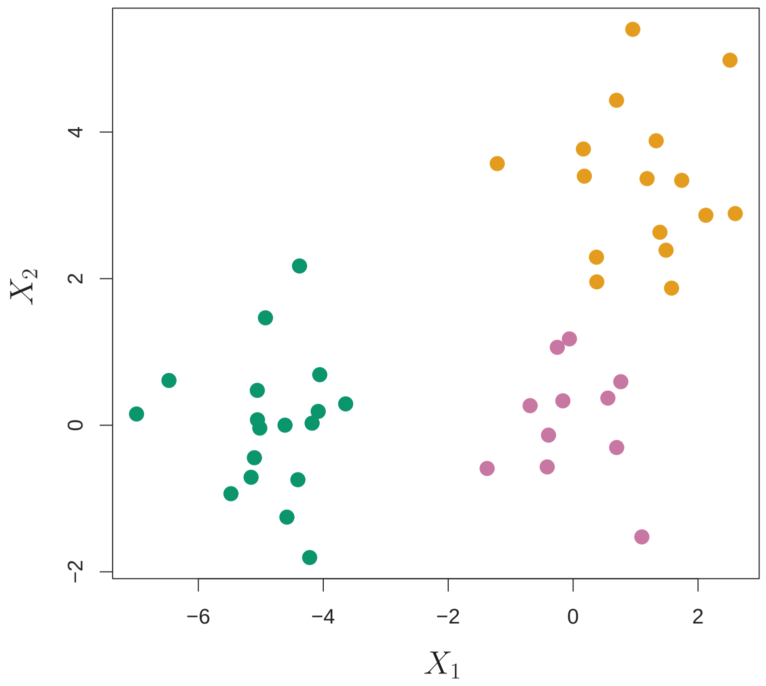

"cut" the dendrogram to produce clusters

Image from James et al., Introduction to Statistical Learning, 2013

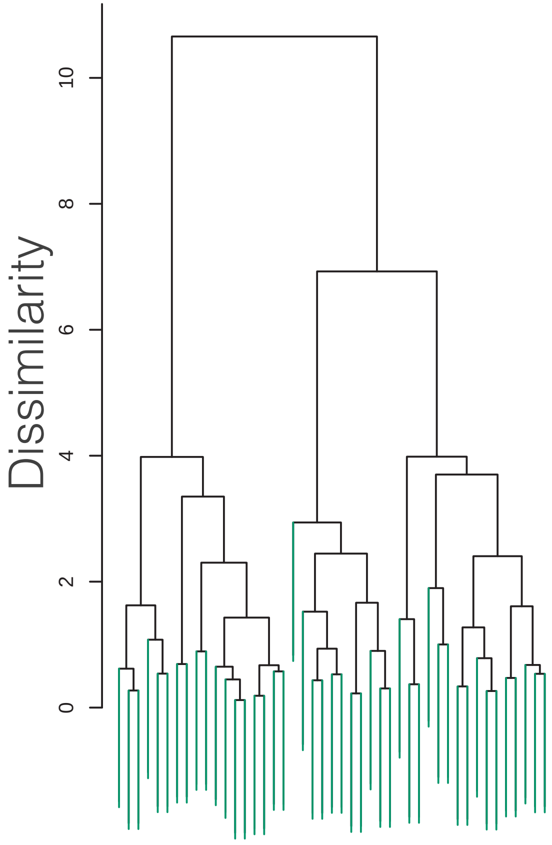
# Example of agglomerative clustering

With complete linkage and Euclidean distance

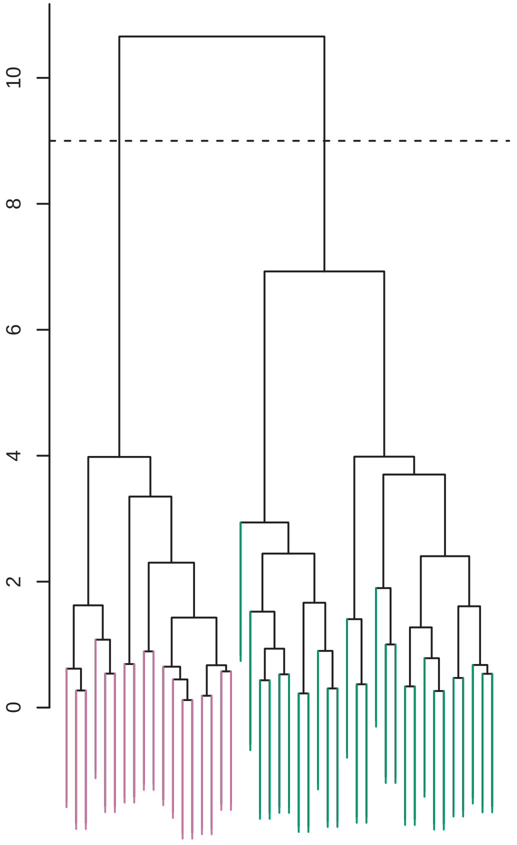
**Data in 2-D feature space**



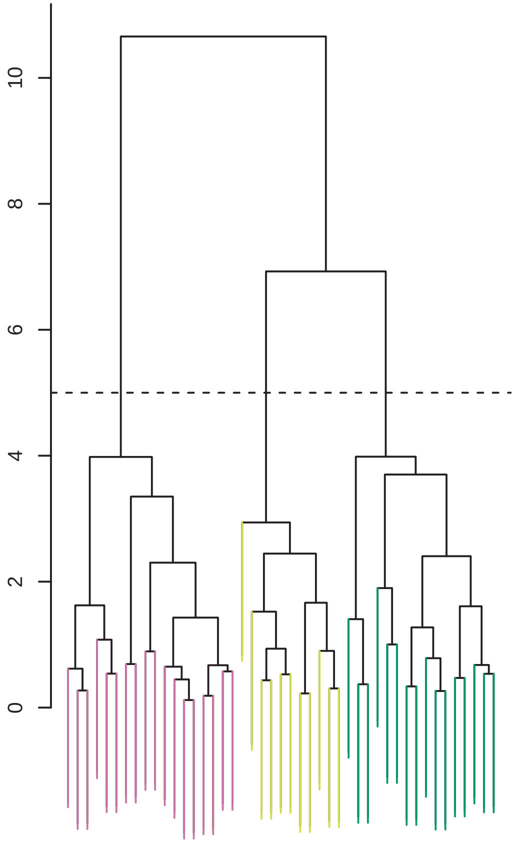

**Original Dendrogram**




**Dendrogram cut for 2 clusters**



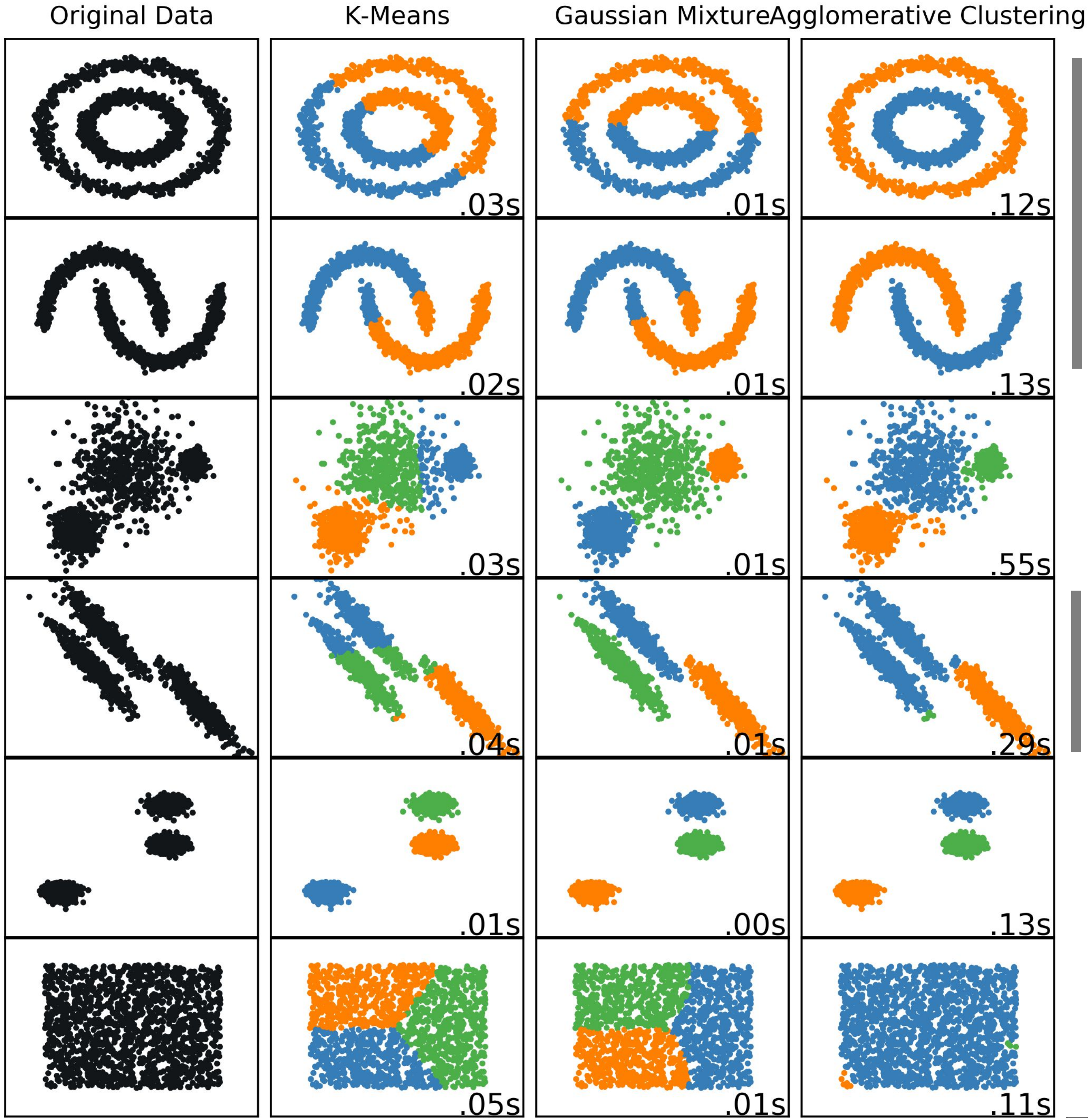
**Dendrogram cut for 3 clusters**



Note: colors do not directly map to plot on the left

Image from James et al., Introduction to Statistical Learning, 2013

# Examples: Agglomerative clustering




Need to choose where to cut the dendrogram

Can be slow since all pairwise distances between clusters need to be evaluated

Performs well when clusters are well-separated

Struggles when intercluster distance is not sufficient to distinguish between clusters

# DBSCAN Clustering

## Density-based spatial clustering of applications with noise

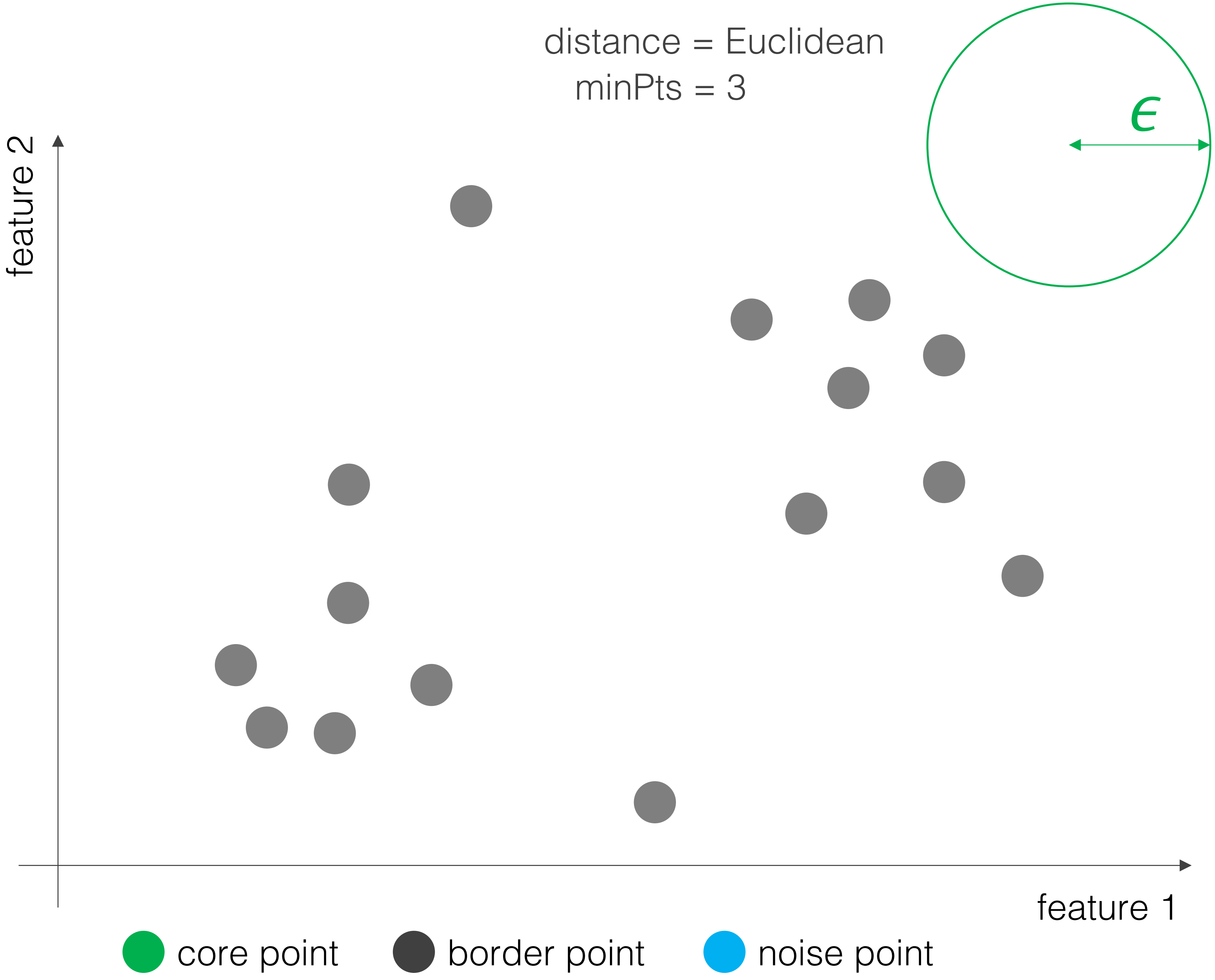
By Martin Ester, Hans-Peter Kriegel, Jörg Sander, and Xiaowei Xu, 1996

# DBSCAN

**Parameters**:
1. Distance measure
2. The radius of a neighbor, $\epsilon$
3. ‘minPts’: The number of neighbors for a point to be considered a core point

**Types of points**:
- **Core**: a point with at least minPts neighbors
- **Border**: a non-core point that neighbors a core point
- **Noise**: Other points

**Algorithm**:
1. Label core and border points
2. Group neighboring core points
3. Add border points that are neighbors of core points



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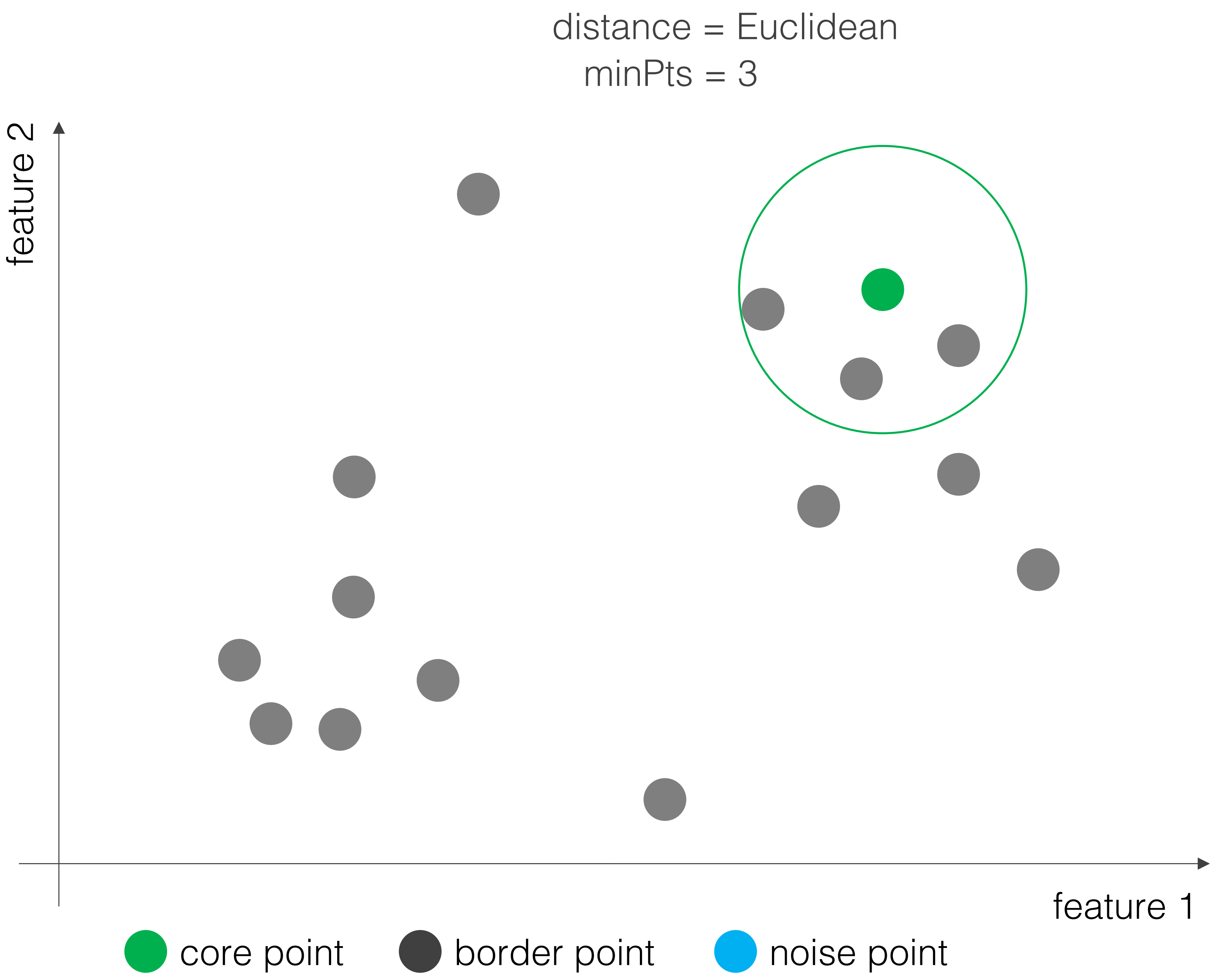

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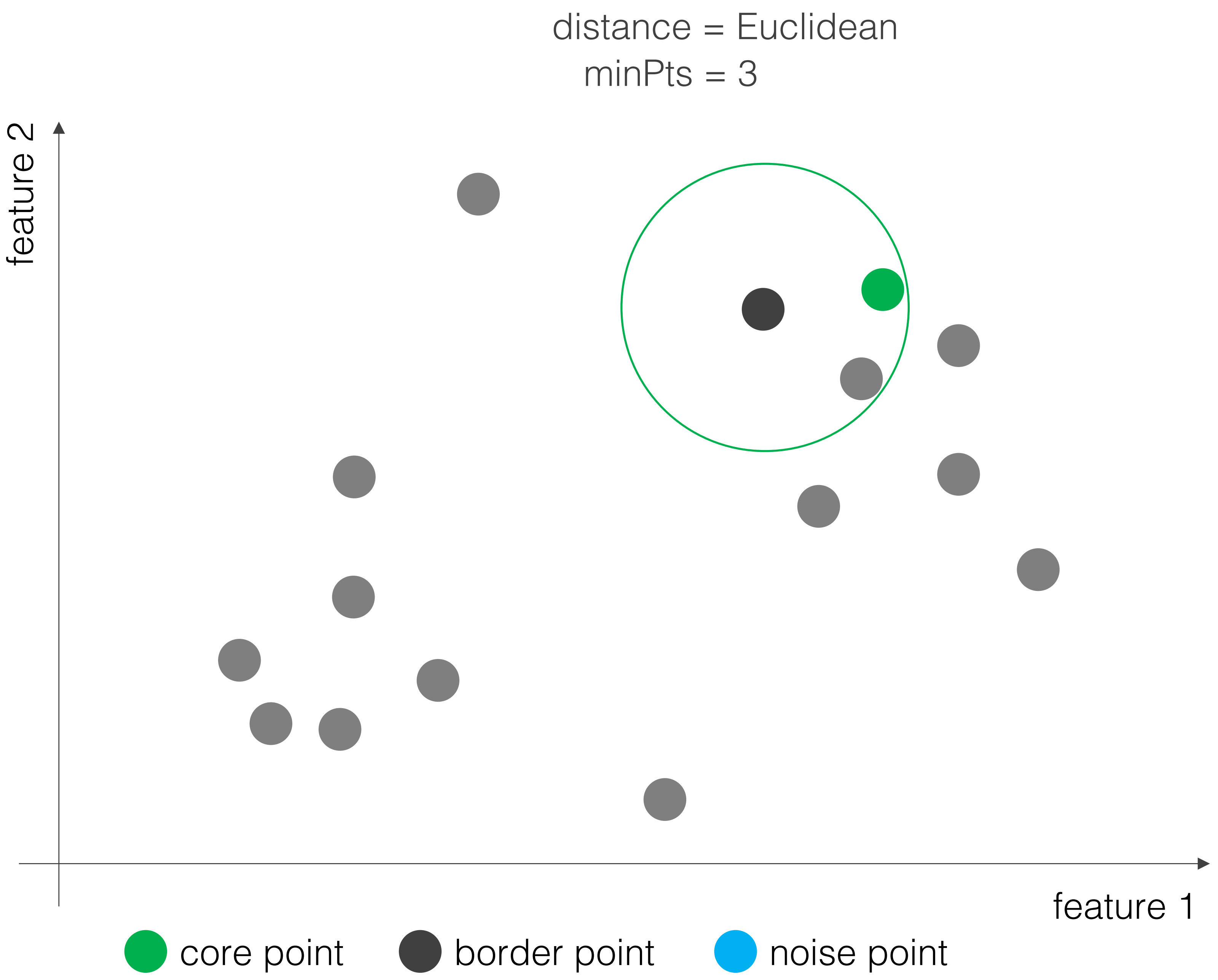

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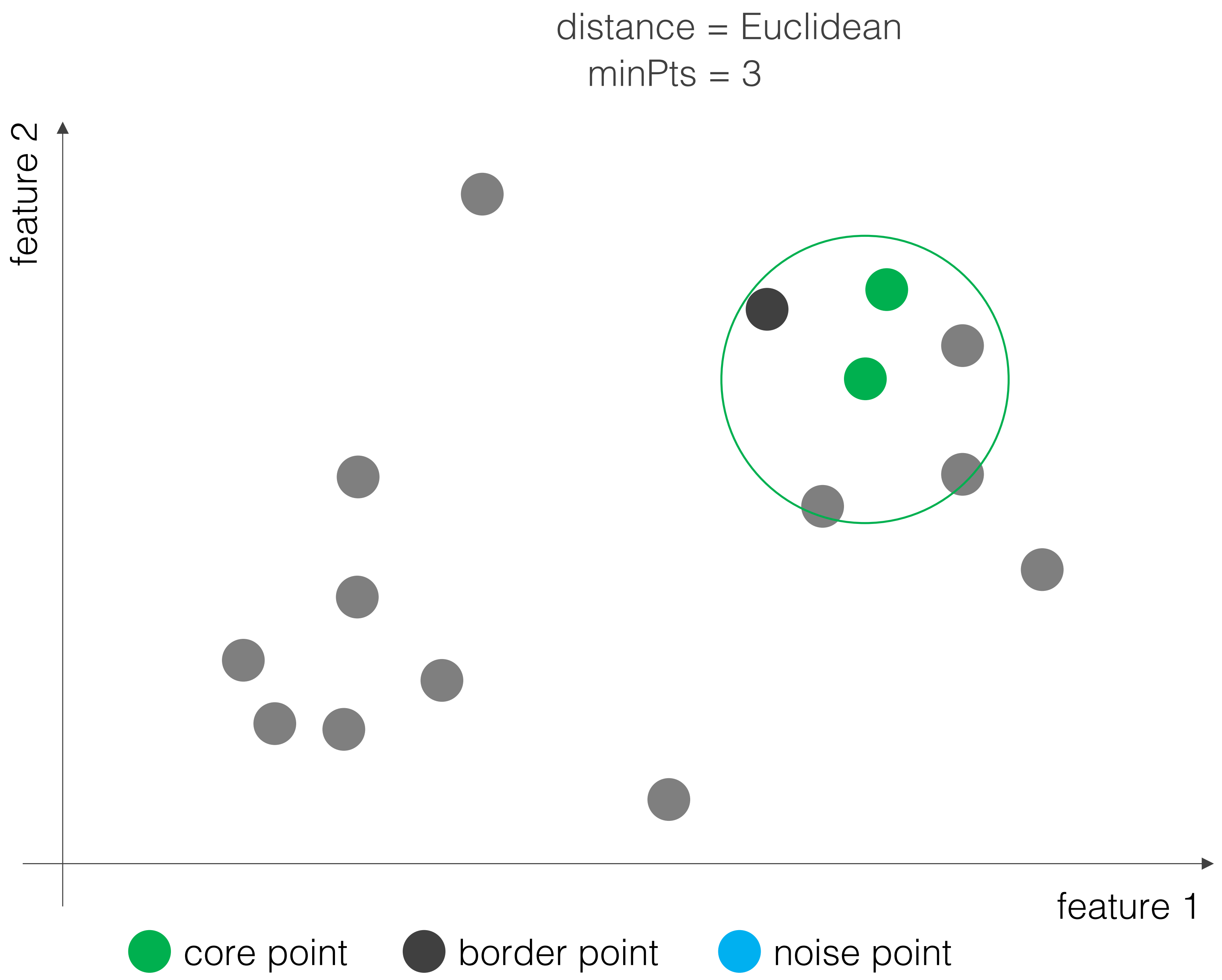

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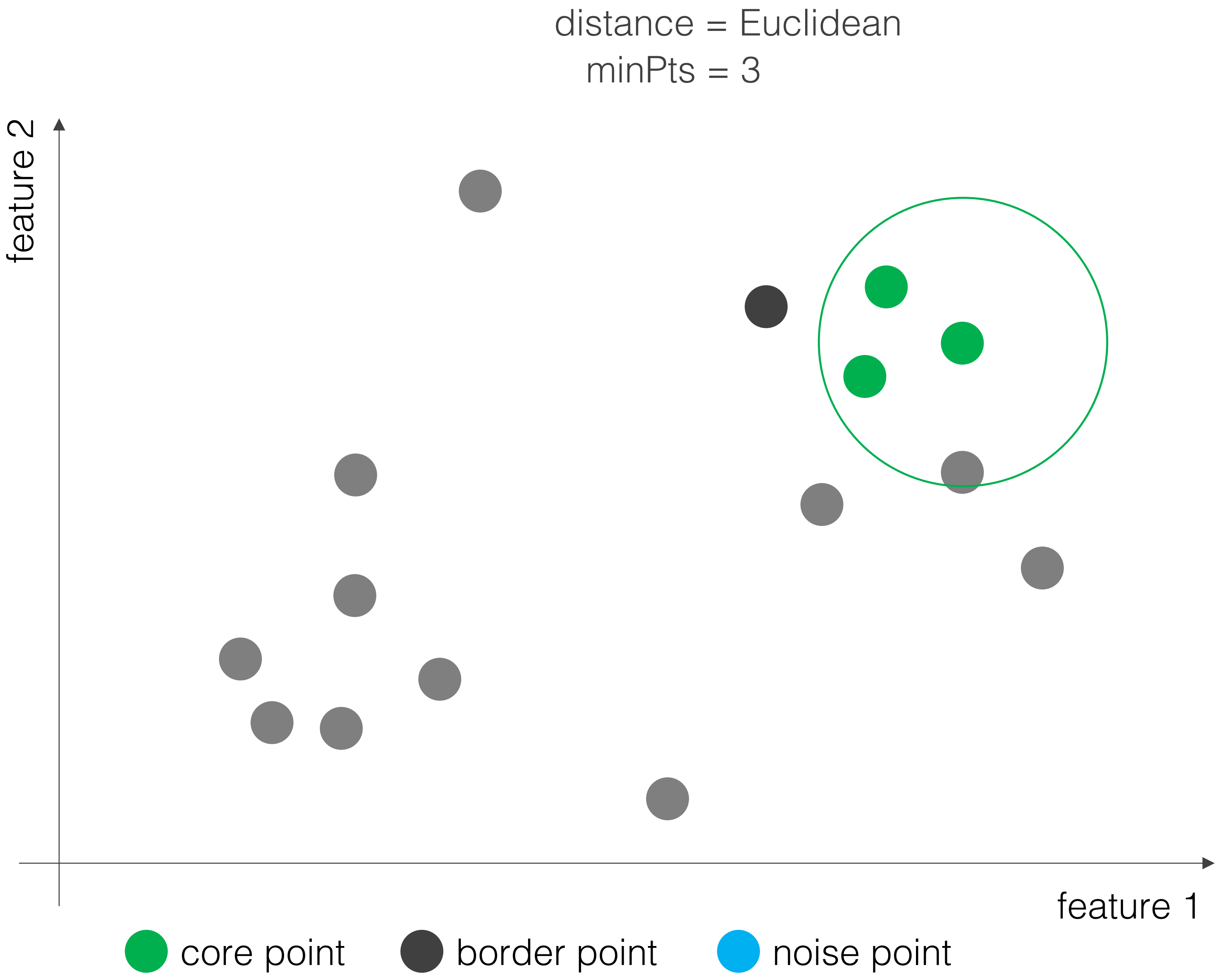

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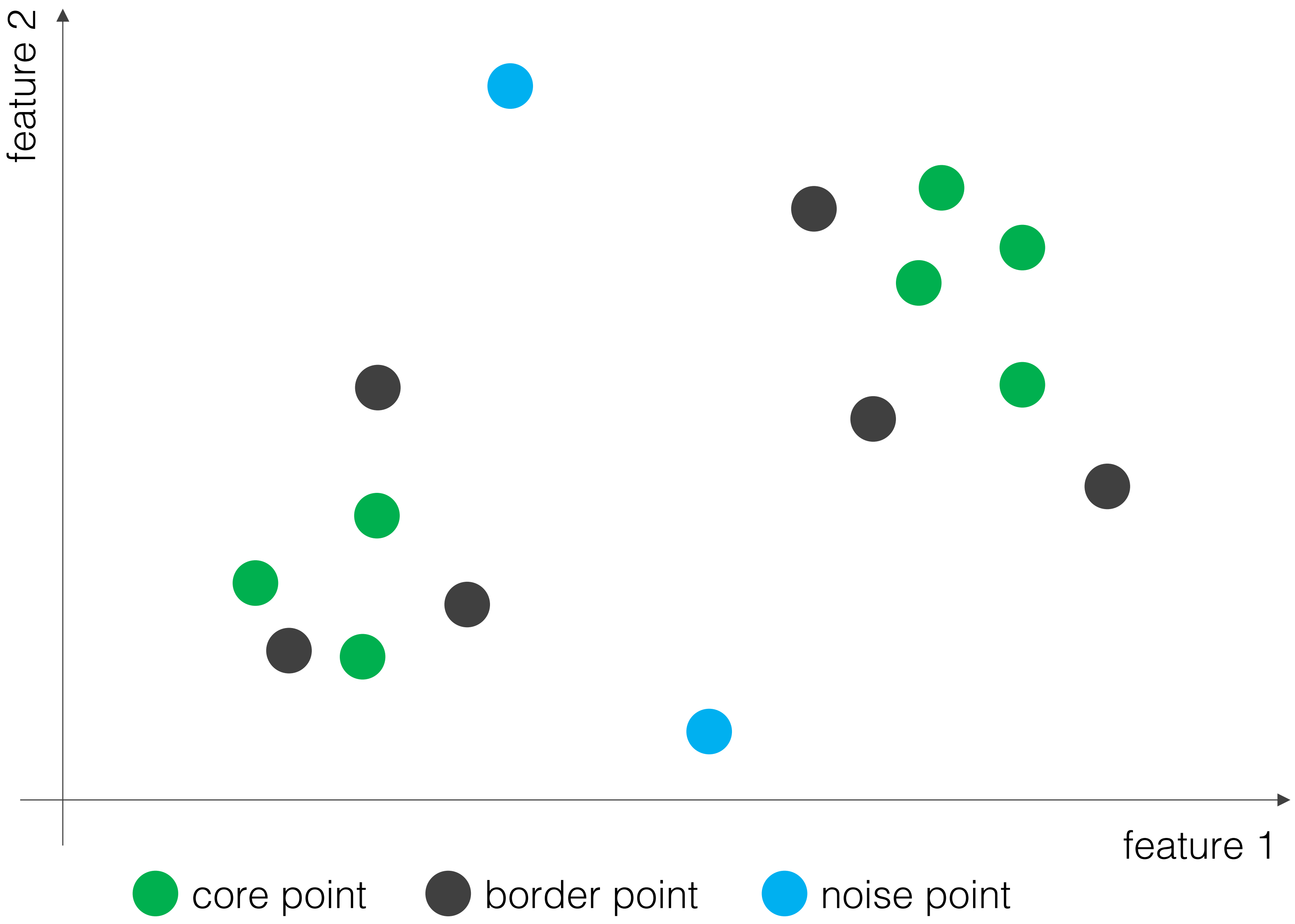

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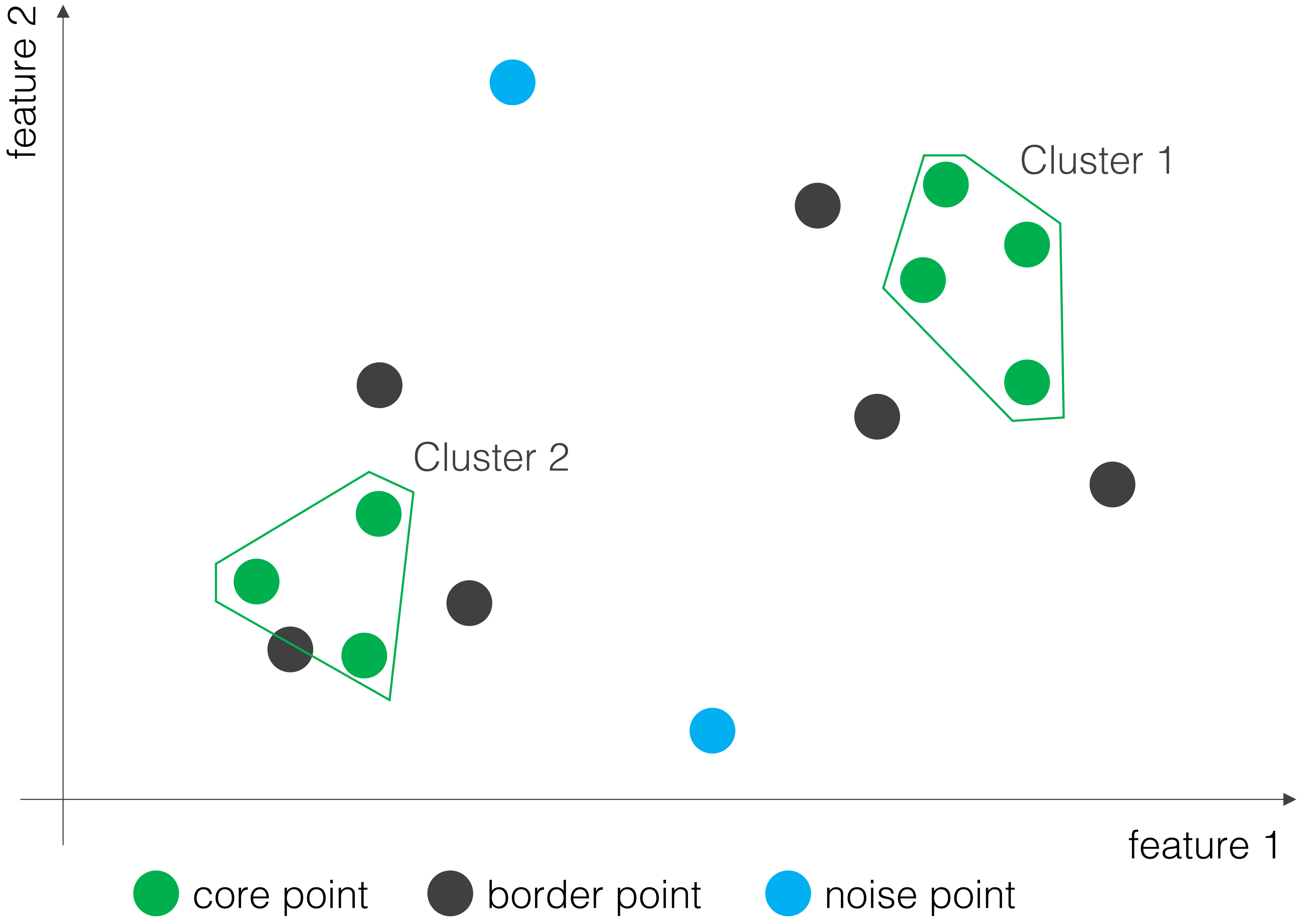

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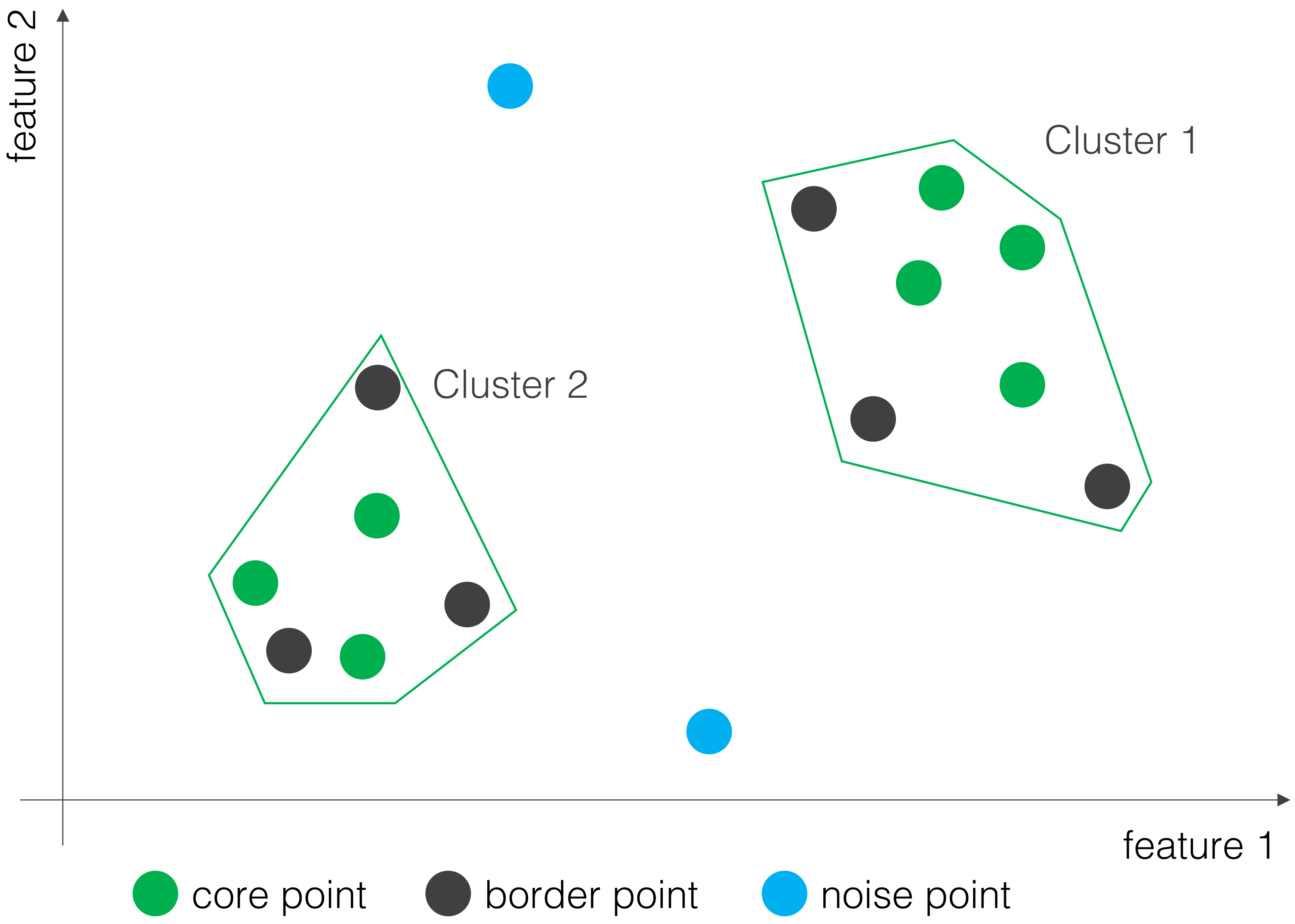


# DBSCAN

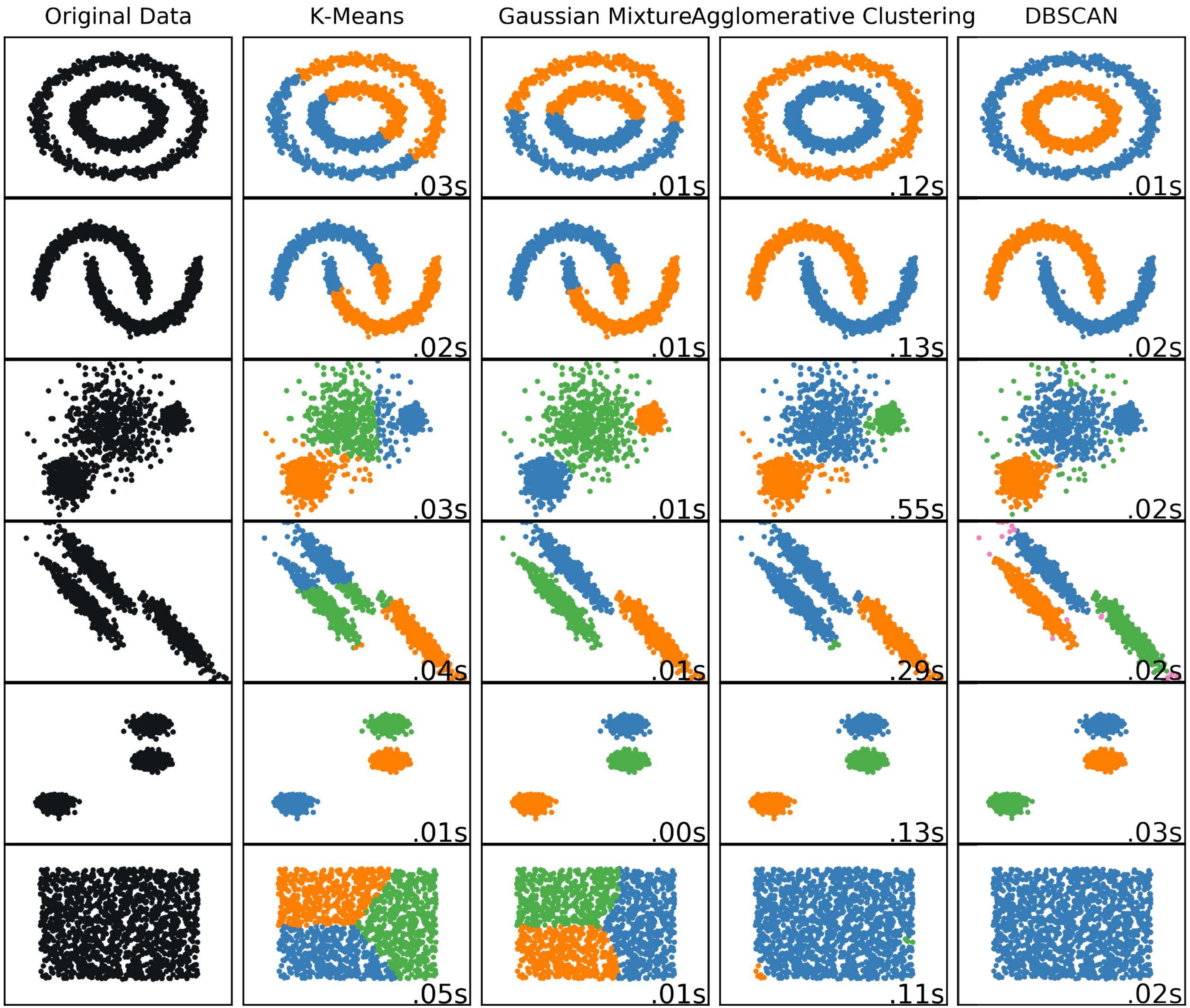
- The number of clusters is chosen as part of the algorithm
- Can find arbitrarily shaped clusters
- Robust to outliers

- Cannot handle significant variation in cluster density
- Not entirely deterministic (border points reachable from more than one cluster may be assigned to either)

# Examples: DBSCAN

Need to choose the density parameters

Does not require selecting the number of clusters beforehand



# Spectral Clustering

Graph-based clustering based on data similarity

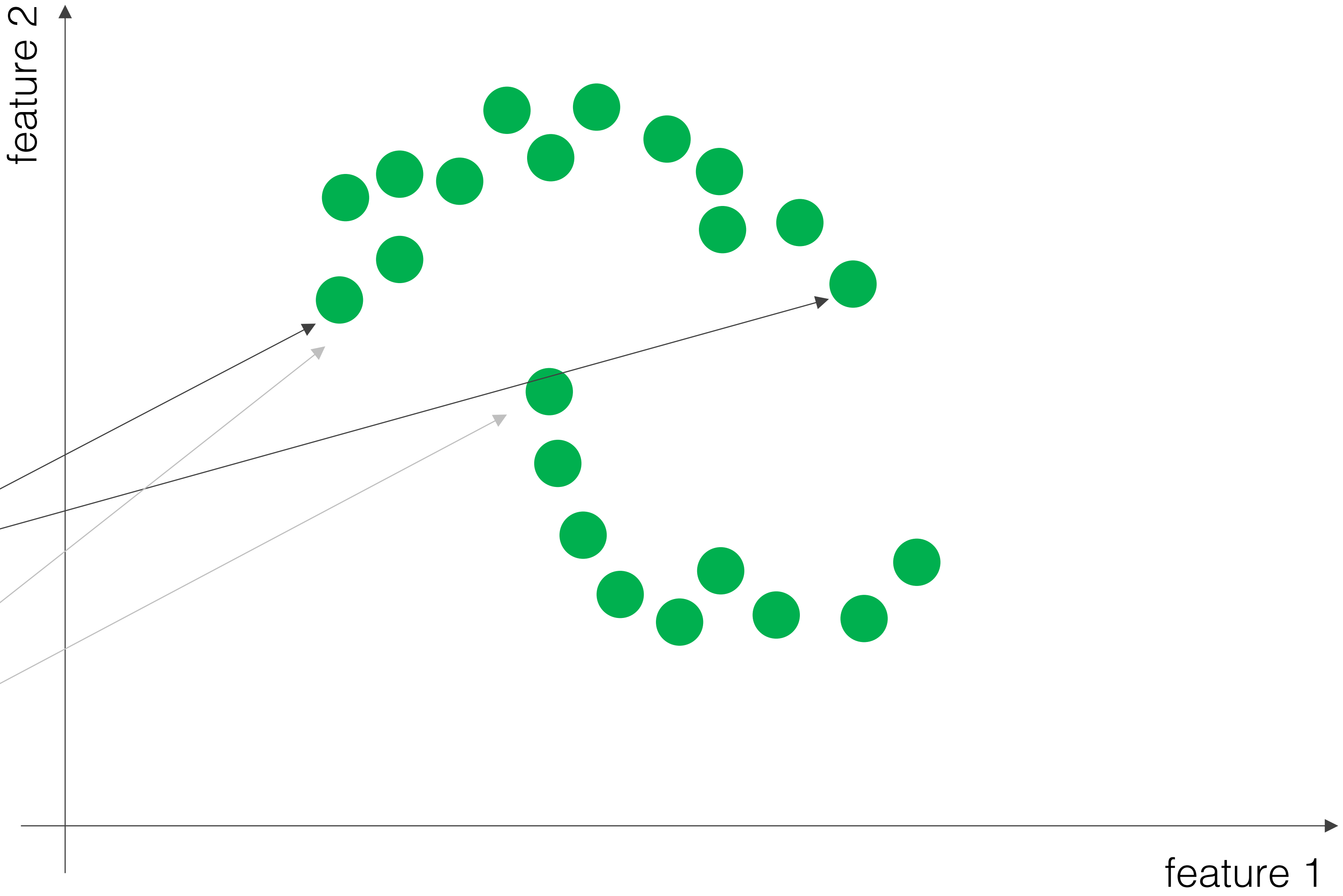
# Spectral Clustering

Focuses on **connectedness** instead of compactness

The location alone does not determine **similarity** or "**affinity**"

These two points are likely connected by a cluster

These two points are NOT likely connected by a cluster




Concept from Sebastian Thrun and Peter Norvig

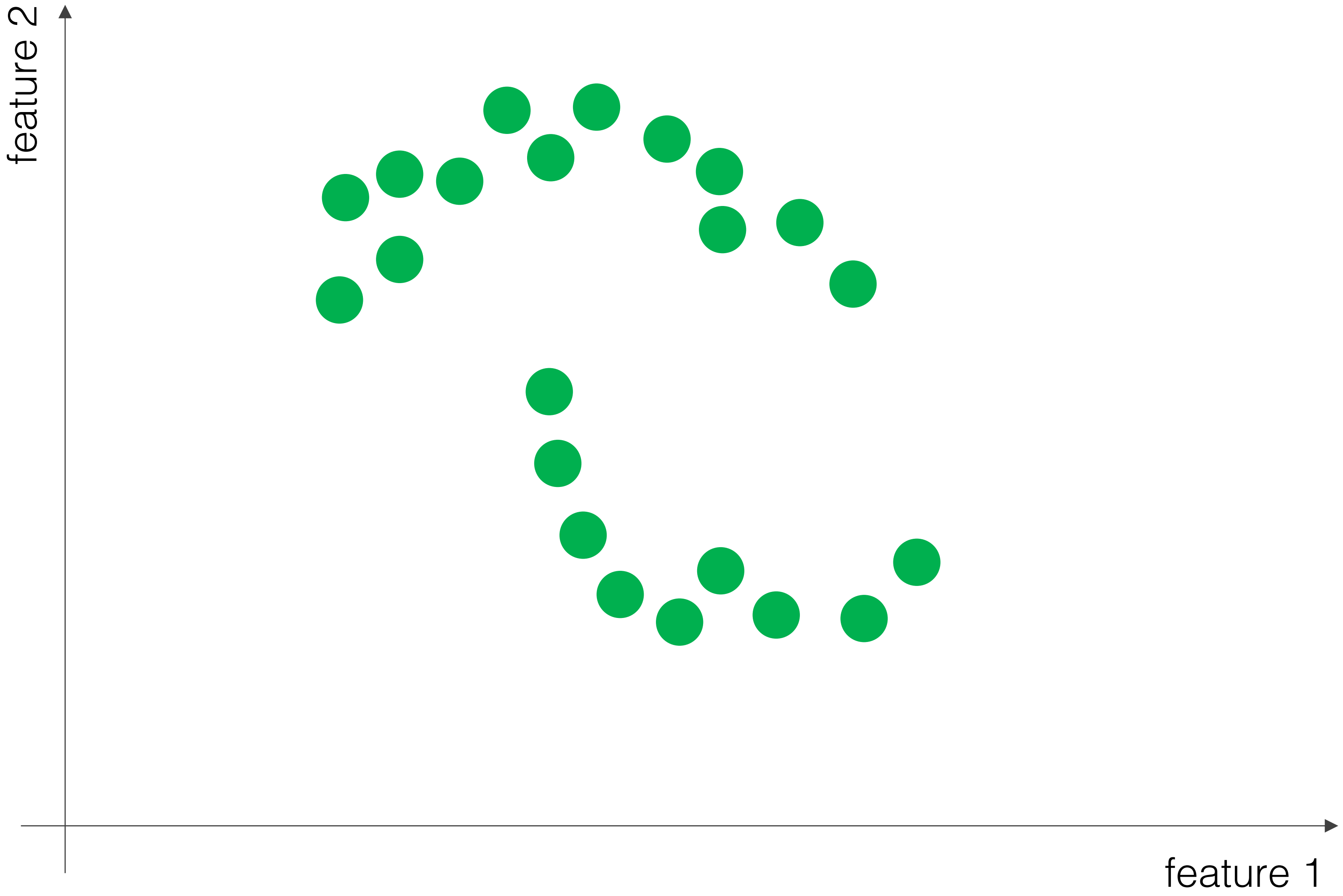
# Spectral Clustering

Define **similarity** or **affinity** as the opposite of distance:

$$A(\boldsymbol{a}, \boldsymbol{b}) = -d(\boldsymbol{a}, \boldsymbol{b})$$

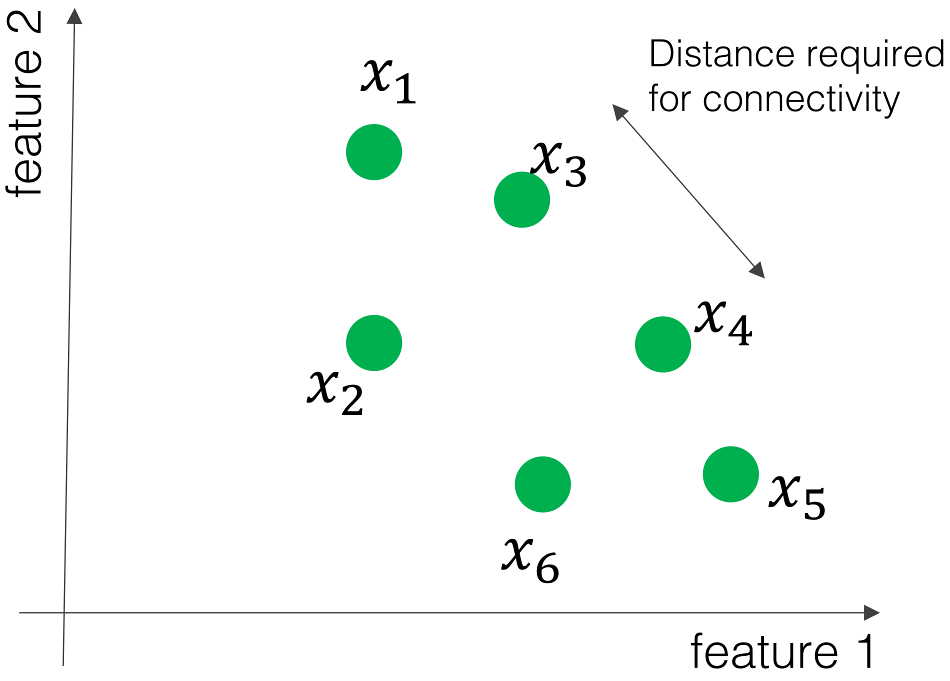
For example, using Euclidean distance, we could define affinity as:

$$A(\boldsymbol{a}, \boldsymbol{b}) = -\|\boldsymbol{a} - \boldsymbol{b}\|_2$$

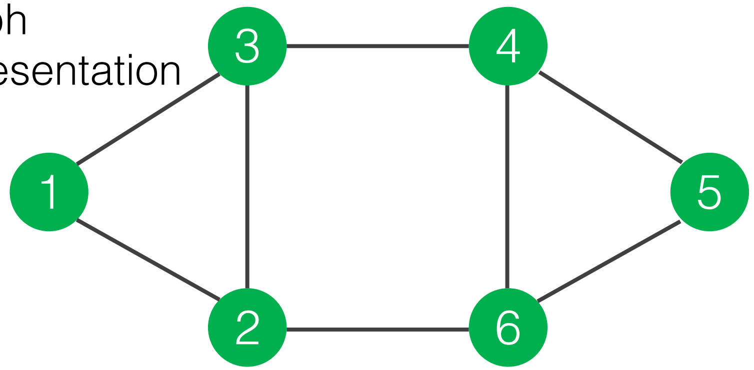



Concept from Sebastian Thrun and Peter Norvig

# Spectral Clustering




Graph representation




**Affinity Matrix (A)**

| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ |
|---|---|---|---|---|---|---|
| $x_1$ | 0 | 1 | 1 | 0 | 0 | 0 |
| $x_2$ | 1 | 0 | 1 | 0 | 0 | 1 |
| $x_3$ | 1 | 1 | 0 | 1 | 0 | 0 |
| $x_4$ | 0 | 0 | 1 | 0 | 1 | 1 |
| $x_5$ | 0 | 0 | 0 | 1 | 0 | 1 |
| $x_6$ | 0 | 1 | 0 | 1 | 1 | 0 |

If distance between points < threshold, consider there to be an “edge” connecting them in the graph

A vertex is not connected to itself

**Degree Matrix (D)**

| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ |
|---|---|---|---|---|---|---|
| $x_1$ | 2 | 0 | 0 | 0 | 0 | 0 |
| $x_2$ | 0 | 3 | 0 | 0 | 0 | 0 |
| $x_3$ | 0 | 0 | 3 | 0 | 0 | 0 |
| $x_4$ | 0 | 0 | 0 | 3 | 0 | 0 |
| $x_5$ | 0 | 0 | 0 | 0 | 3 | 0 |
| $x_6$ | 0 | 0 | 0 | 0 | 0 | 2 |

The sum of edges connected to each vertex

Concept from Sebastian Thrun and Peter Norvig

# Spectral Clustering

**Degree Matrix (D)**

| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ |
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**Affinity Matrix (A)**

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| $x_2$ | 1 | 0 | 1 | 0 | 0 | 1 |
| $x_3$ | 1 | 1 | 0 | 1 | 0 | 0 |
| $x_4$ | 0 | 0 | 1 | 0 | 1 | 1 |
| $x_5$ | 0 | 0 | 0 | 1 | 0 | 1 |
| $x_6$ | 0 | 1 | 0 | 1 | 1 | 0 |

**Graph Laplacian Matrix (L)**

| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ |
|---|---|---|---|---|---|---|
| $x_1$ | 2 | -1 | -1 | 0 | 0 | 0 |
| $x_2$ | -1 | 3 | -1 | 0 | 0 | -1 |
| $x_3$ | -1 | -1 | 3 | -1 | 0 | 0 |
| $x_4$ | 0 | 0 | -1 | 3 | -1 | -1 |
| $x_5$ | 0 | 0 | 0 | -1 | 3 | -1 |
| $x_6$ | 0 | -1 | 0 | -1 | -1 | 2 |

$$\mathbf{D} - \mathbf{A} = \mathbf{L}$$

# Spectral Clustering

**Graph Laplacian Matrix (L)**

| | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ |
|---|---|---|---|---|---|---|
| $x_1$ | 2 | -1 | -1 | 0 | 0 | 0 |
| $x_2$ | -1 | 3 | -1 | 0 | 0 | -1 |
| $x_3$ | -1 | -1 | 3 | -1 | 0 | 0 |
| $x_4$ | 0 | 0 | -1 | 3 | -1 | -1 |
| $x_5$ | 0 | 0 | 0 | -1 | 3 | -1 |
| $x_6$ | 0 | -1 | 0 | -1 | -1 | 2 |

**L**

**Eigenvectors of L**

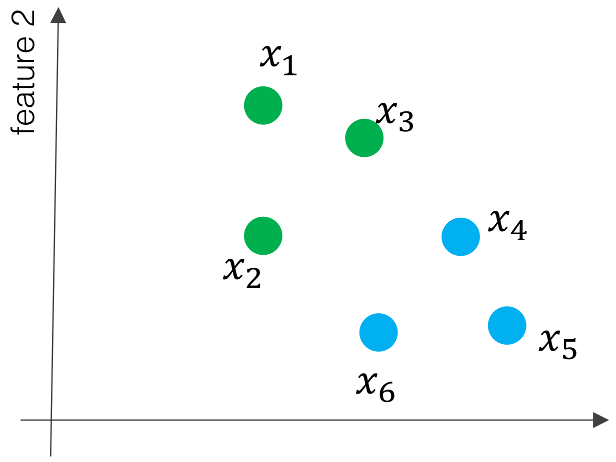
| $\mathbf{u}_1$ | $\mathbf{u}_2$ | $\mathbf{u}_3$ | $\mathbf{u}_4$ | $\mathbf{u}_5$ | $\mathbf{u}_6$ |
|---|---|---|---|---|---|
| 0.4 | 0.6 | 0.0 | 0.6 | 0.3 | 0.0 |
| 0.4 | 0.3 | 0.4 | -0.4 | -0.5 | 0.5 |
| 0.4 | 0.3 | -0.4 | -0.4 | -0.1 | -0.6 |
| 0.4 | -0.3 | -0.5 | -0.1 | 0.3 | 0.6 |
| 0.3 | -0.4 | -0.2 | 0.5 | -0.6 | -0.1 |
| 0.5 | -0.5 | 0.5 | -0.1 | 0.4 | -0.3 |

$\lambda_i =$

| | | | | | |
|---|---|---|---|---|---|
| -0.1 | 1.0 | 2.7 | 3.3 | 4.1 | 4.8 |

**Eigenvalues of L**

| | $\mathbf{u}_2$ |
|---|---|
| $x_1$ | **0.6** |
| $x_2$ | **0.3** |
| $x_3$ | **0.3** |
| $x_4$ | **-0.3** |
| $x_5$ | **-0.4** |
| $x_6$ | **-0.5** |

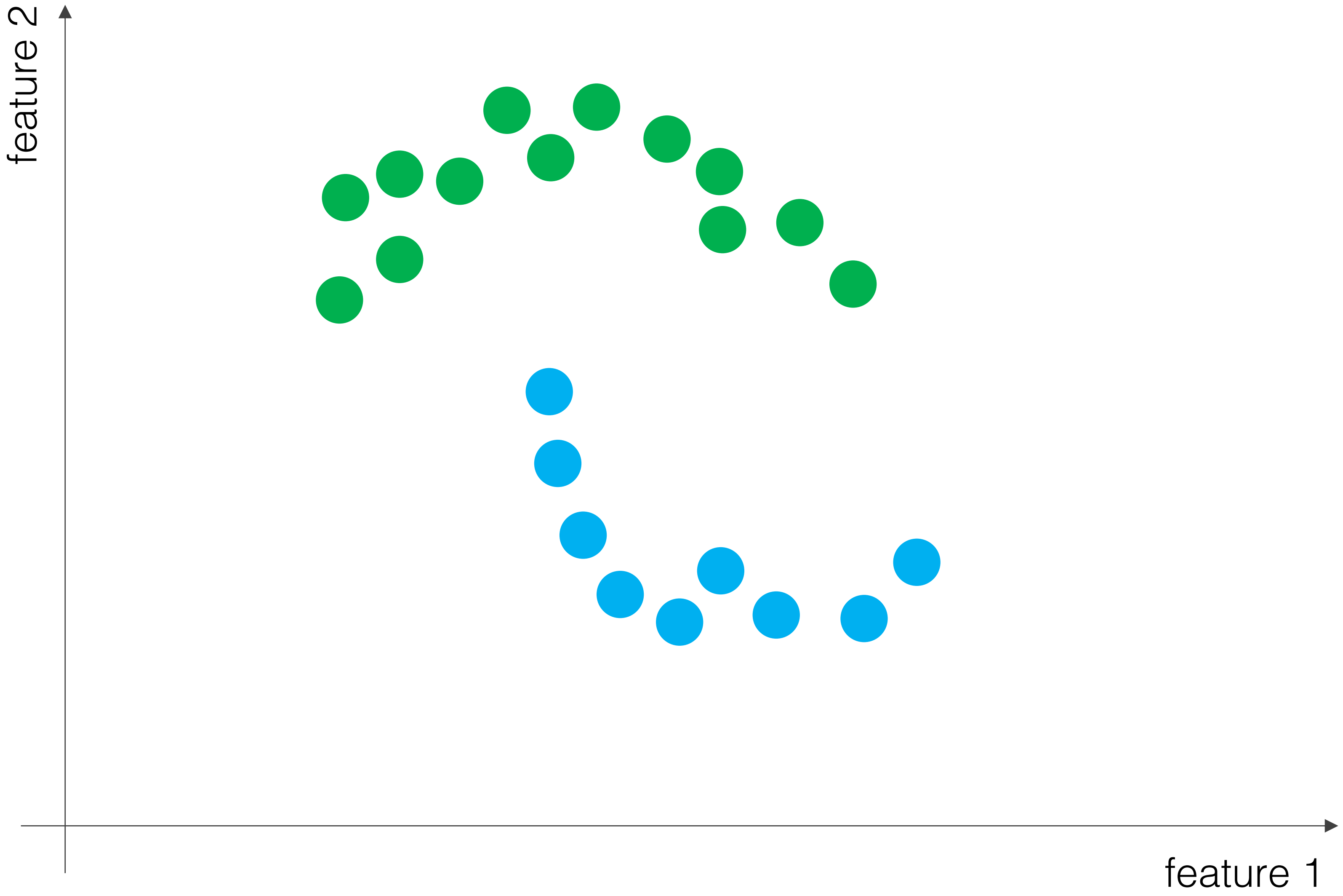



Get the eigenvectors of the Laplacian matrix, cluster points based on the eigenvectors (typically using k-means)

# Spectral Clustering

**Algorithm**

1. Construct a graph representation of your data
2. Perform clustering based on the eigenvalues of the Laplacian matrix (often with K-means)



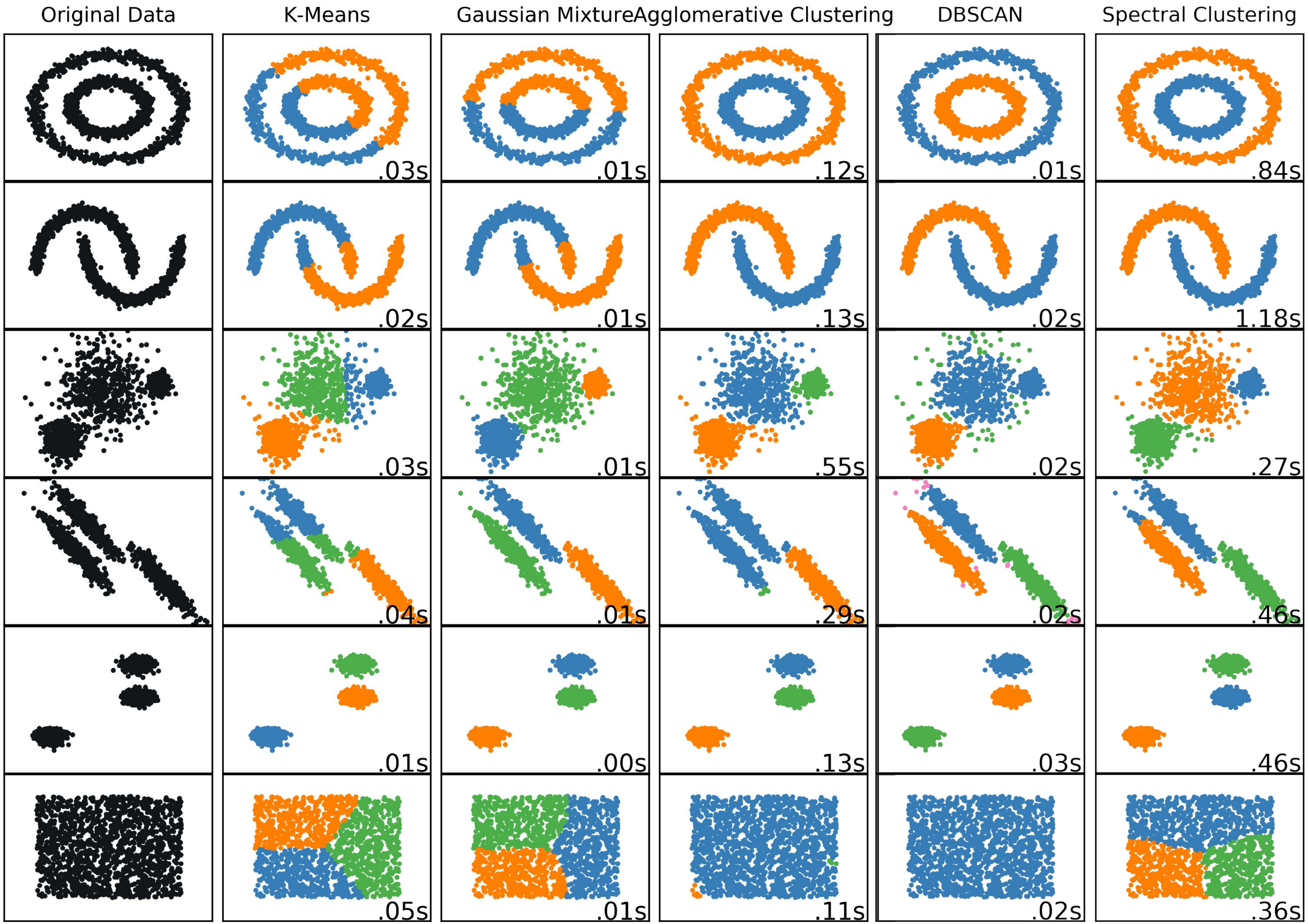

Concept from Sebastian Thrun and Peter Norvig

# Examples: Spectral Clustering

Makes few assumptions about data, so often produces good clustering results

Slow for large datasets

Requires specifying number of clusters



# Types of clustering algorithms

## Methods

Centroid-based clustering (e.g. **K-Means**)
Distribution-based clustering (e.g. **Gaussian mixture model**)
Density-based clustering (e.g. **DBSCAN**)
Hierarchical clustering (e.g. **agglomerative clustering**)
Graph-based clustering (e.g. **spectral clustering**)

## Cluster assignment

**Hard clustering**
**Soft clustering** (a.k.a. fuzzy clustering)

# Clustering choices:

1. How should the data be scaled?

2. How many clusters to estimate?

3. How do we measure dissimilarity?

4. How do we evaluate “fit” of the clusters?

Image from James et al., Introduction to Statistical Learning, 2013