Clustering

Cynthia Rudin

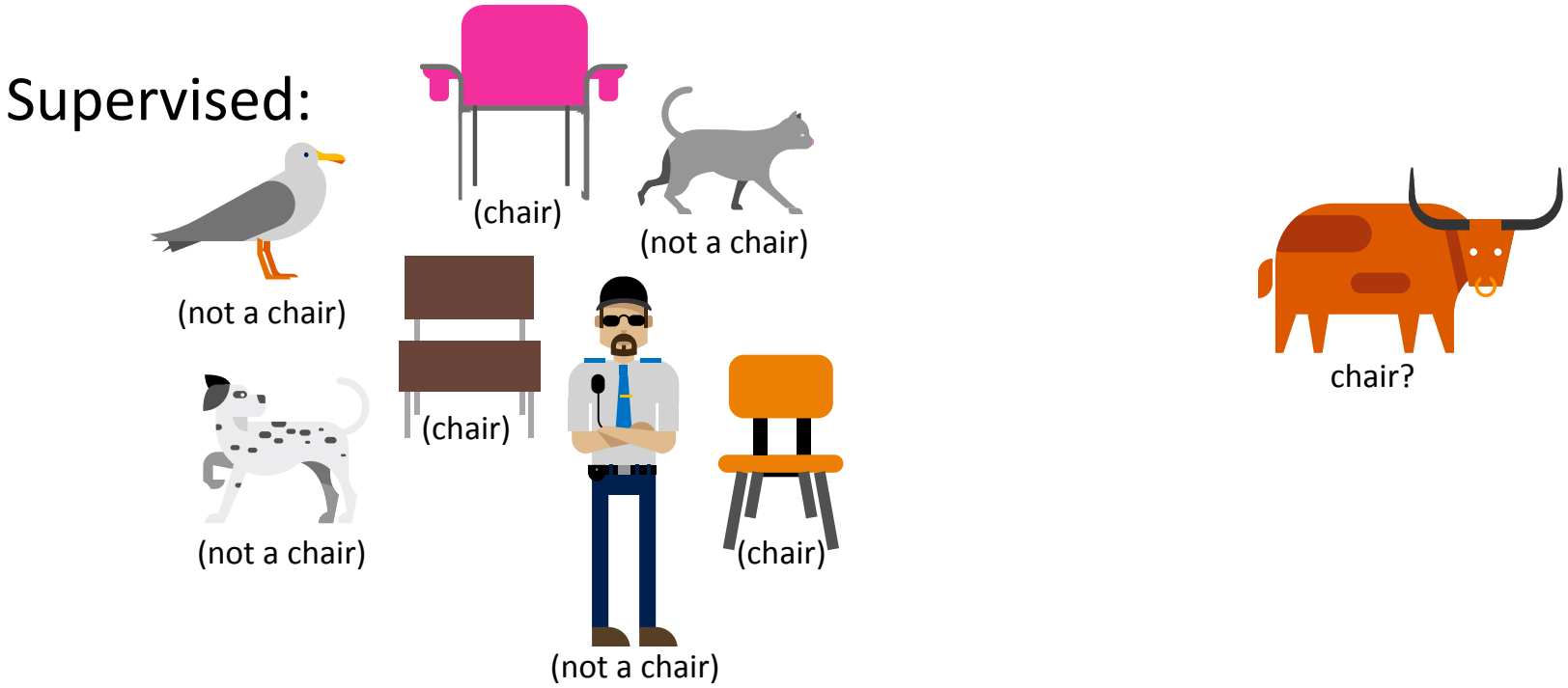
Duke Machine Learning

Clustering

- K-Means clustering algorithm and examples
- K-Means derivation
- Hierarchical agglomerative clustering algorithm and examples
- Comparison

Unsupervised Learning

- "Unsupervised" means that the training data has no ground truth labels to learn from.



Unsupervised Learning

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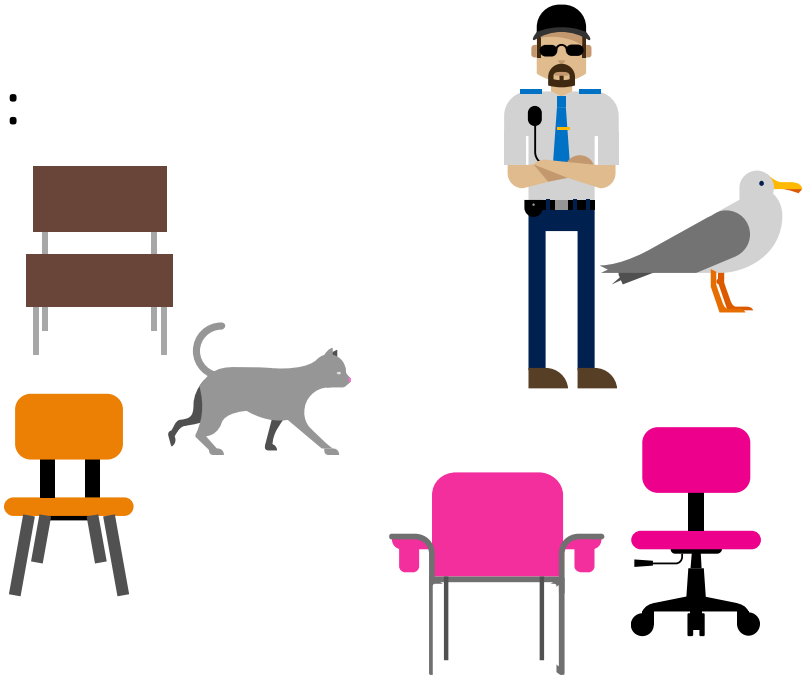

Unsupervised Learning

- “Unsupervised” means that the training data has no ground truth labels to learn from.

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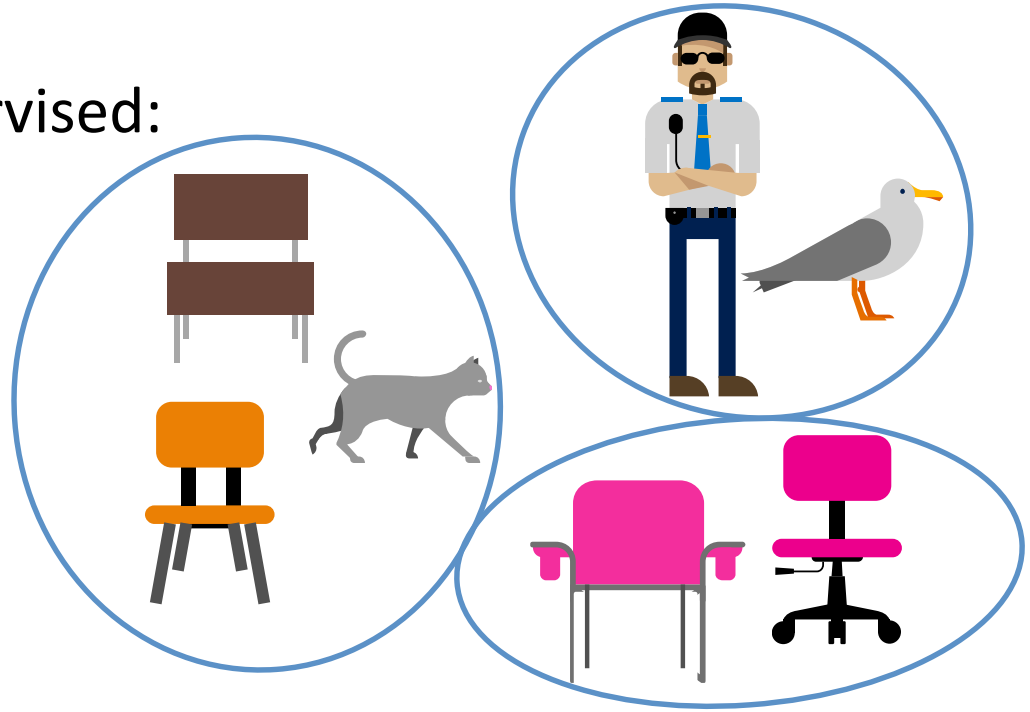
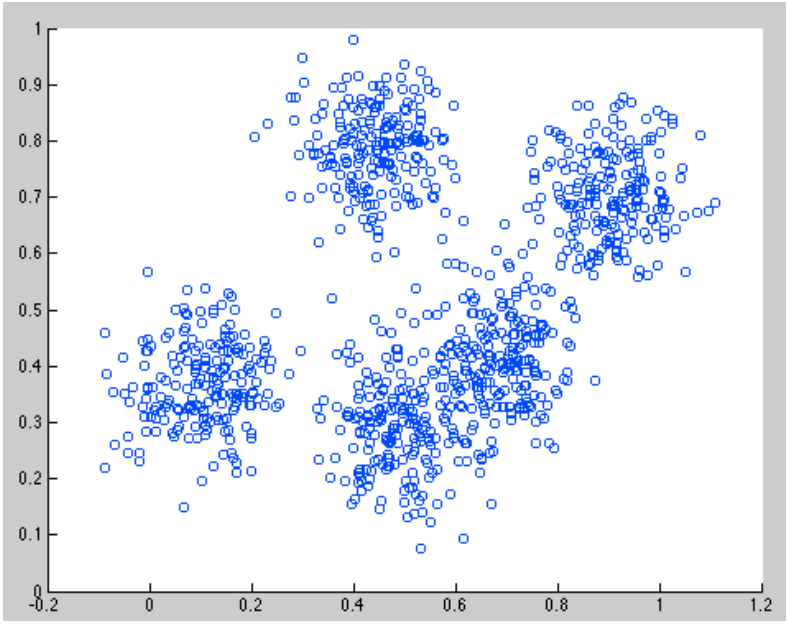


Unsupervised Learning

- “Unsupervised” means that the training data has no ground truth labels to learn from.
- Clustering is an key unsupervised problem.

Clustering

- Data within a cluster should be similar to other members of the cluster.



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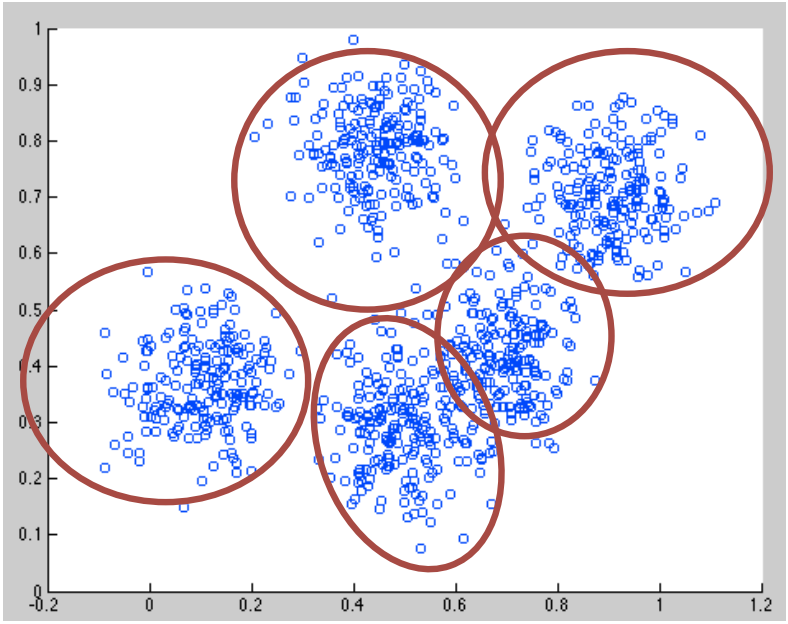

Clustering

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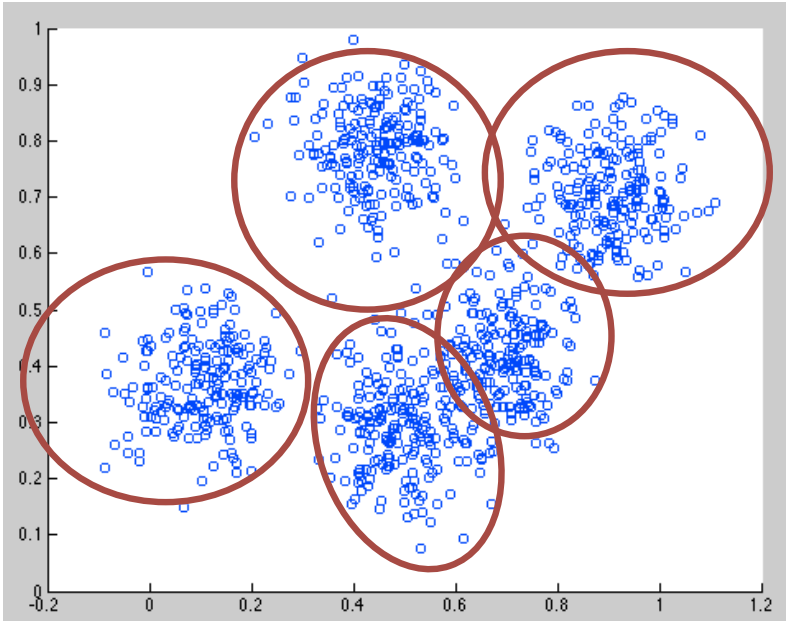
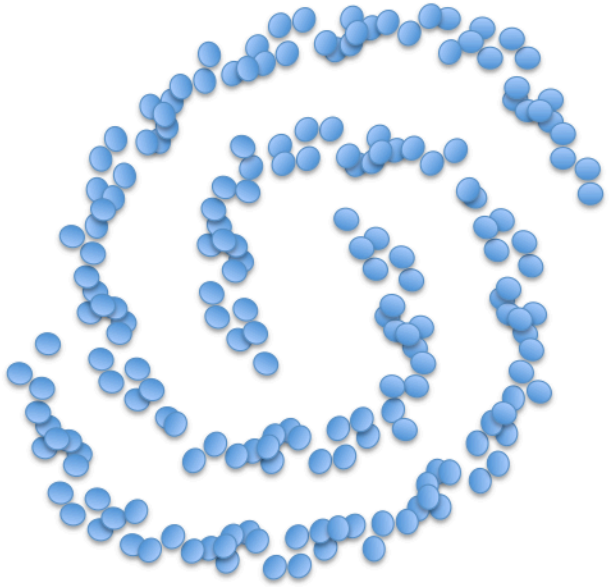




Clustering

Applications include:

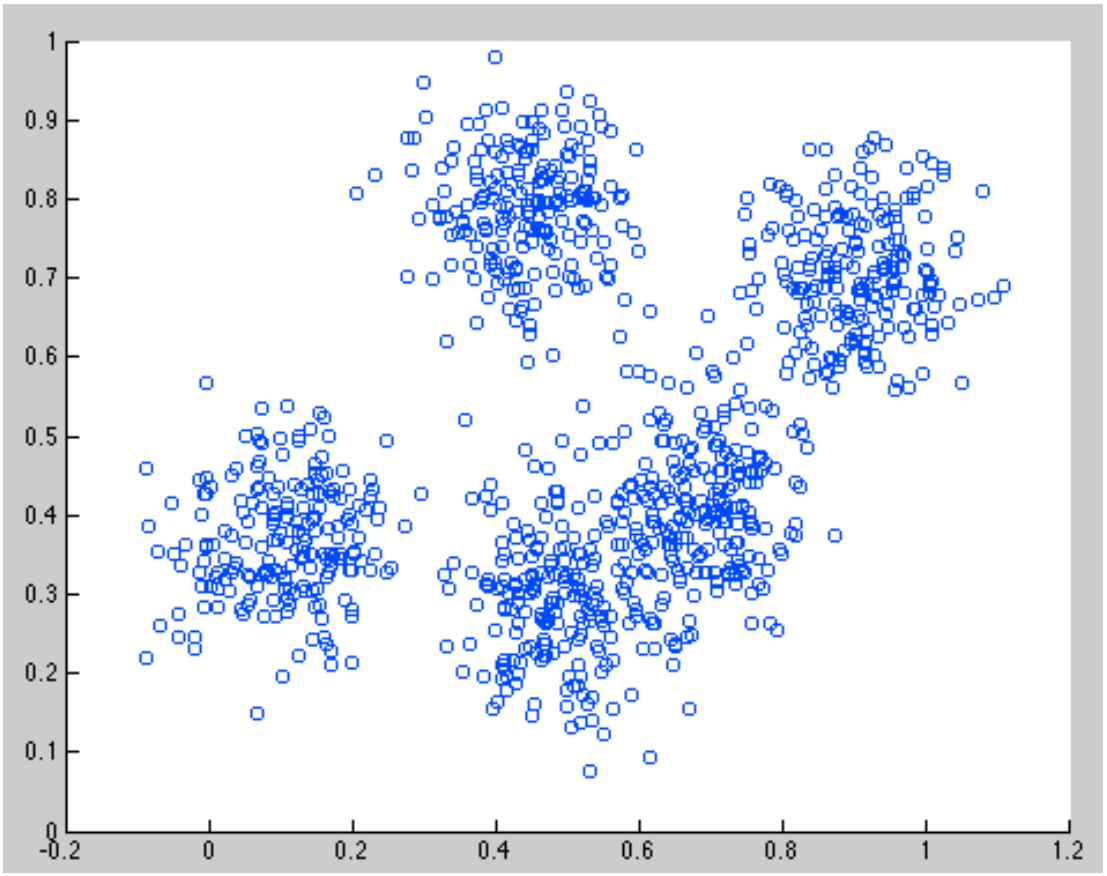
- Automatically grouping documents/webpages into topics
  - For instance, grouping news stories from today into categories
- Clustering large number of products
  - E.g., etsy products
- Clustering customers into those with similar purchase behavior

K-Means Clustering

Clustering

- K-means clustering
  - Input number of clusters, randomly initialize centers
  - Assign all points to the closest cluster center
  - Change cluster centers to be in the middle of its points
  - Repeat until convergence

K-Means in action



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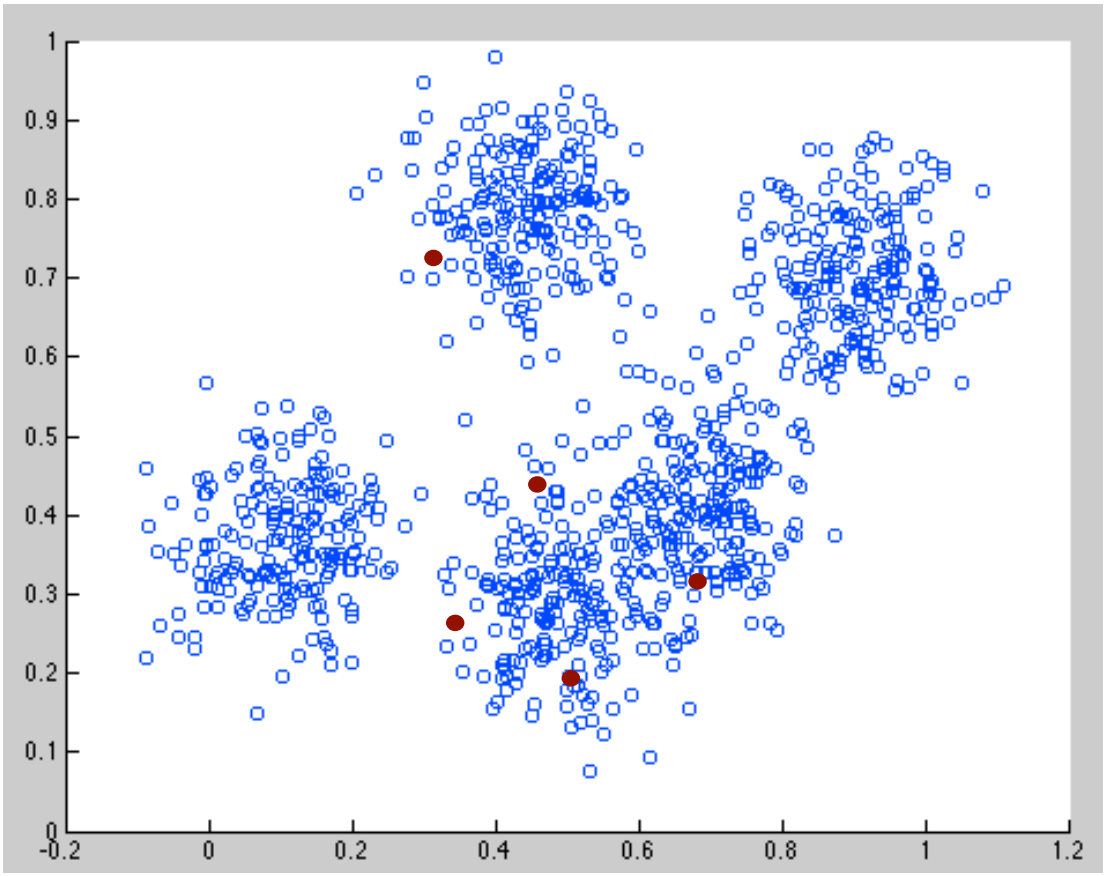

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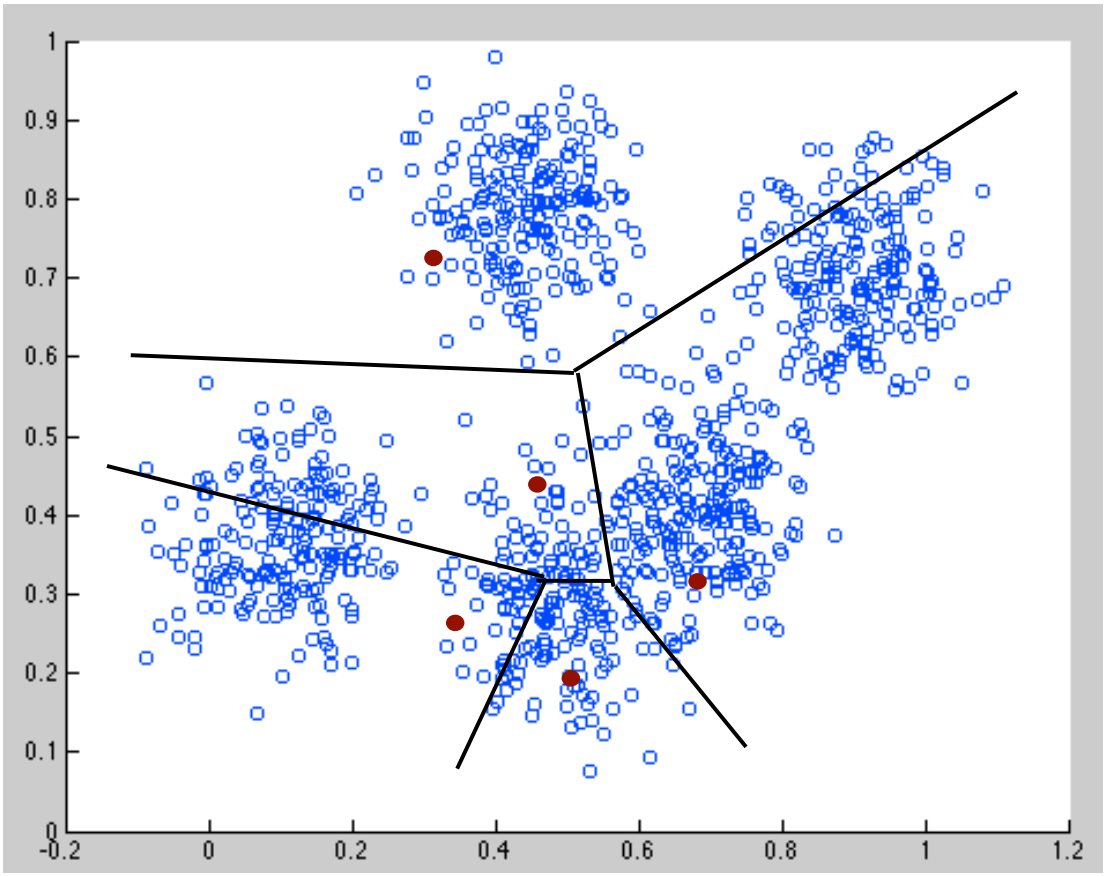

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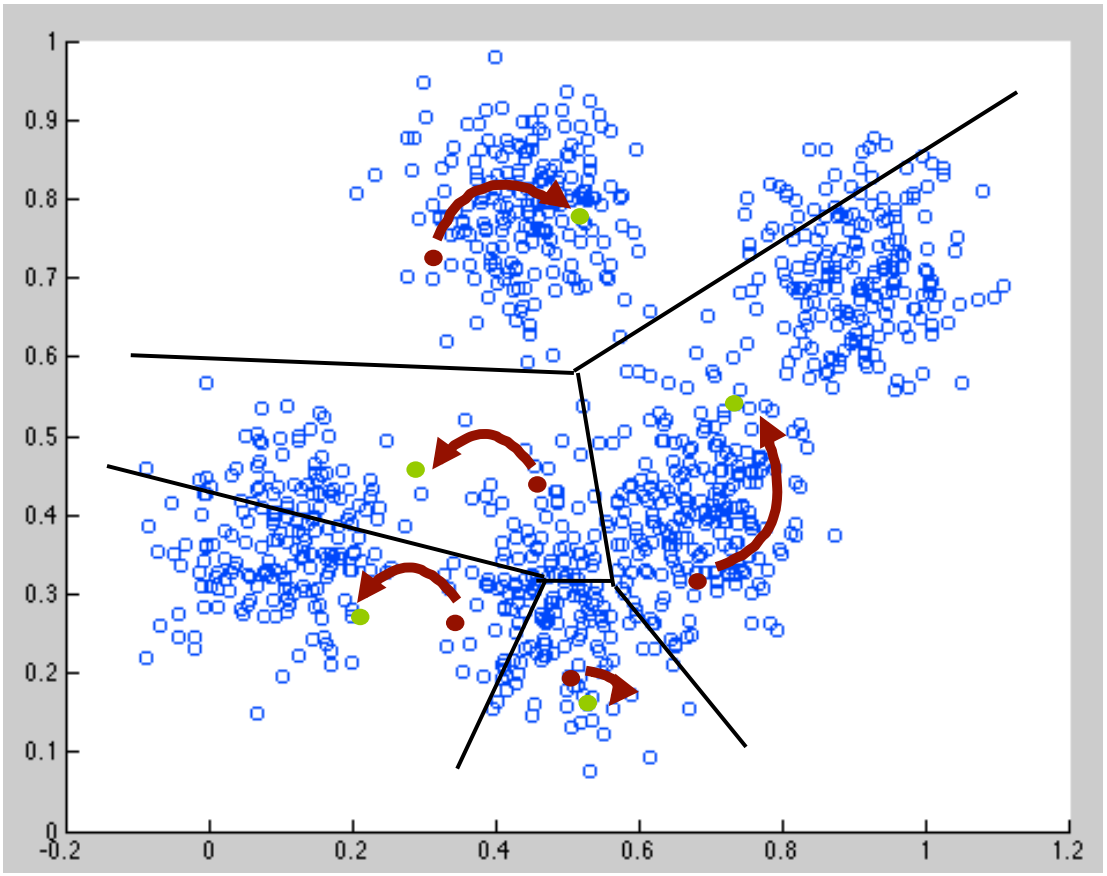

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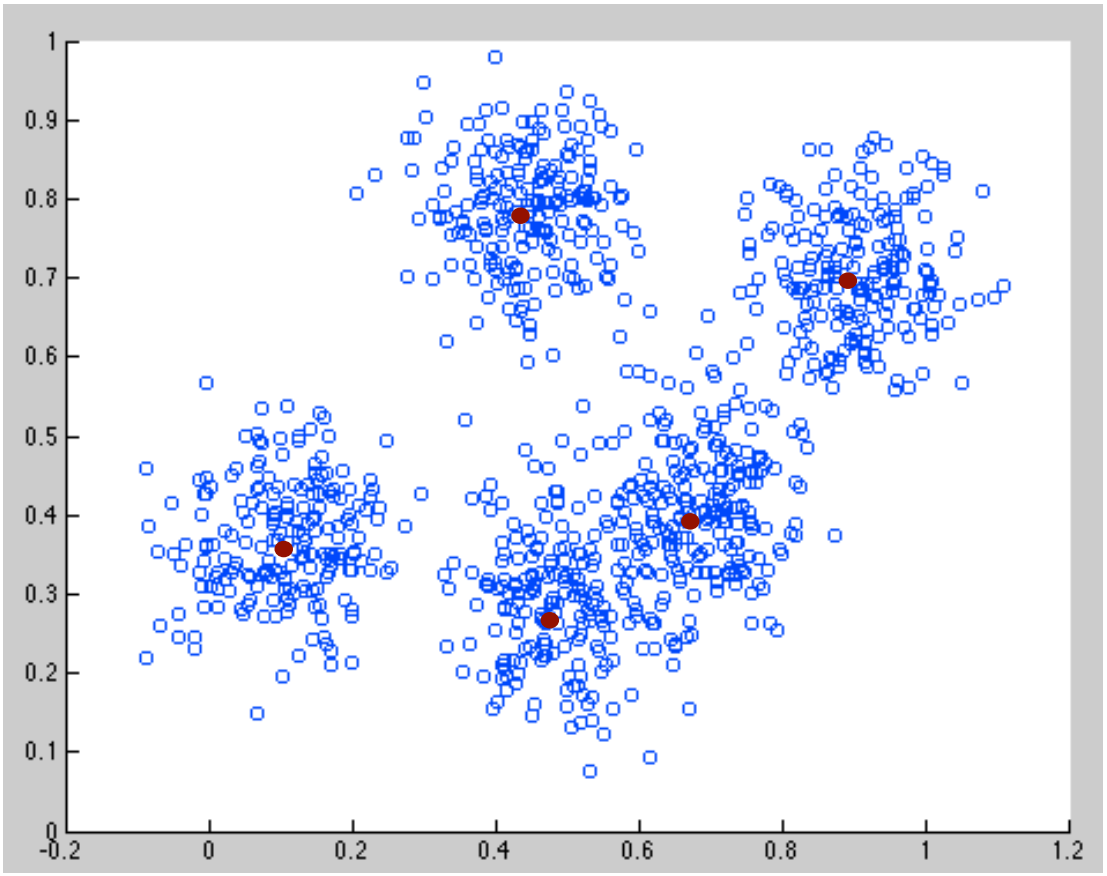

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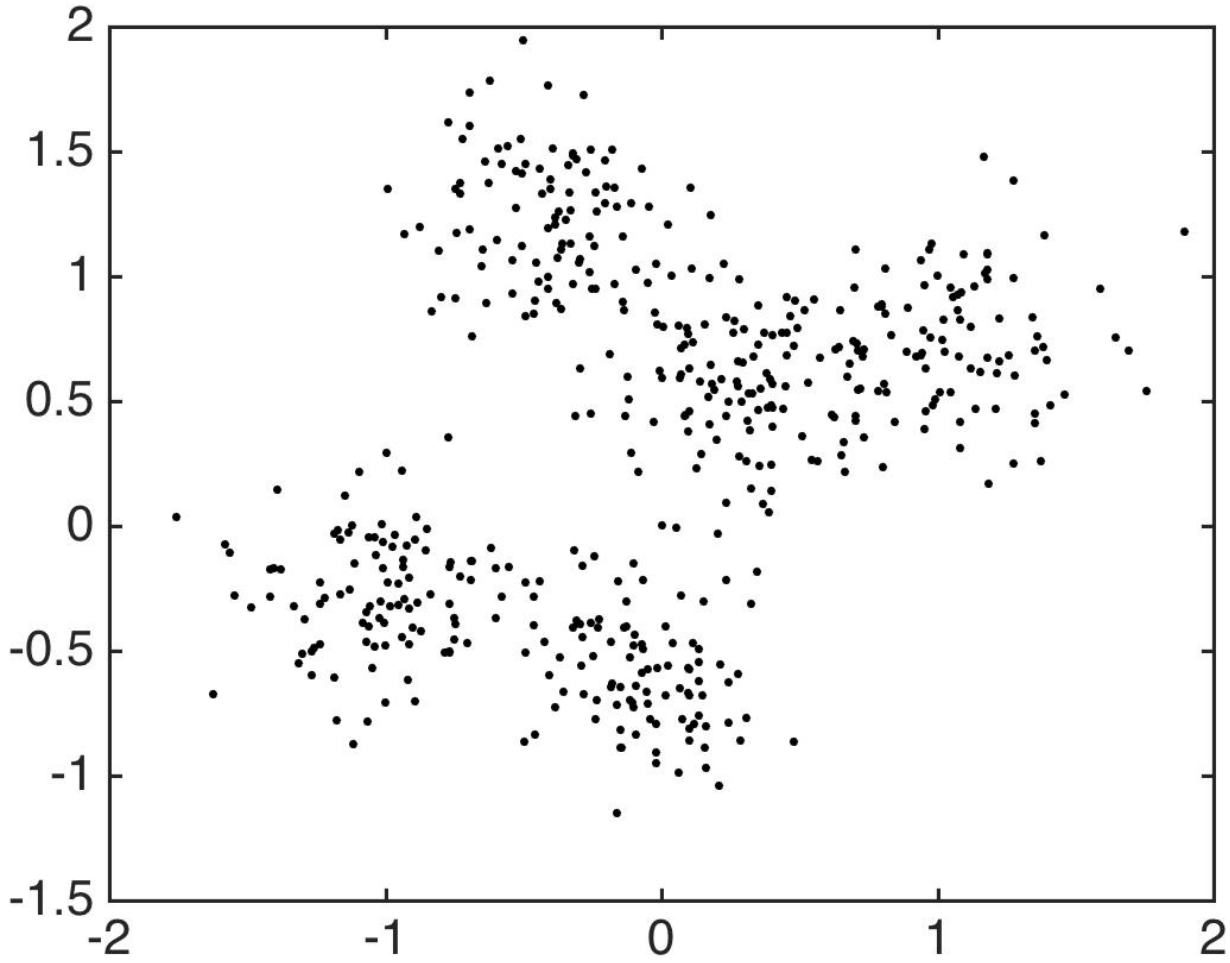
Ready to see it?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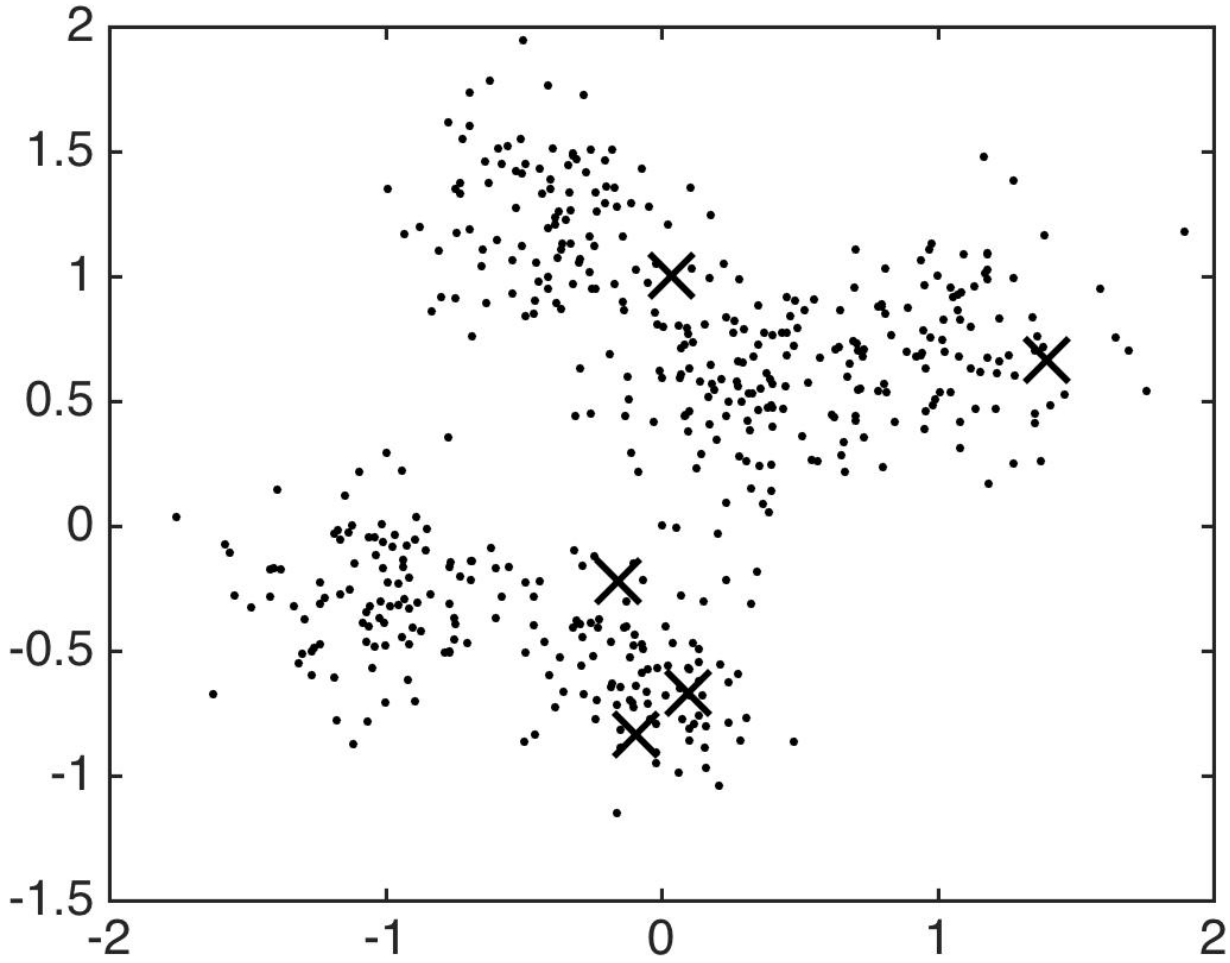
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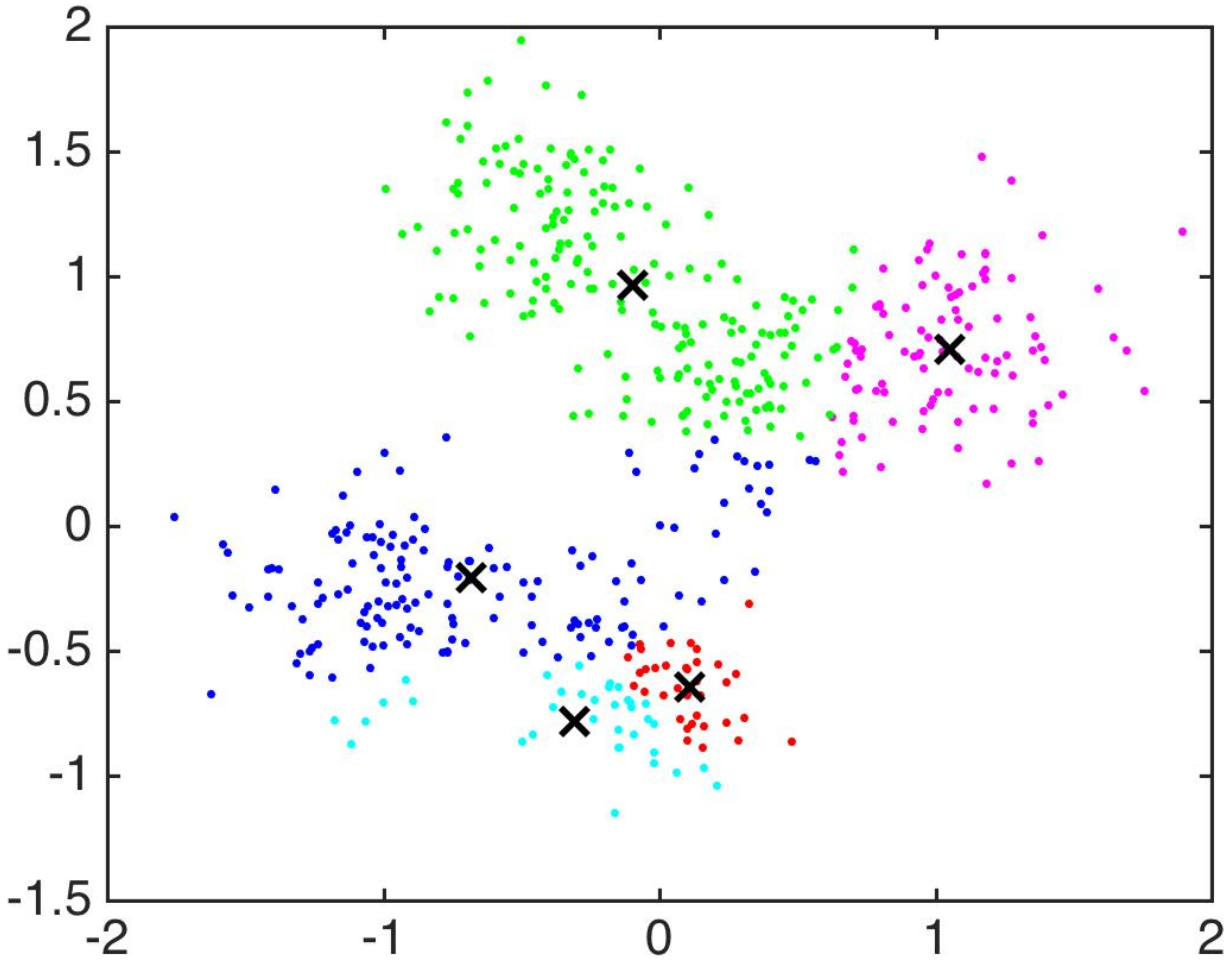
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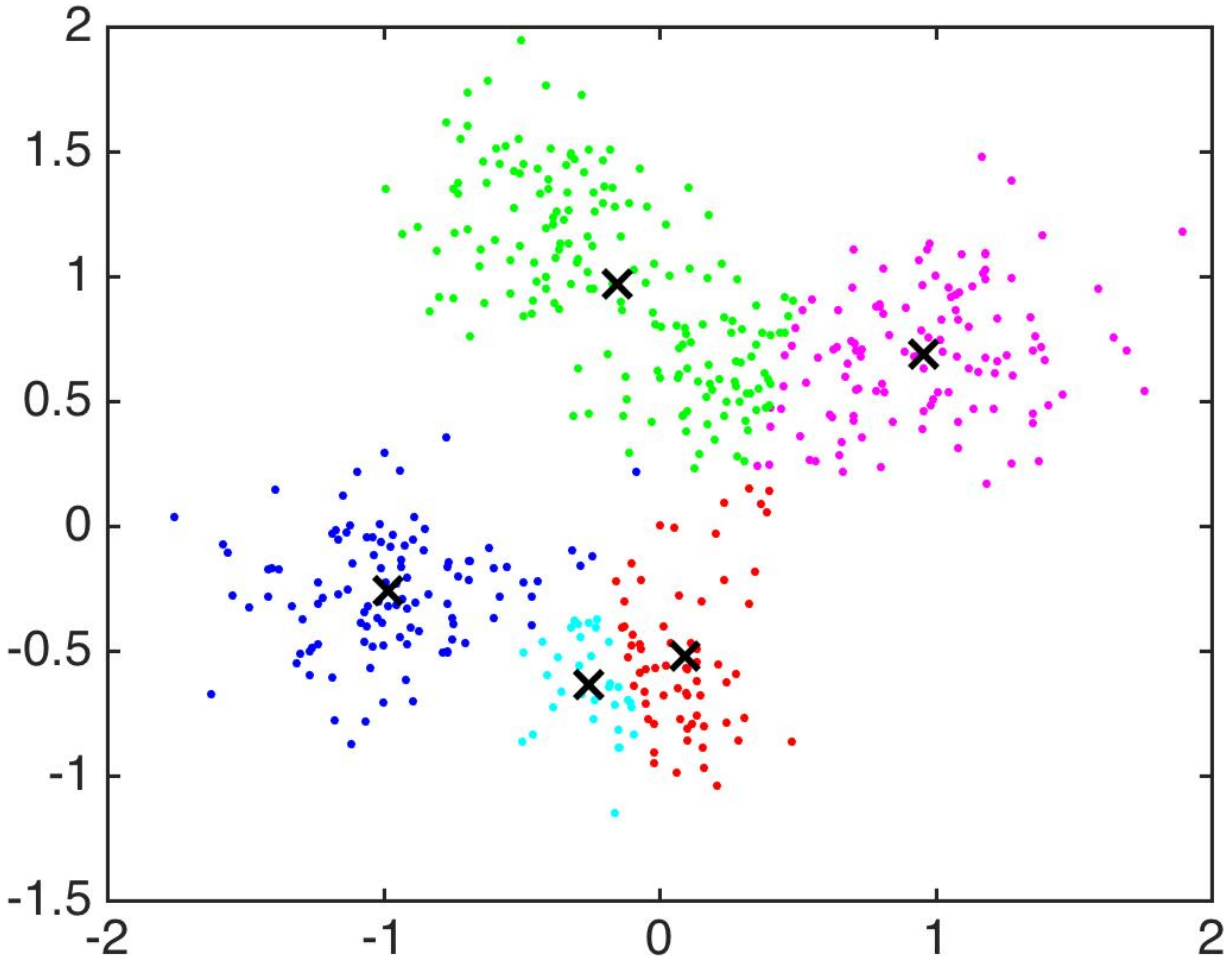
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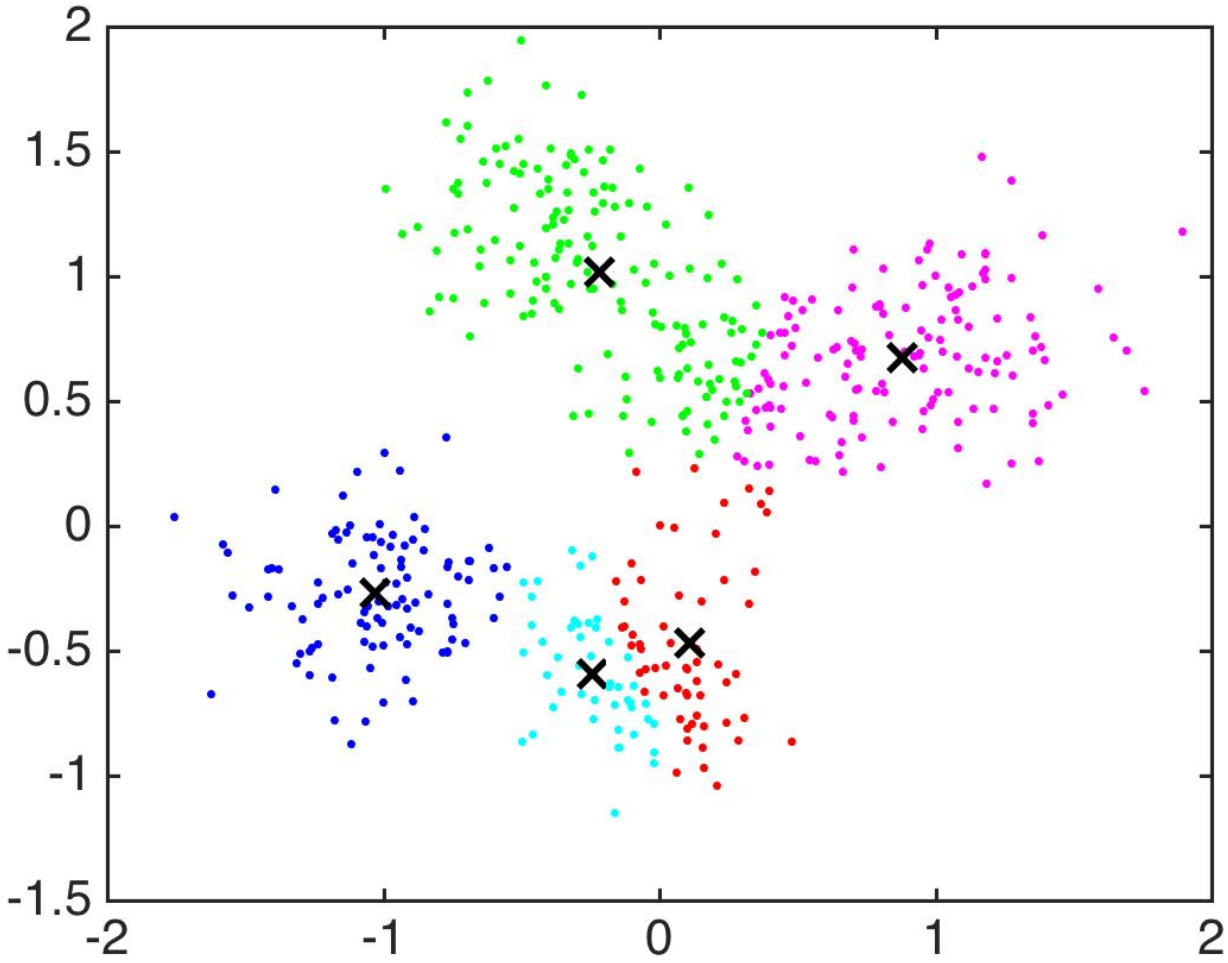
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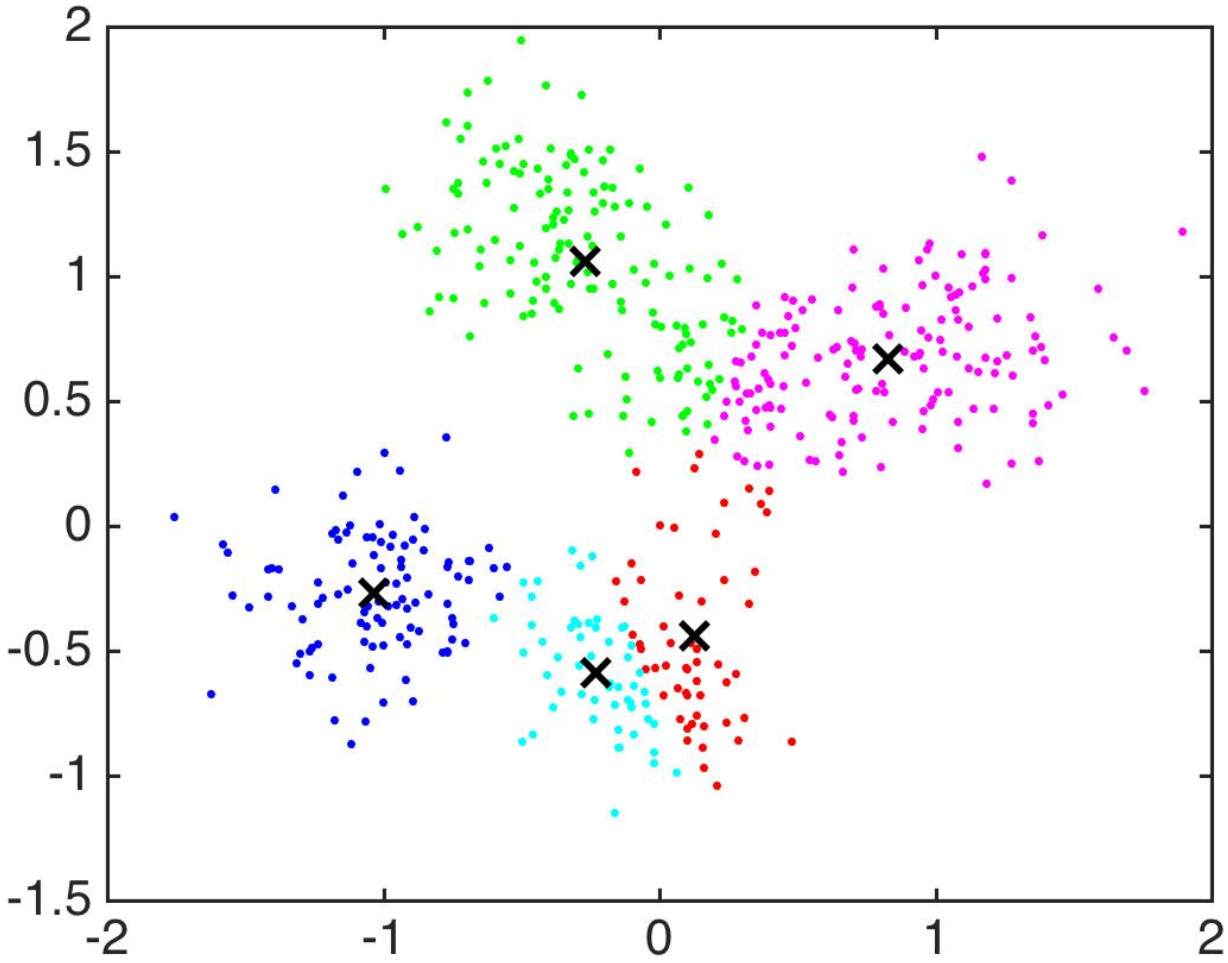
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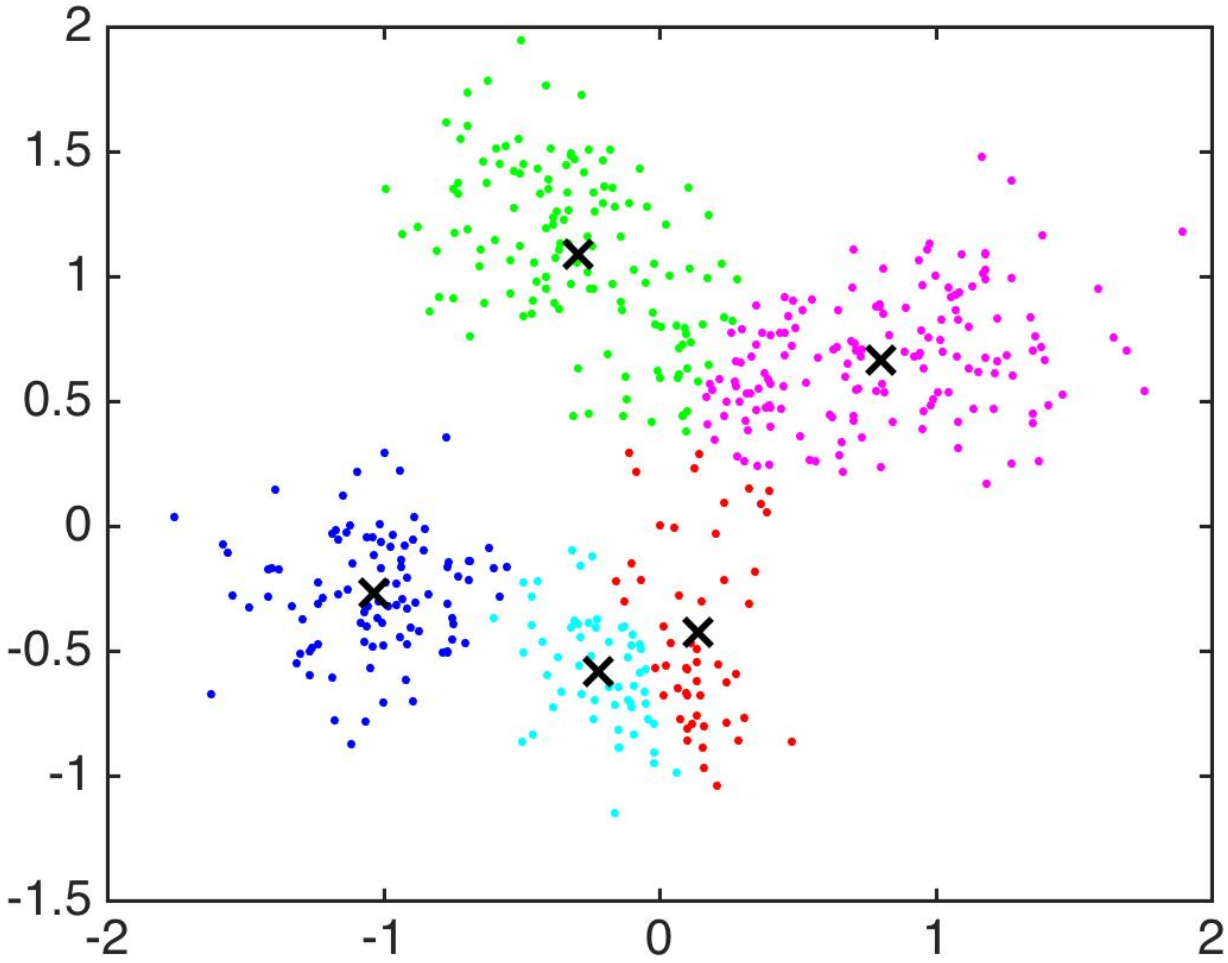
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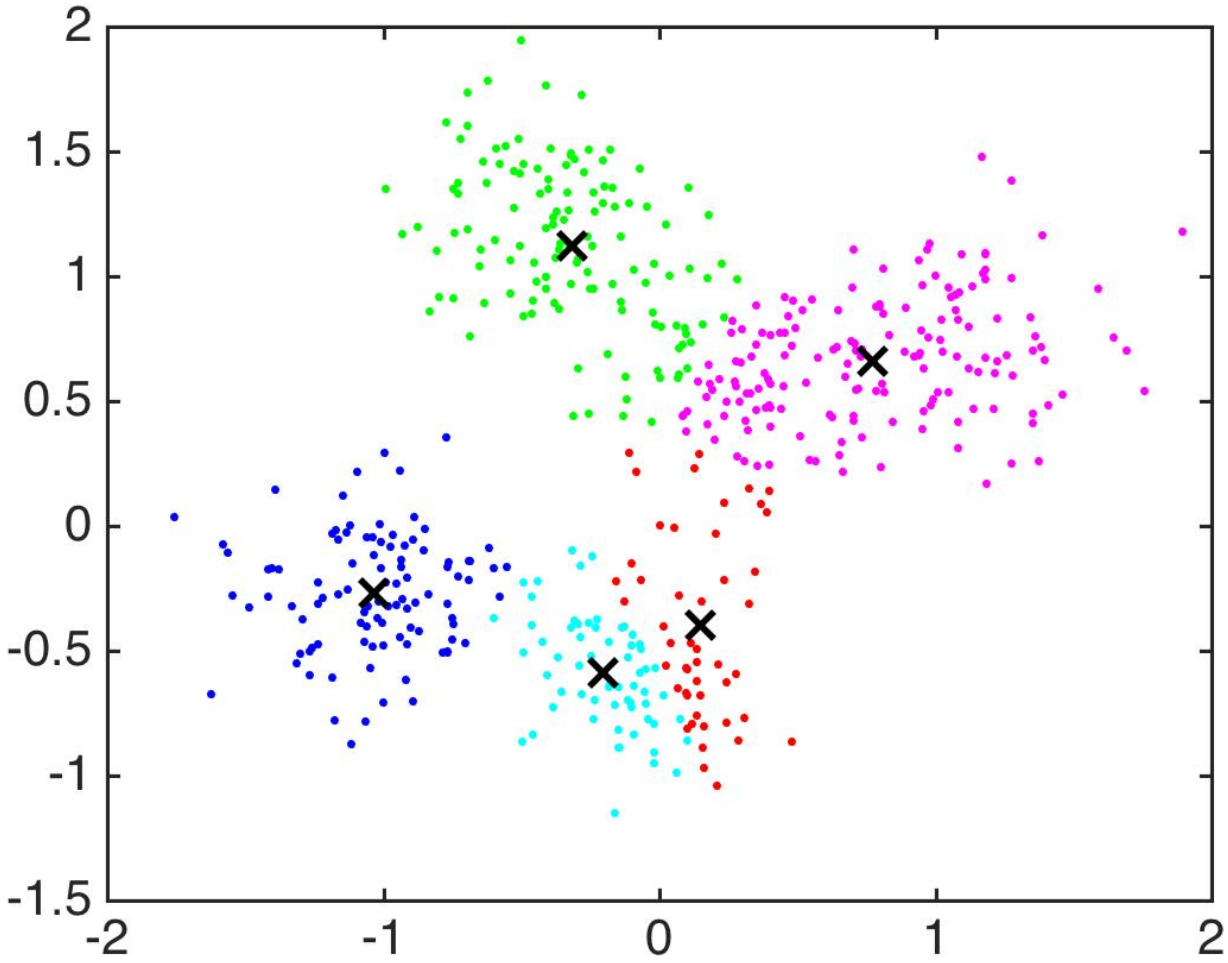
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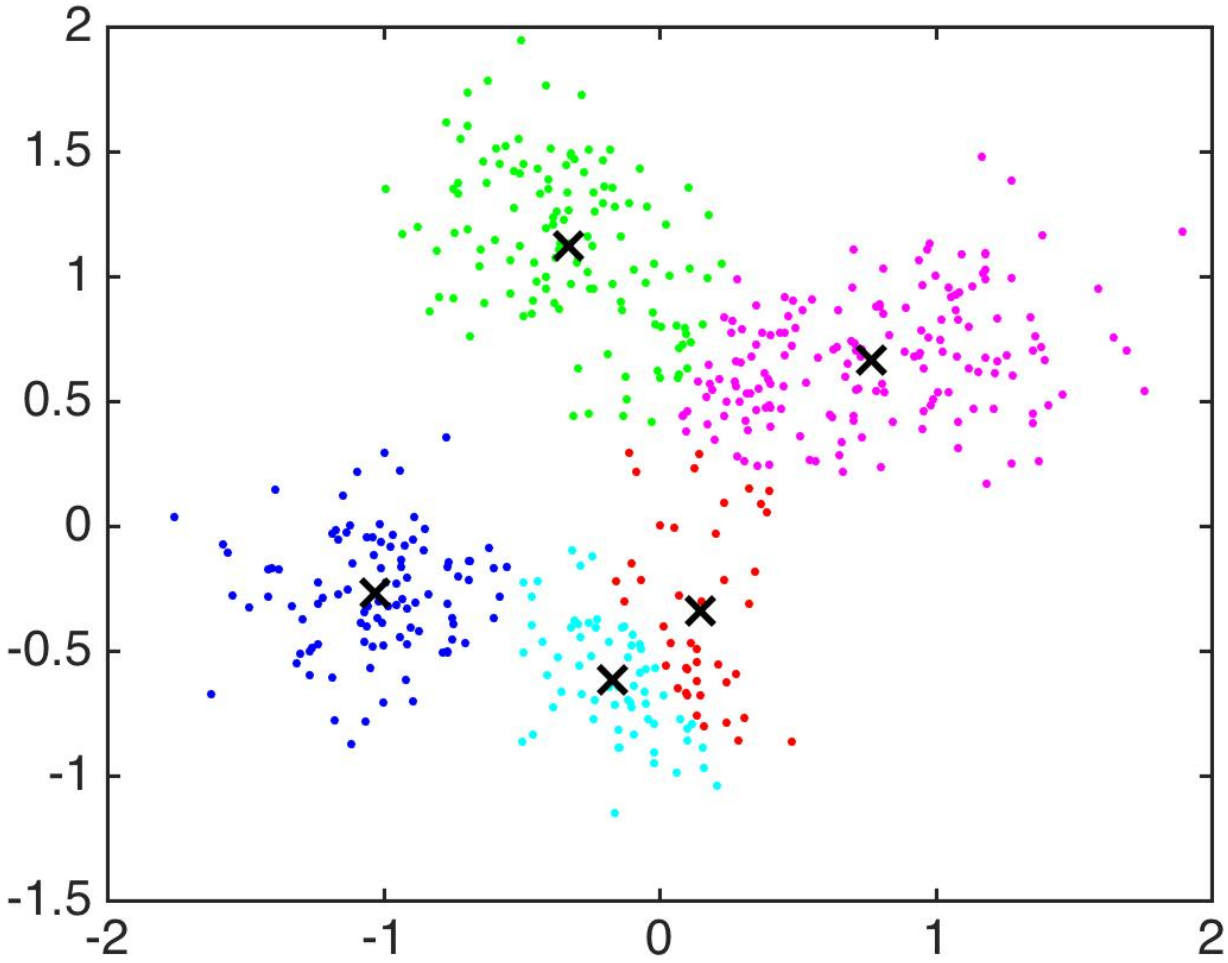
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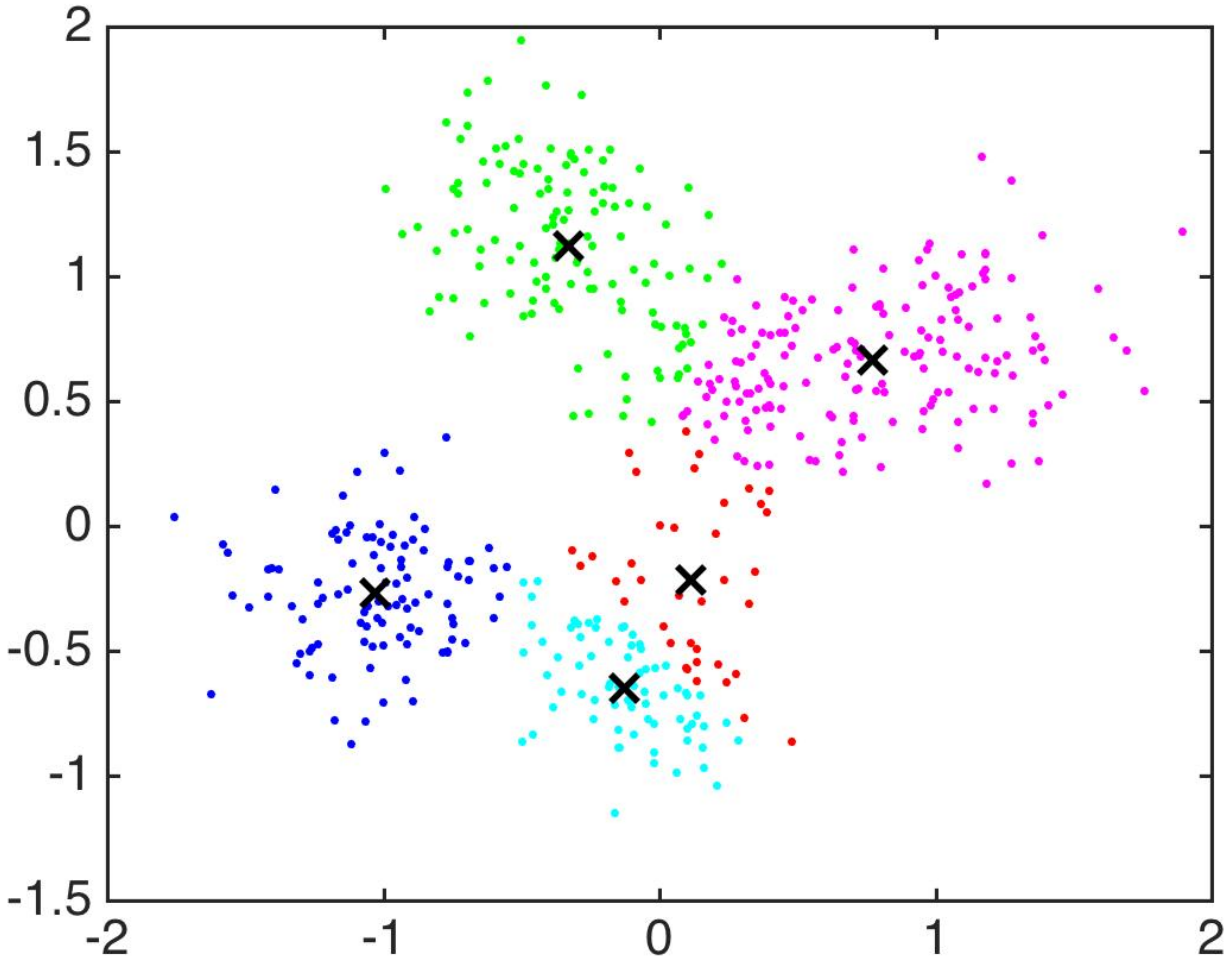
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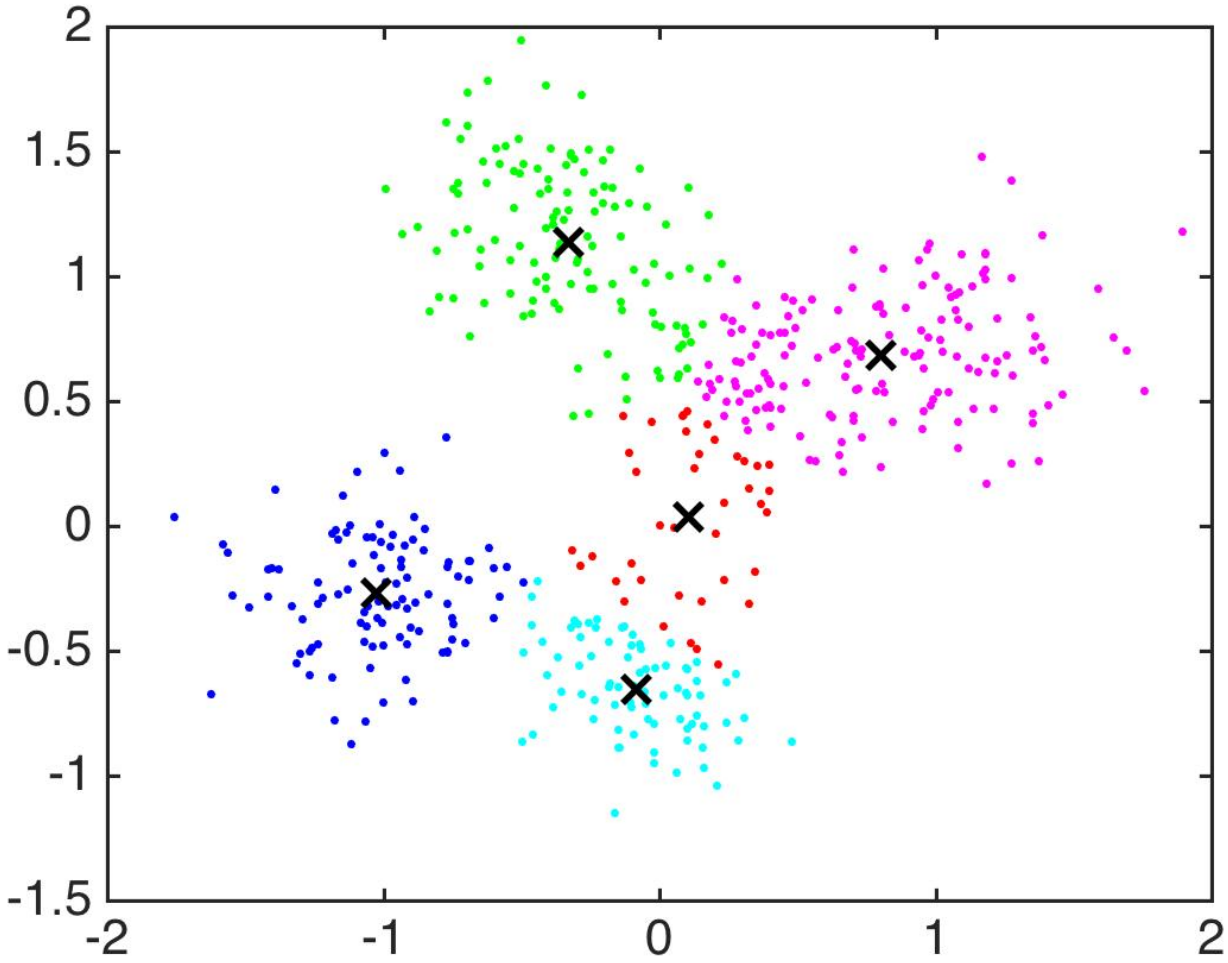
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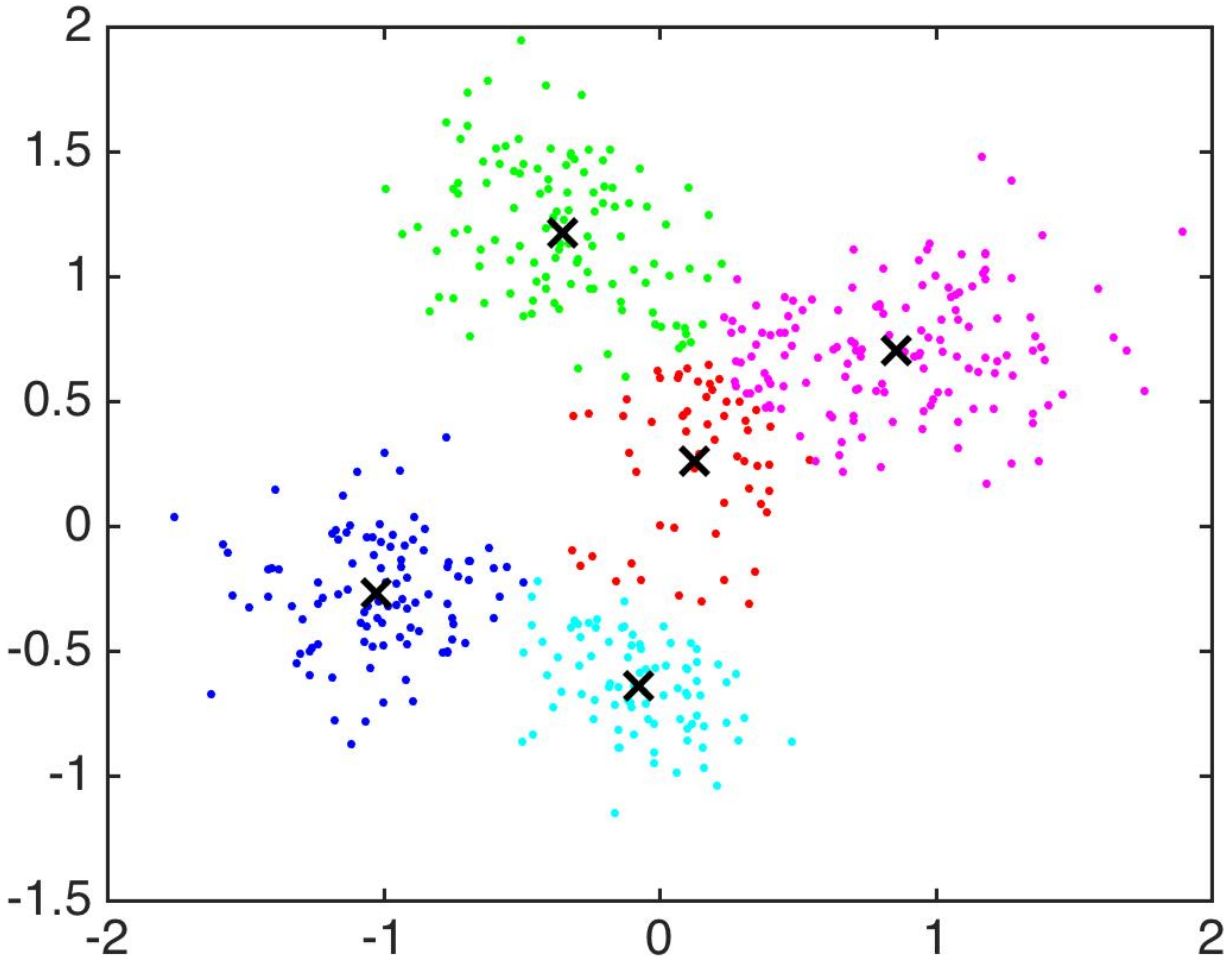
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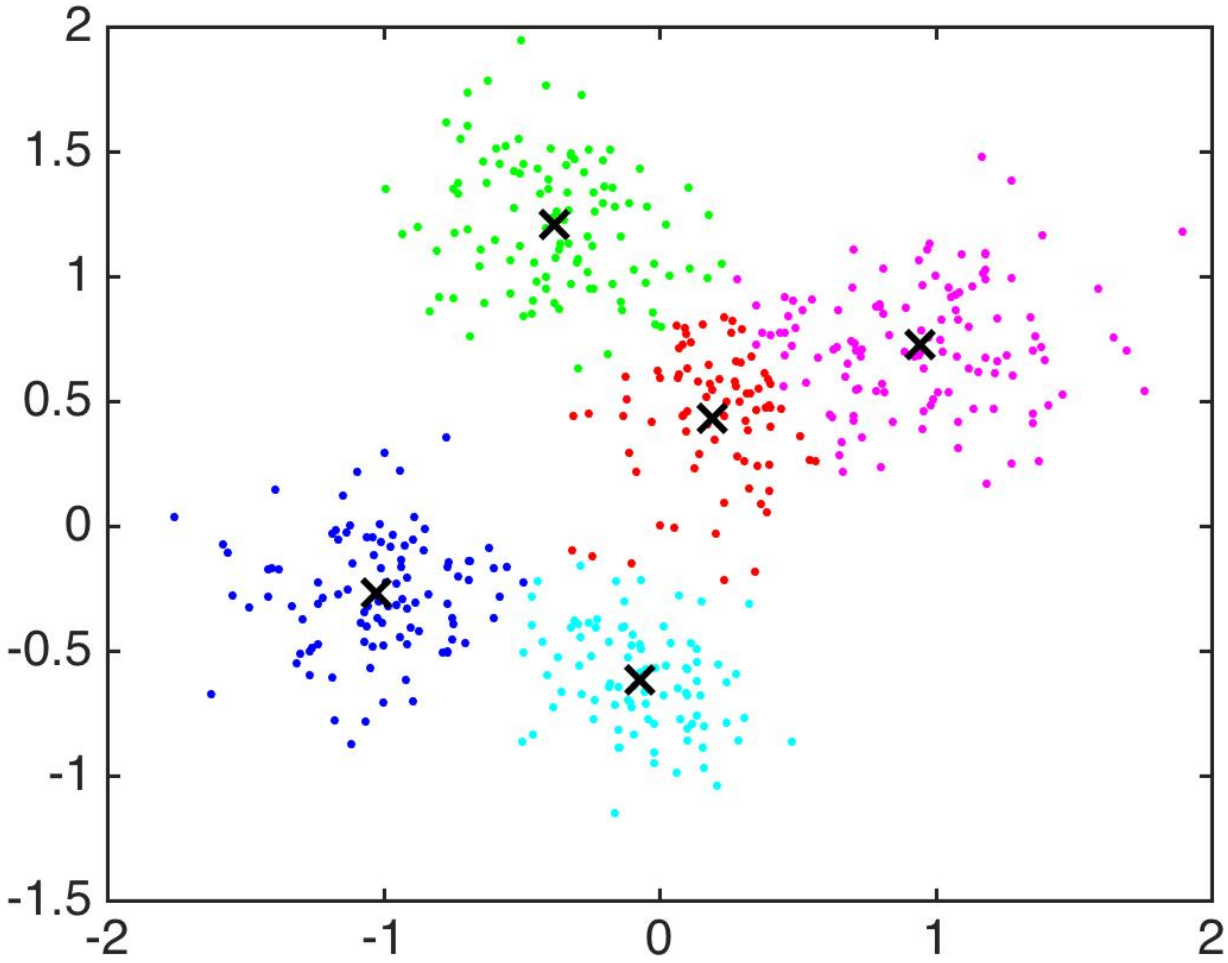
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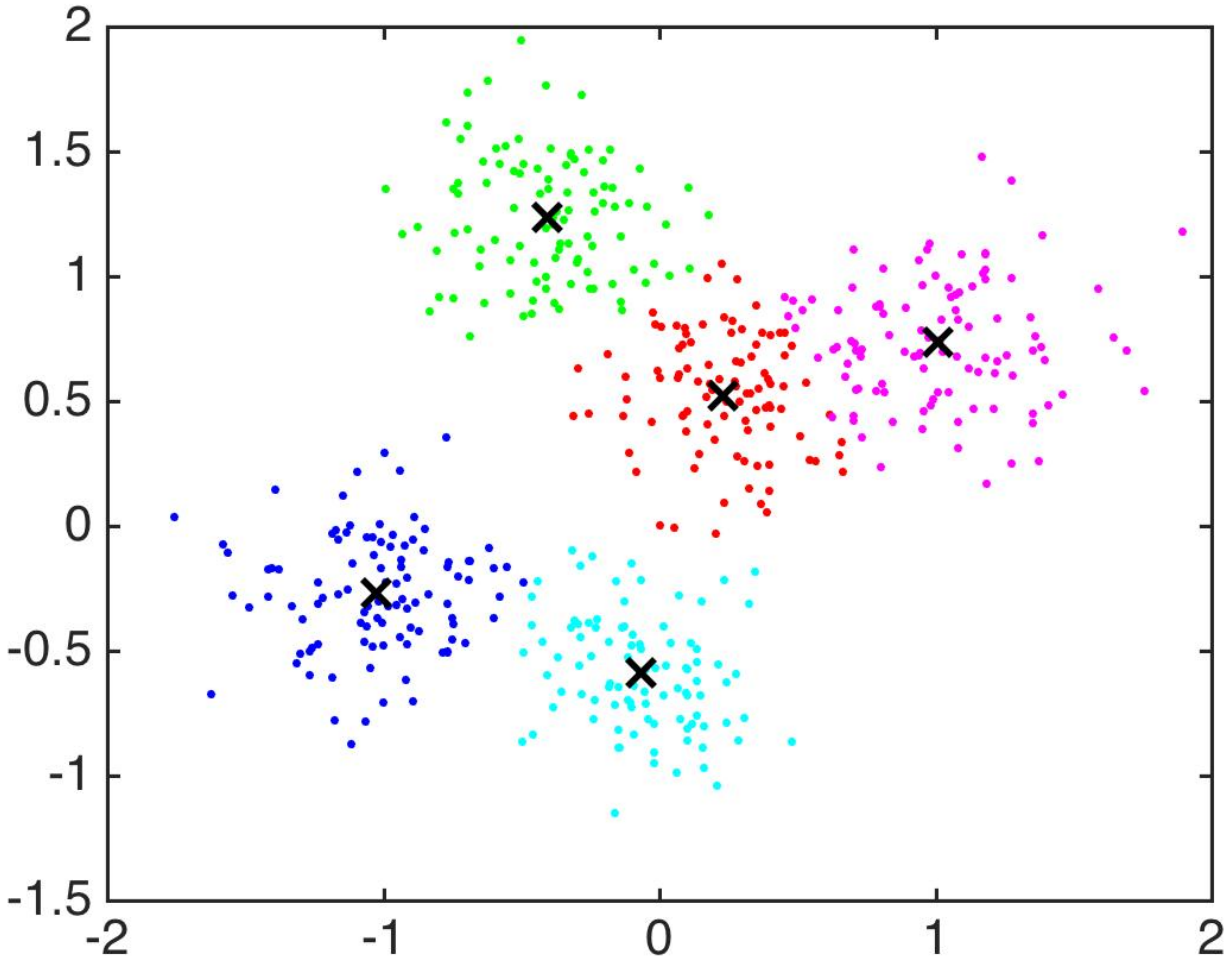
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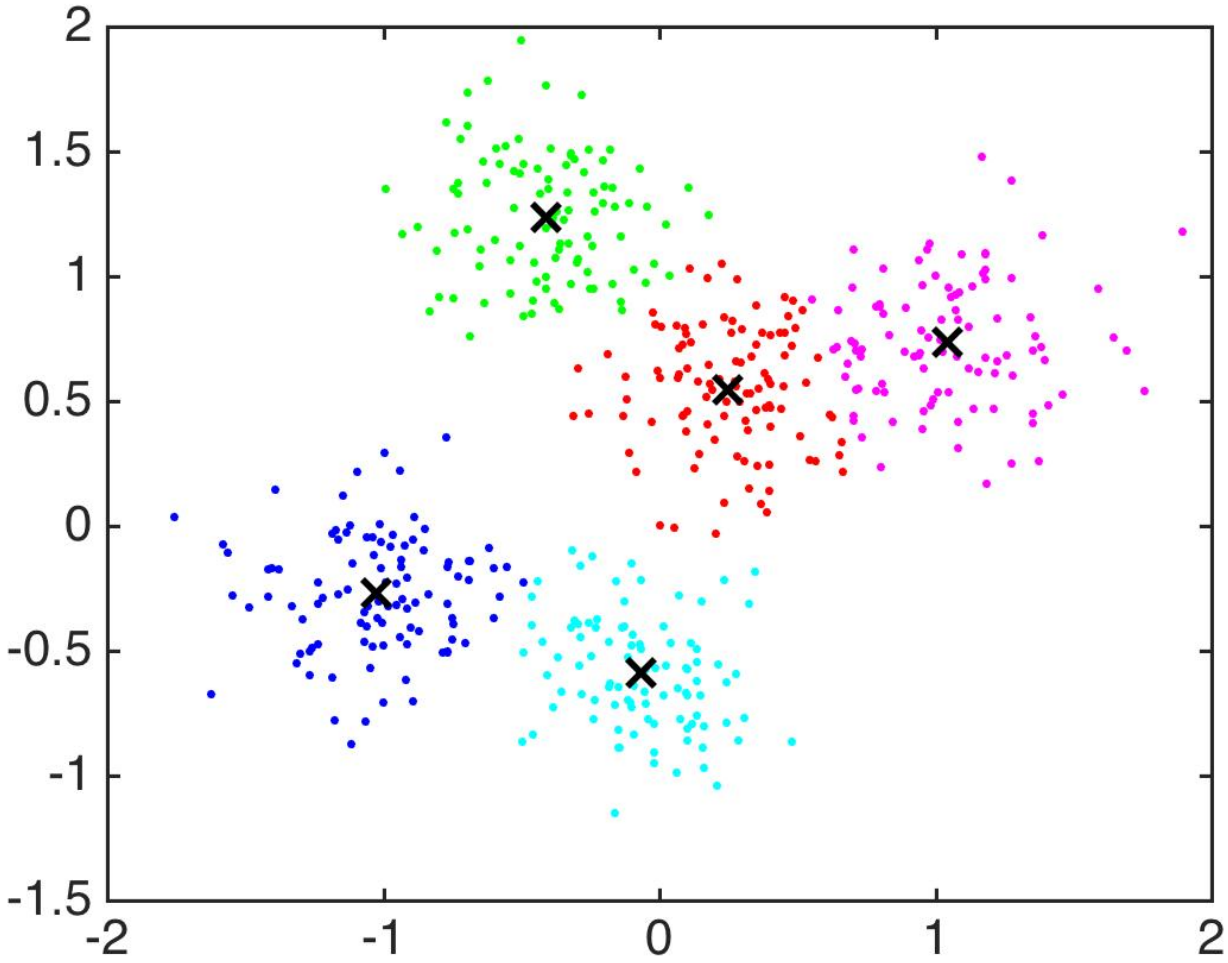
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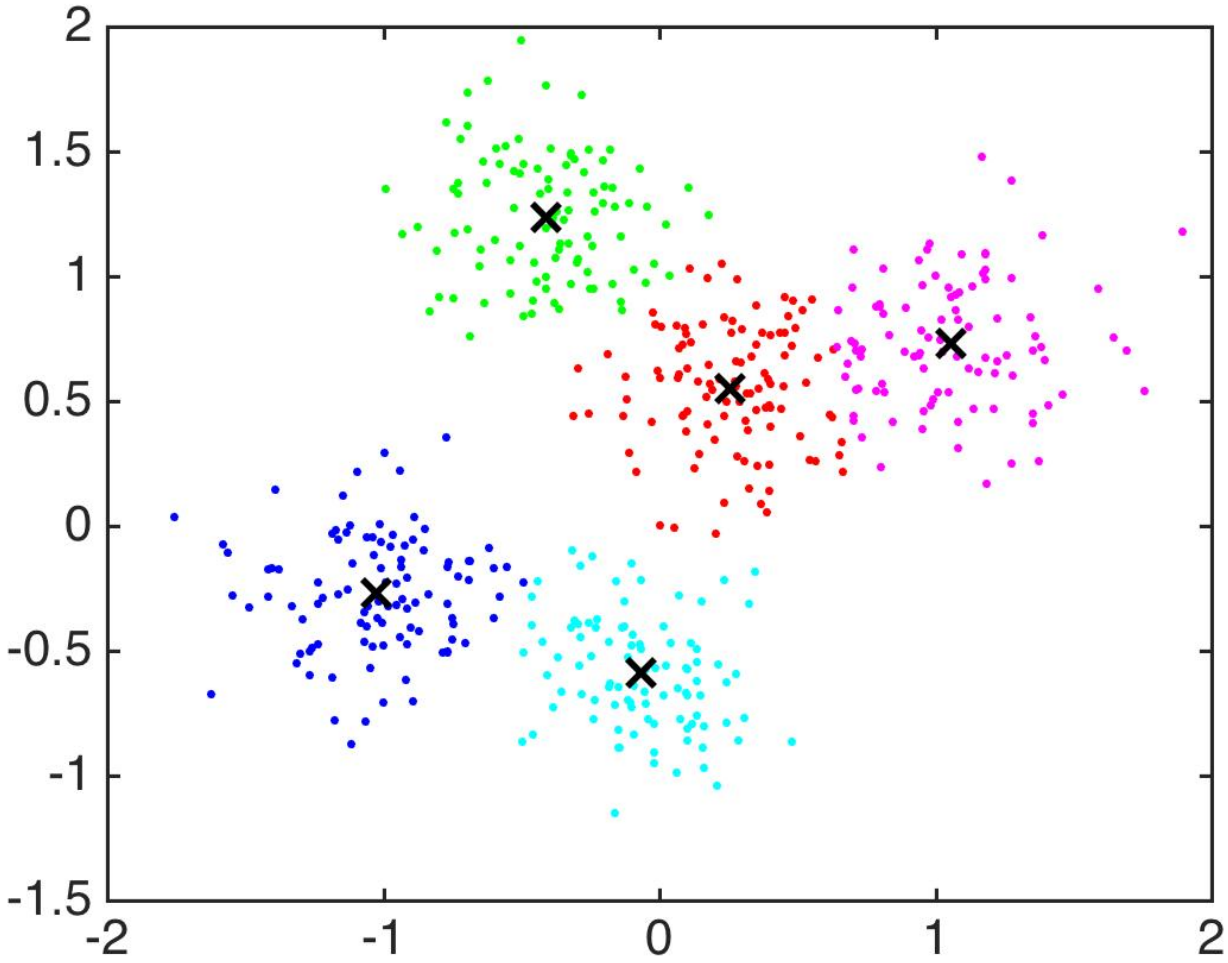
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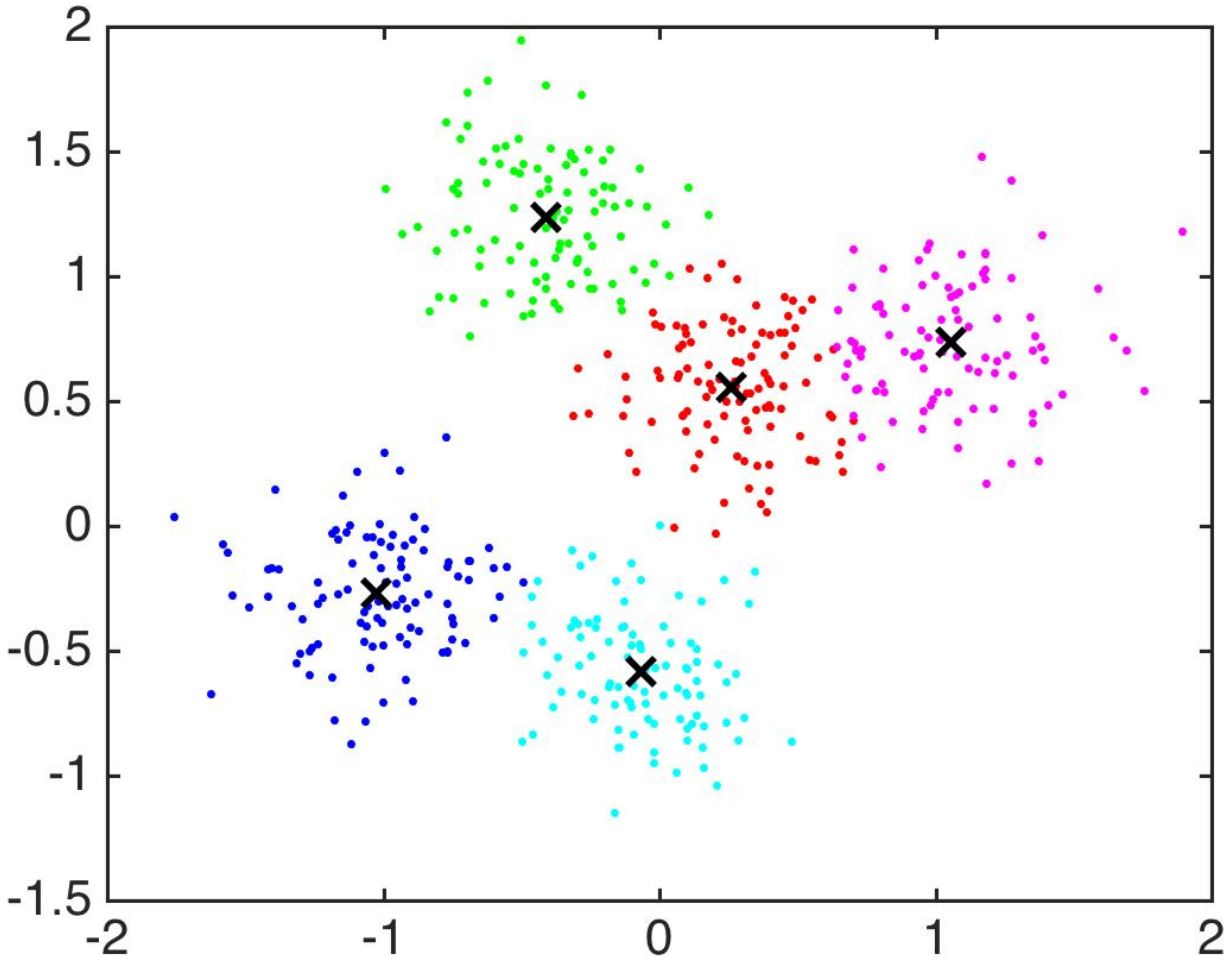
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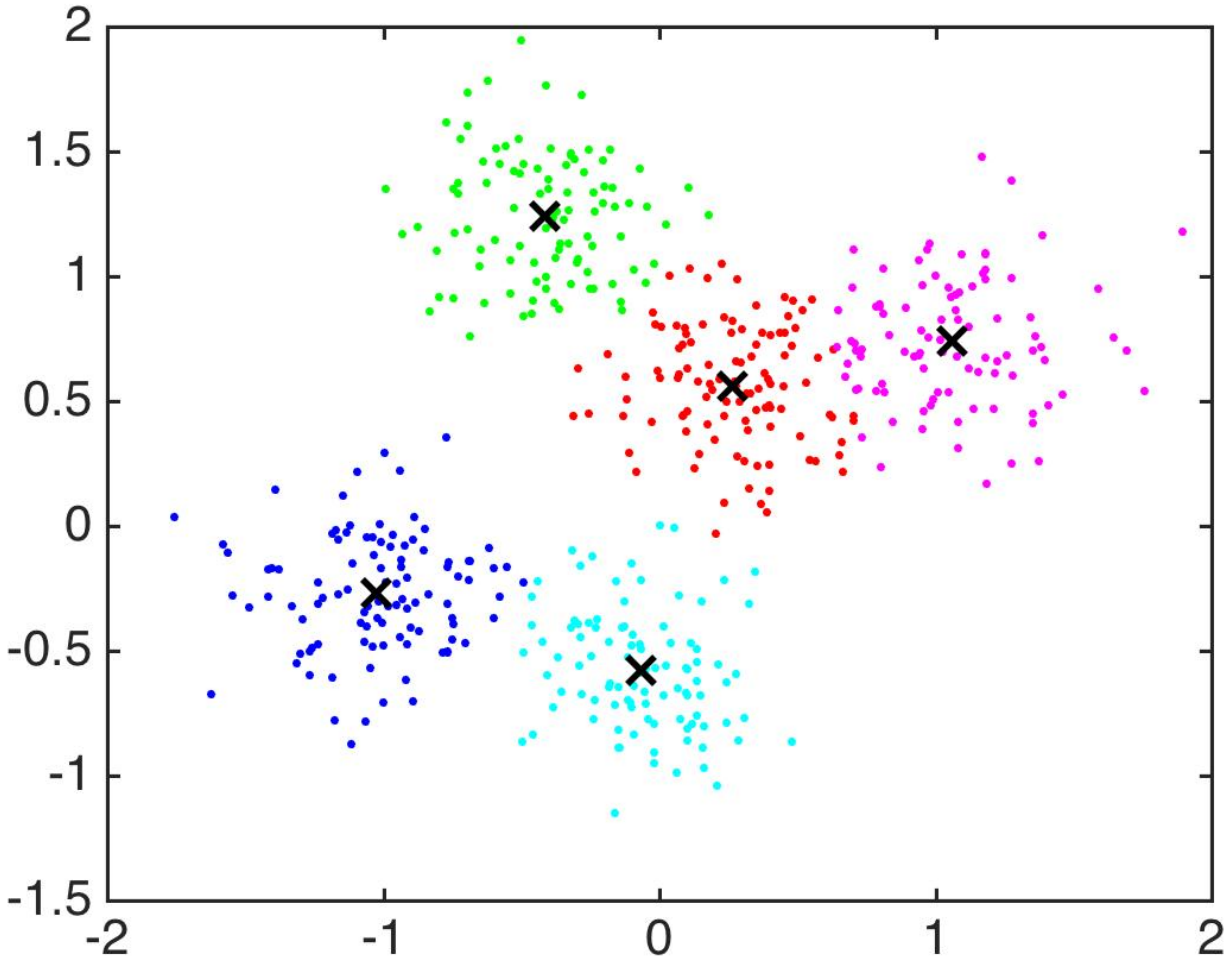
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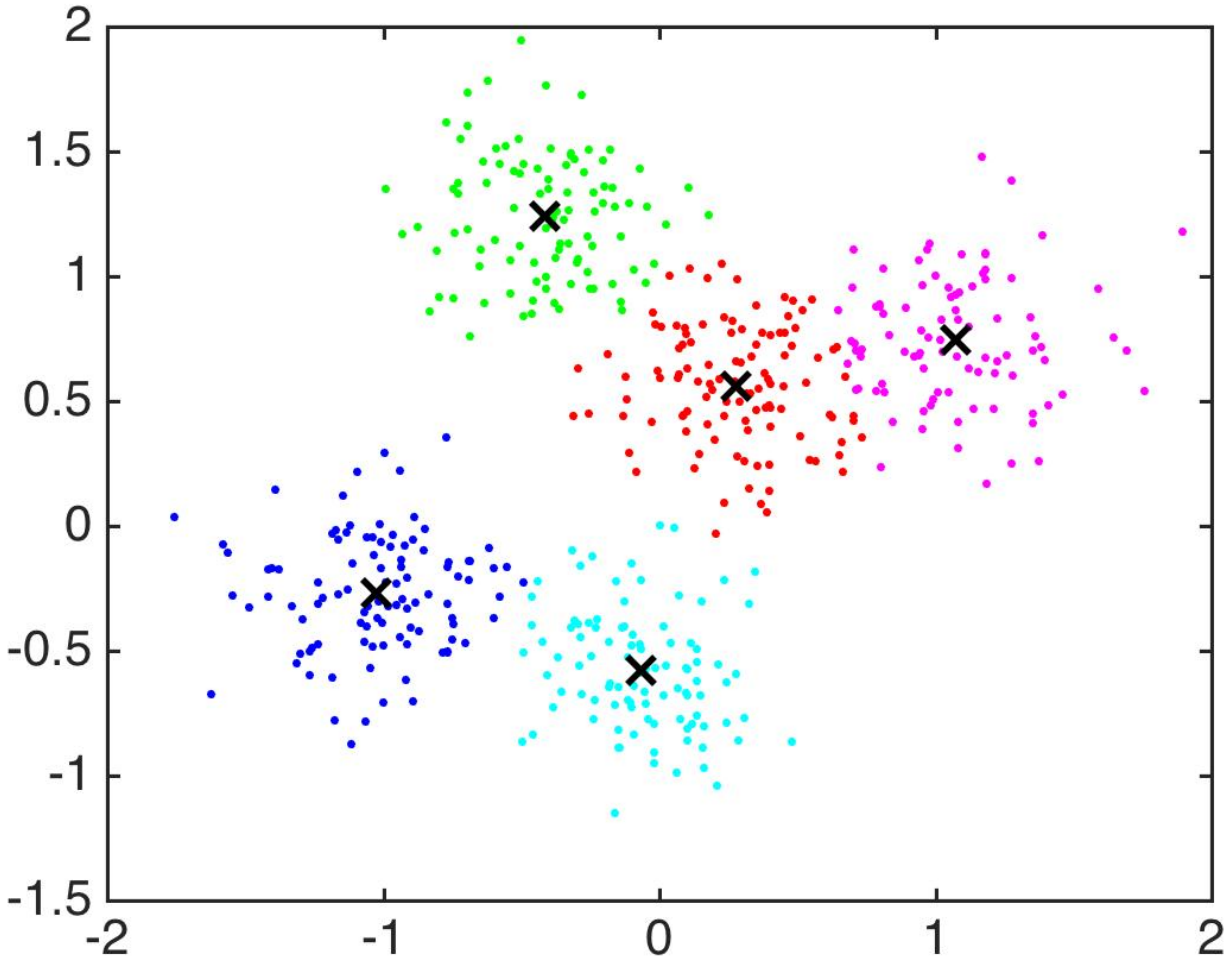
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K-Means Actual Goal

Input: Data set $x_1,\ldots,x_n$, number of clusters K
Output: Cluster centers $c_1,..,c_K$
Goal: Minimize

$$\left(\text{dist}(x_i, c_k)\right)$$

K-Means Actual Goal

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Output: Cluster centers $c_1,..,c_K$
Goal: Minimize

$$\text{cost}(c_1,...,c_K) = \sum_i \min_k \left(\text{dist}(x_i, c_k)\right)$$

Global minimization: Try all possible assignments of m points to K clusters:

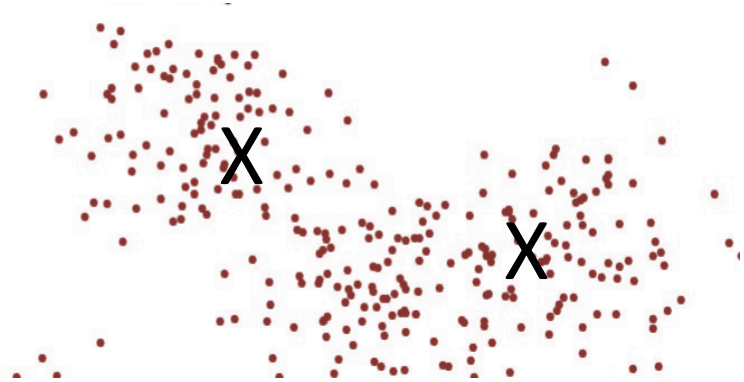
$$\text{Combos}(m,K) = \frac{1}{K!}\sum_{k=1}^{K}(-1)^{K-k}\begin{pmatrix} K \\ k \end{pmatrix}k^n$$

$$\text{Combos}(10,4) = 34K, \quad \text{Combos}(19,4) = 10^{10},...,\text{urg}$$

K-Means Actual Goal

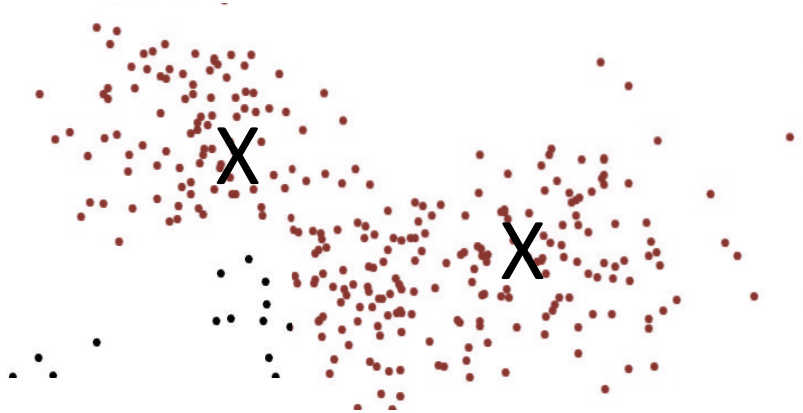
$$\text{cost}(c_1,...,c_K) = \sum_i \min_k \left(\text{dist}(x_i, c_k)\right)$$

K-Means Actual Goal



$$\text{cost}(c_1,\ldots,c_K) = \sum_i \min_k \left(\text{dist}(x_i, c_k)\right)$$

K-Means Actual Goal



$$\text{cost}(c_1,\ldots,c_K) = \sum_{k} \sum_{i:\, x_i \text{ is in cluster}_k} \text{dist}(x_i, c_k)$$

K-Means Actual Goal

$$\text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, \text{c}_1, ..., c_K) = \sum_k \sum_{i: x_i \text{ is in cluster}_k} \text{dist}(\text{x}_i, c_k)$$

$$\text{cost}(\text{c}_1, ..., c_K) = \sum_k \sum_{i: x_i \text{ is in cluster}_k} \text{dist}(\text{x}_i, c_k)$$

K-Means Actual Goal

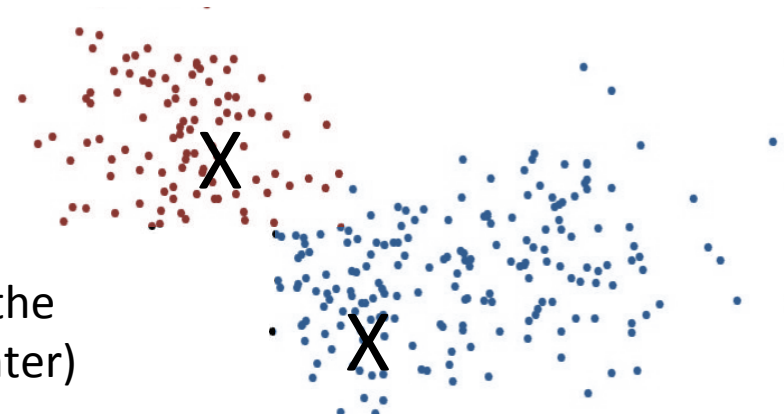
$$\text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, \text{c}_1, ..., c_K) = \sum_k \sum_{i: x_i \text{ is in cluster}_k} \text{dist}(\text{x}_i, c_k)$$

K-Means Actual Goal

$$\text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, c_1, ..., c_K) = \sum_k \sum_{i: x_i \text{ is in cluster}_k} \text{dist}(x_i, c_k)$$

$$\min_{\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k} \text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, c_1, ..., c_K)$$

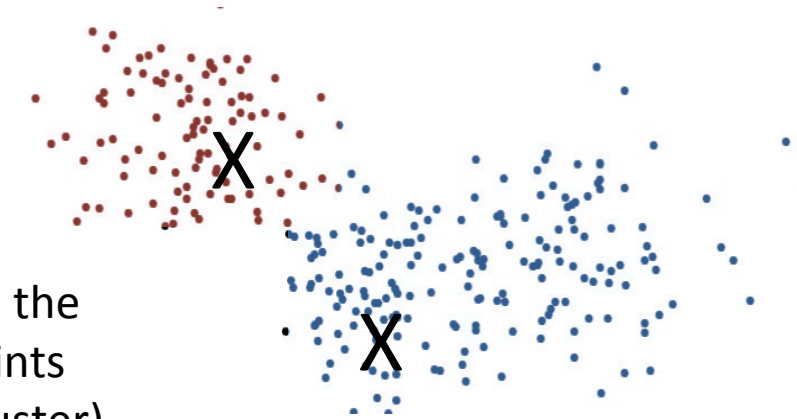
(Assign points to the nearest cluster center)



K-Means Actual Goal

$$\text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, c_1, ..., c_K) = \sum_k \sum_{i:\, x_i \text{ is in cluster}_k} \text{dist}(x_i, c_k)$$

$$\min_{c_1, c_2, .., c_k} \text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, c_1, ..., c_K)$$



(Assign centers to the middle of the points assigned to that cluster)

K-Means Actual Goal

$$\text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, c_1, ..., c_K) = \sum_k \sum_{i:\, x_i \text{ is in cluster}_k} \text{dist}(x_i, c_k)$$

Input: number of clusters K, randomly initialize centers c_k

Until converged:

Assign all points to the closest cluster center

$$\min_{\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k} \text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, c_1, ..., c_K)$$

Change cluster centers to be in the middle of its points

$$\min_{c_1, c_2, .., c_k} \text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, c_1, ..., c_K)$$

K-Means Actual Goal

$$\text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, c_1, ..., c_K) = \sum_k \sum_{i:\, x_i \text{ is in cluster}_k} \text{dist}(x_i, c_k)$$

Does K-Means achieve its goal?

K-Means Actual Goal

$$\text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, c_1, ..., c_K) = \sum_{k} \sum_{i:\, x_i \text{ is in cluster}_k} \text{dist}(x_i, c_k)$$

Does K-Means achieve its goal?

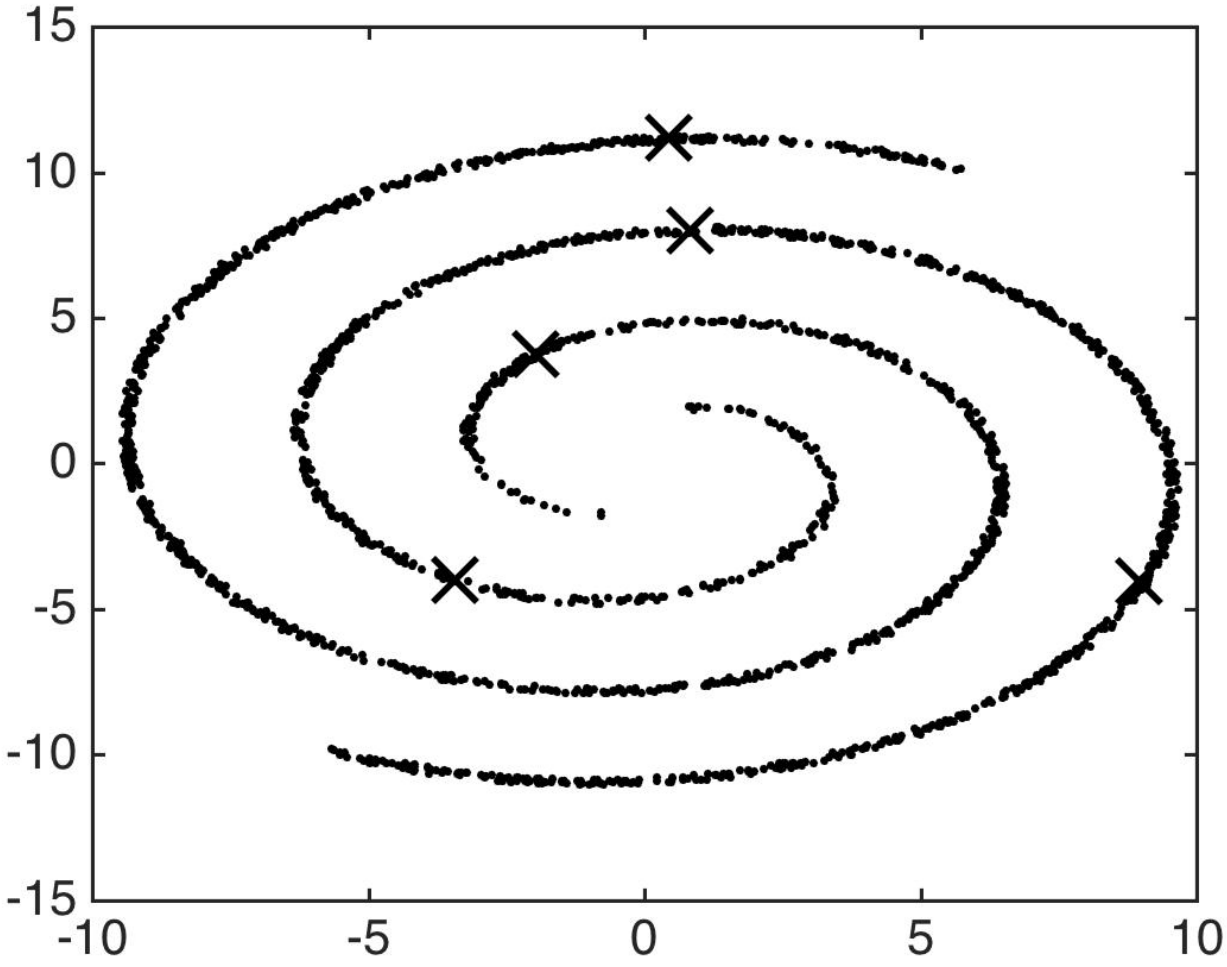
Not always. Might need multiple replicates.

K-Means Actual Goal

$$\text{cost}(\text{cluster}_1, \text{cluster}_2, .., \text{cluster}_k, c_1, ..., c_K) = \sum_{k} \sum_{i:\, x_i \text{ is in cluster}_k} \text{dist}(x_i, c_k)$$

Does K-Means achieve its goal?

Not always. Might need multiple replicates. Even worse than that, its goal might not be the right one…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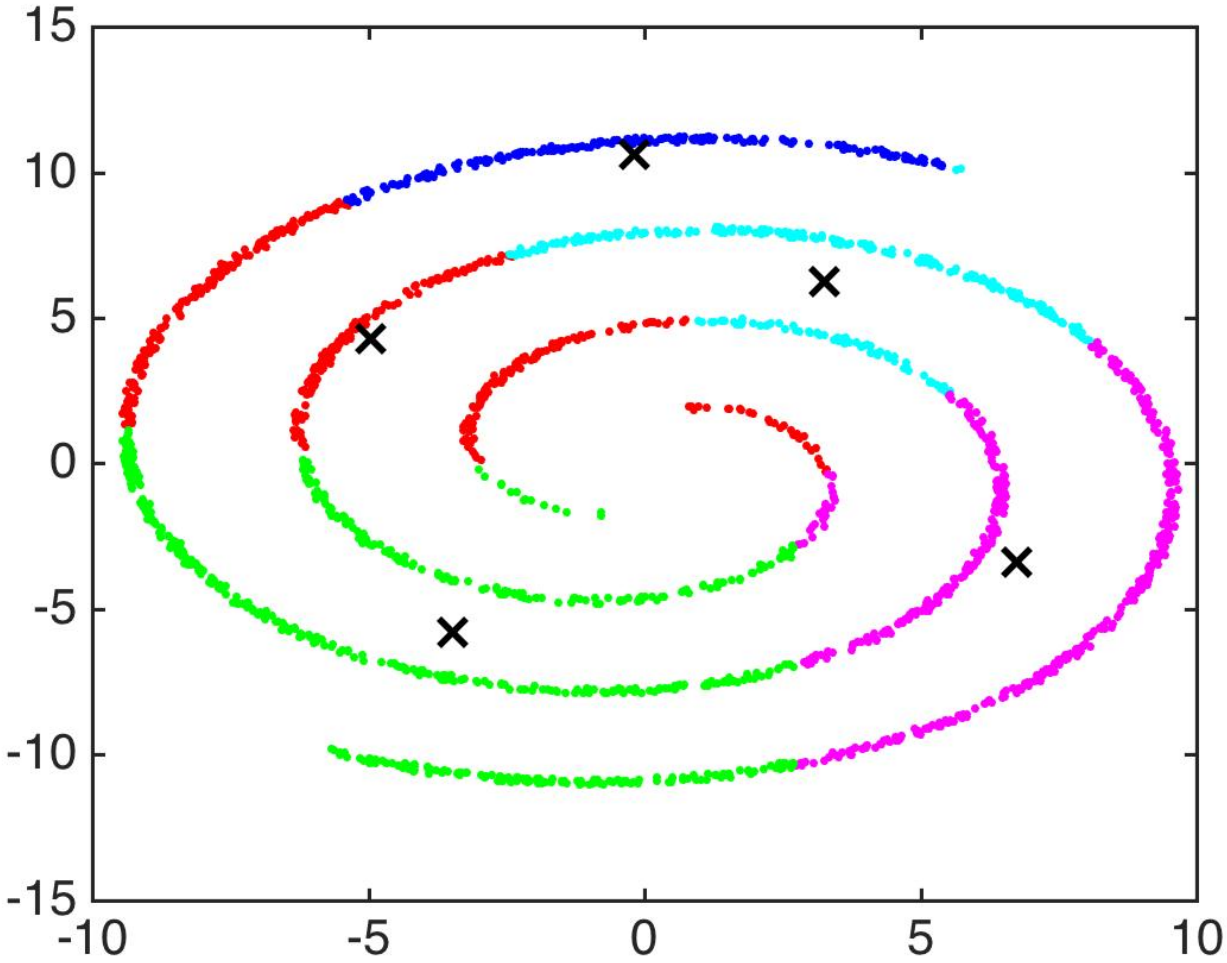
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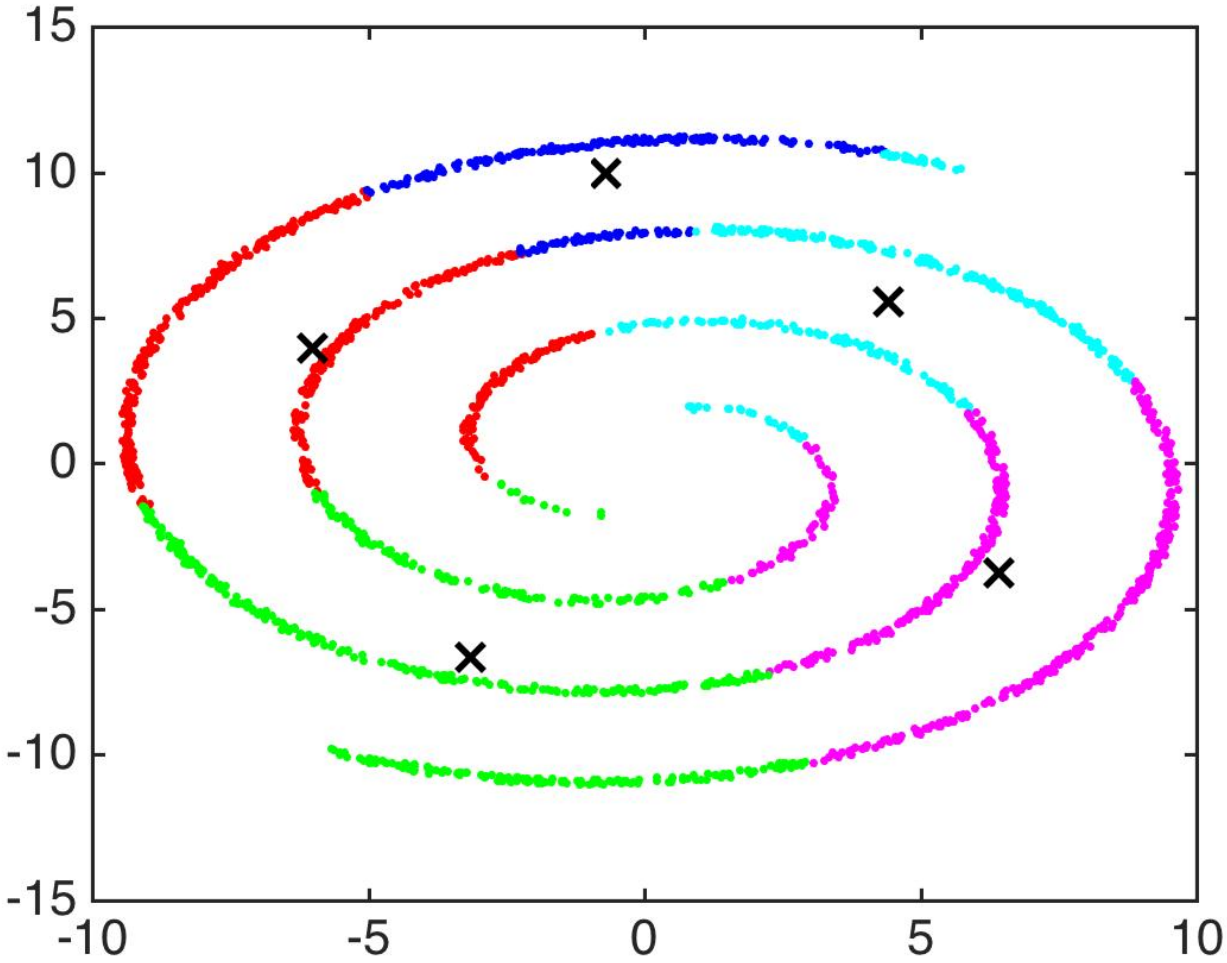
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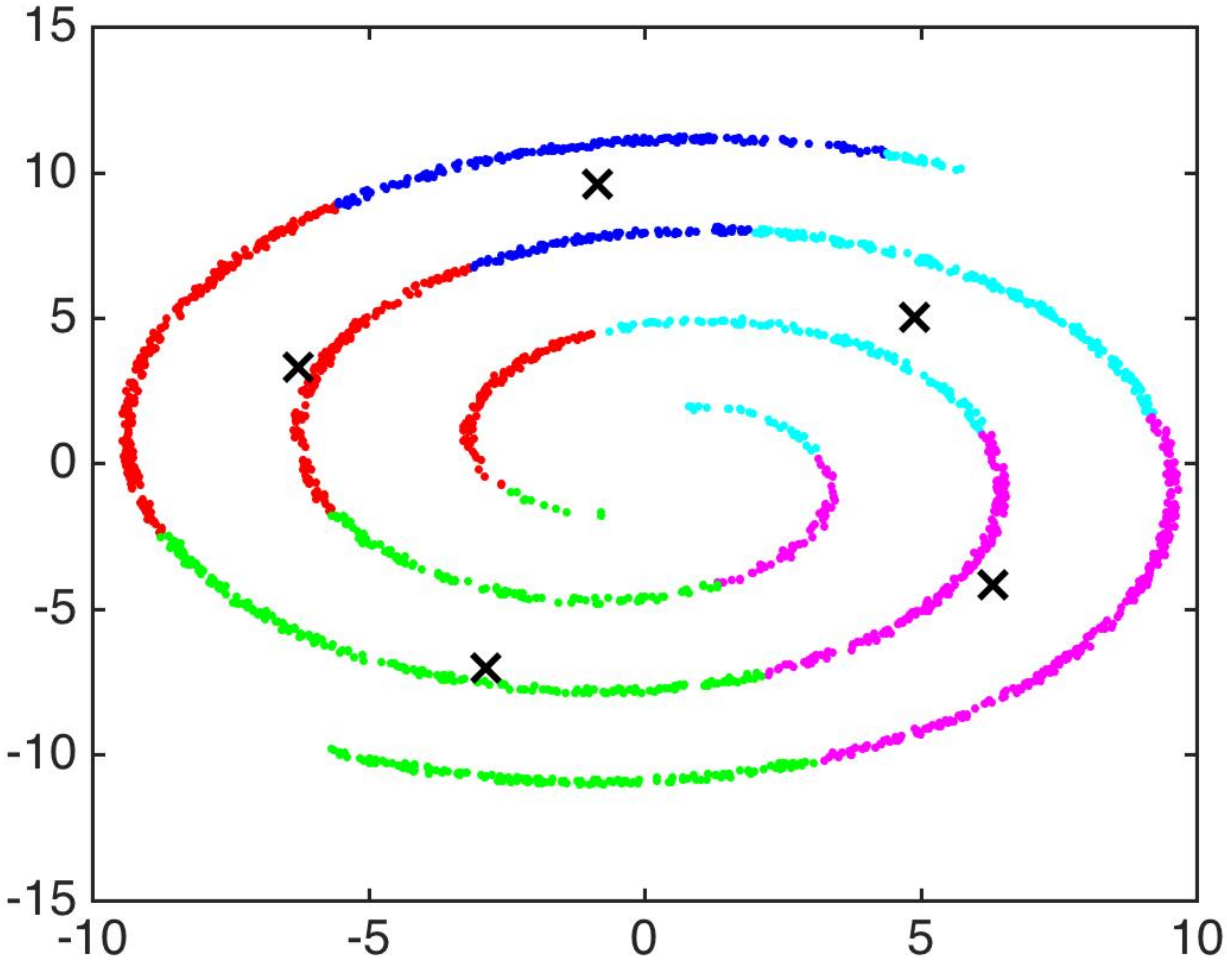
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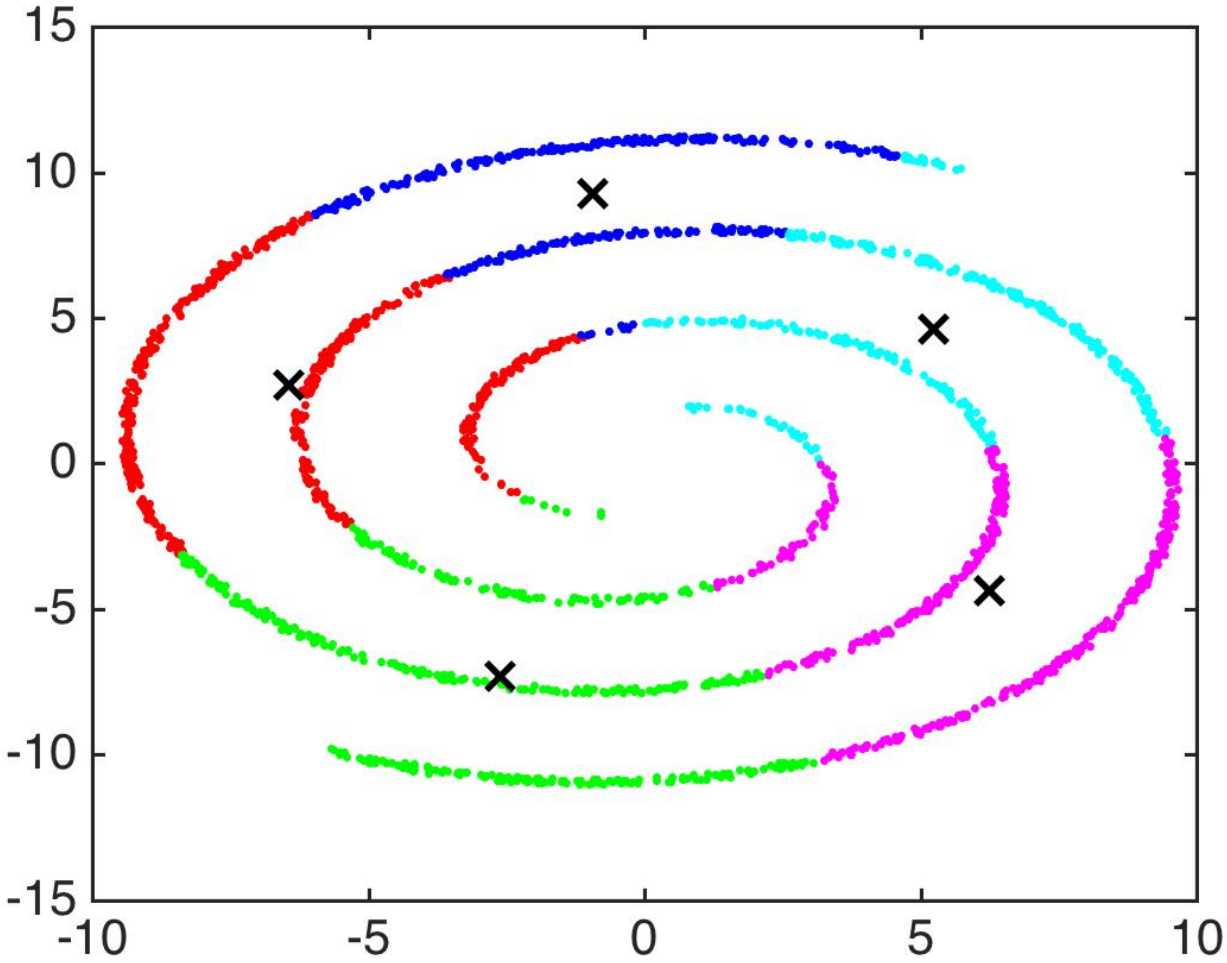
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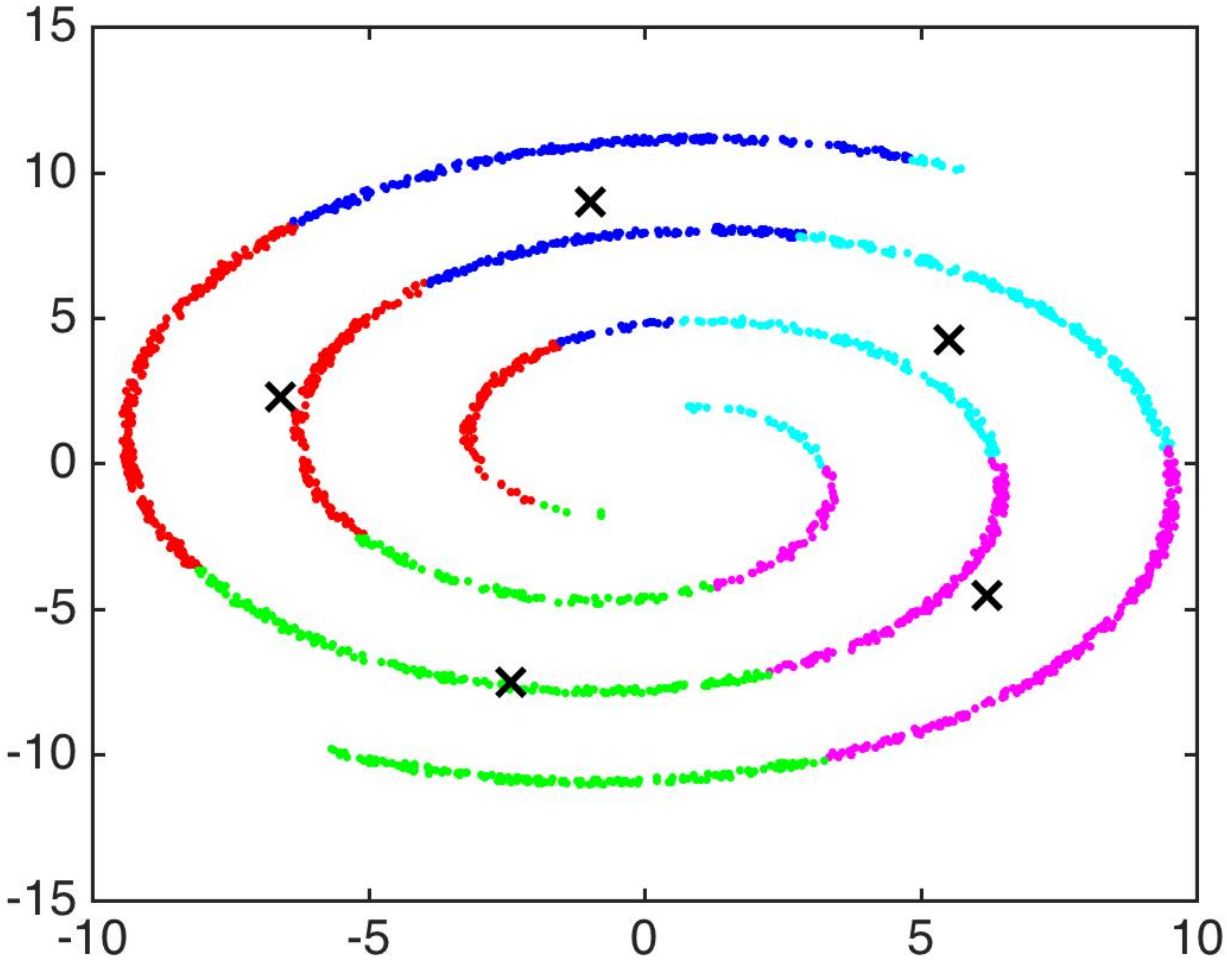
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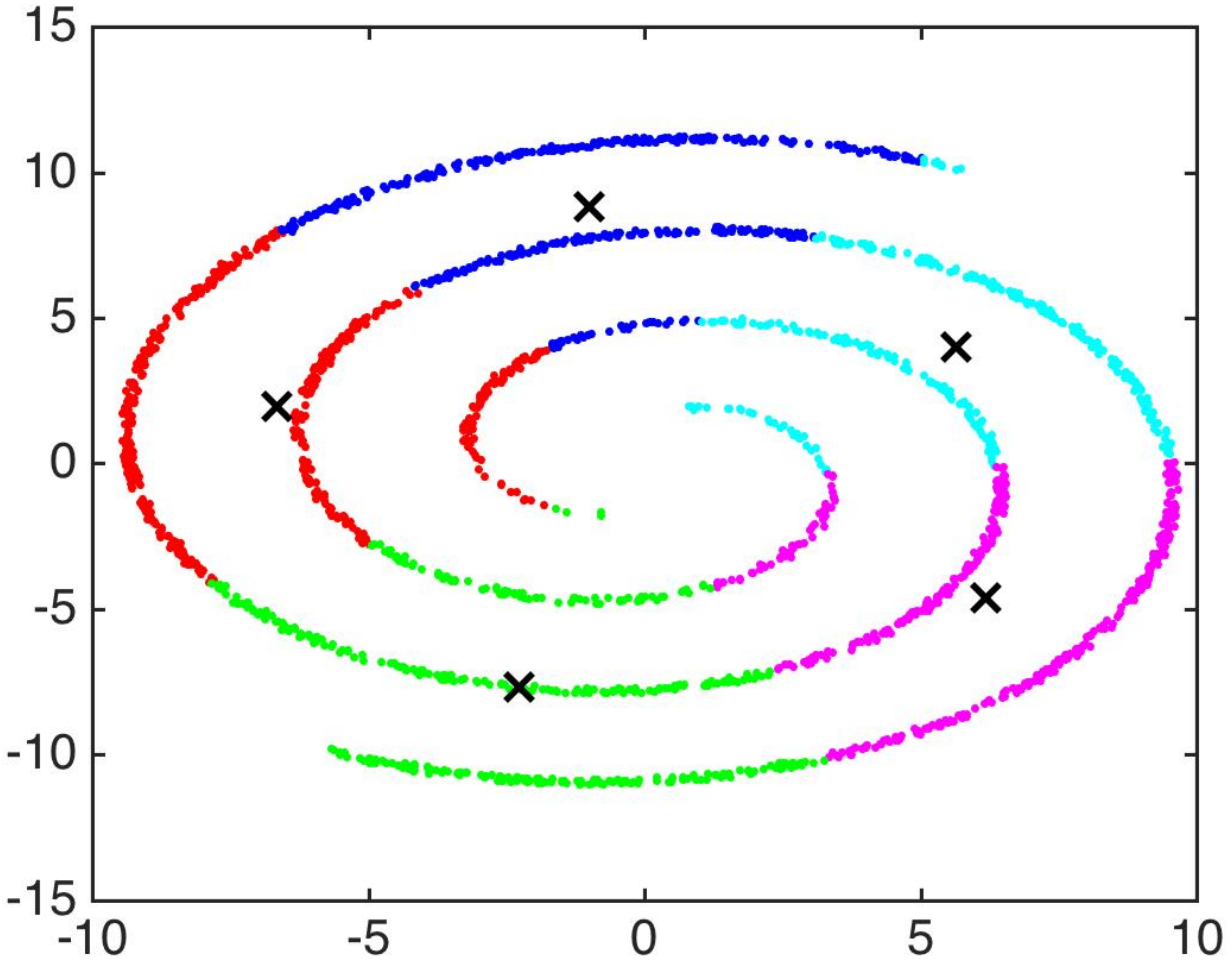
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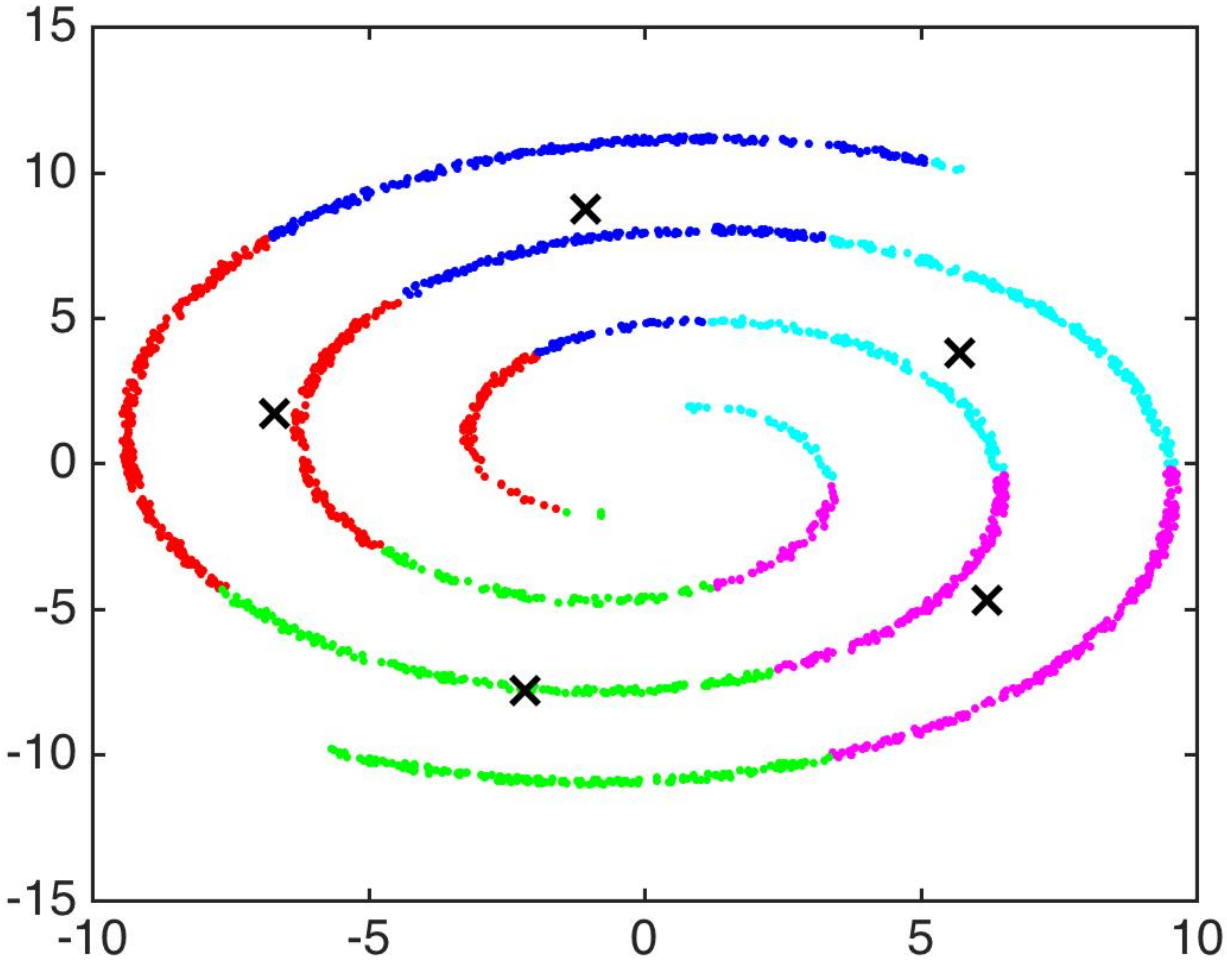
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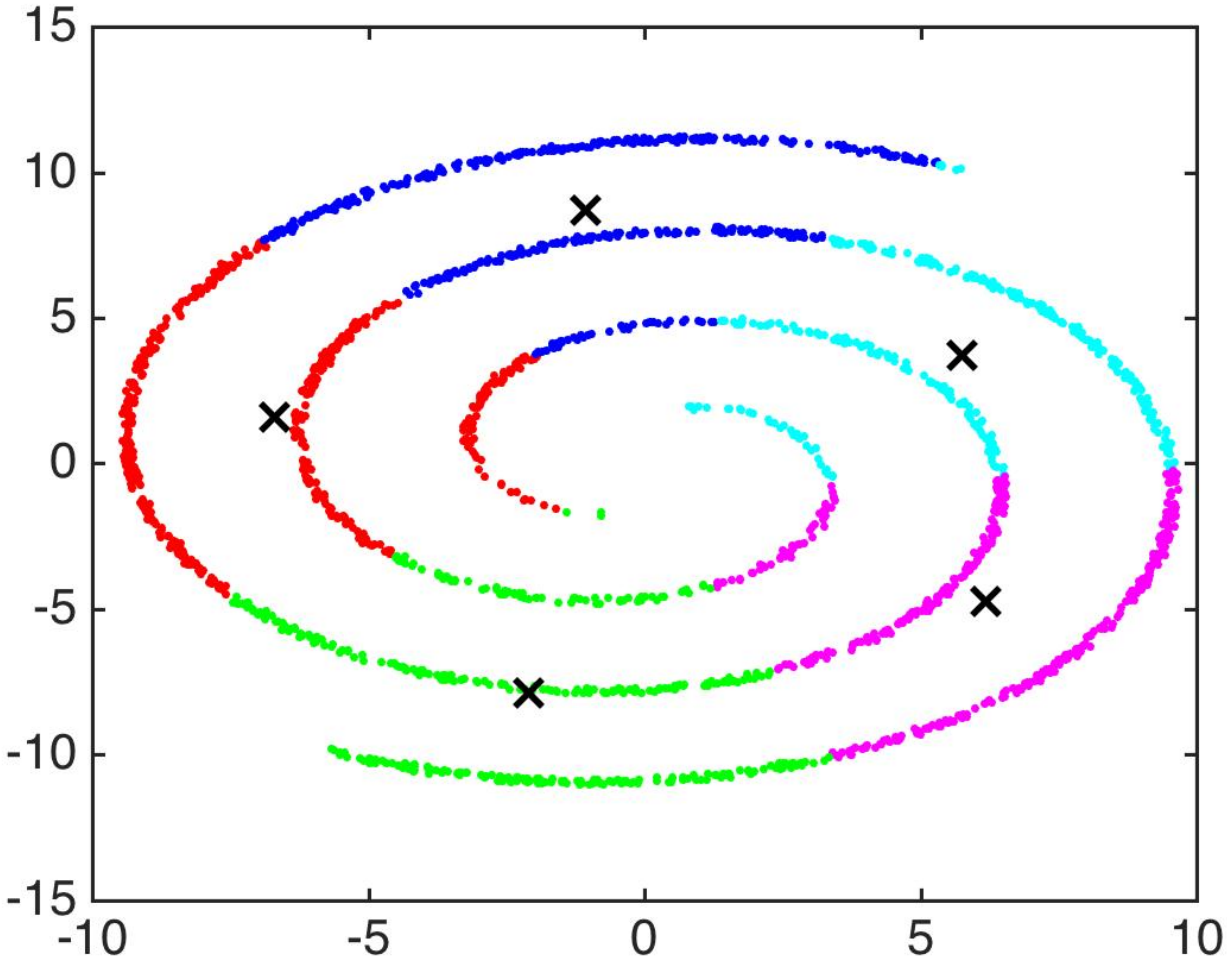
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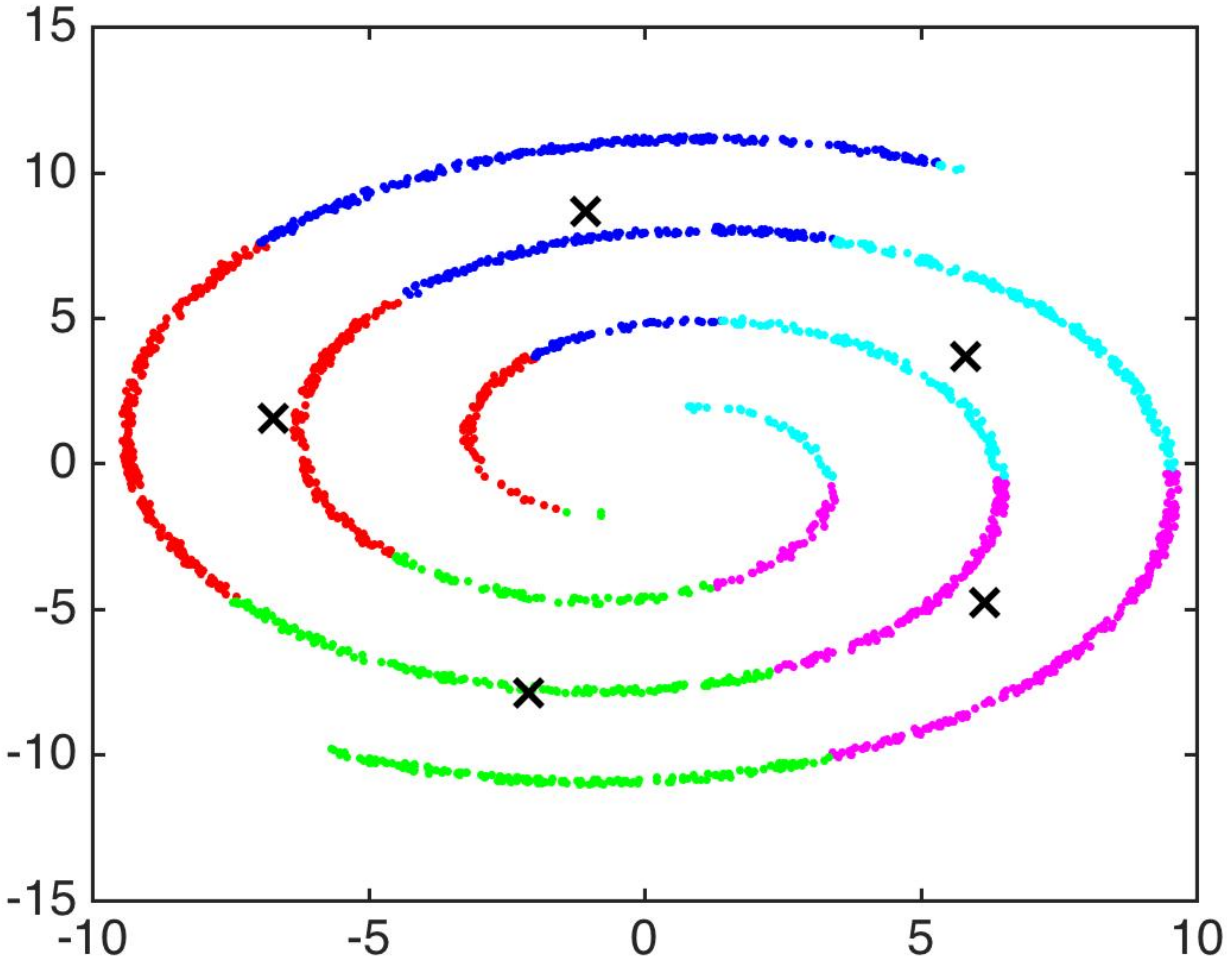
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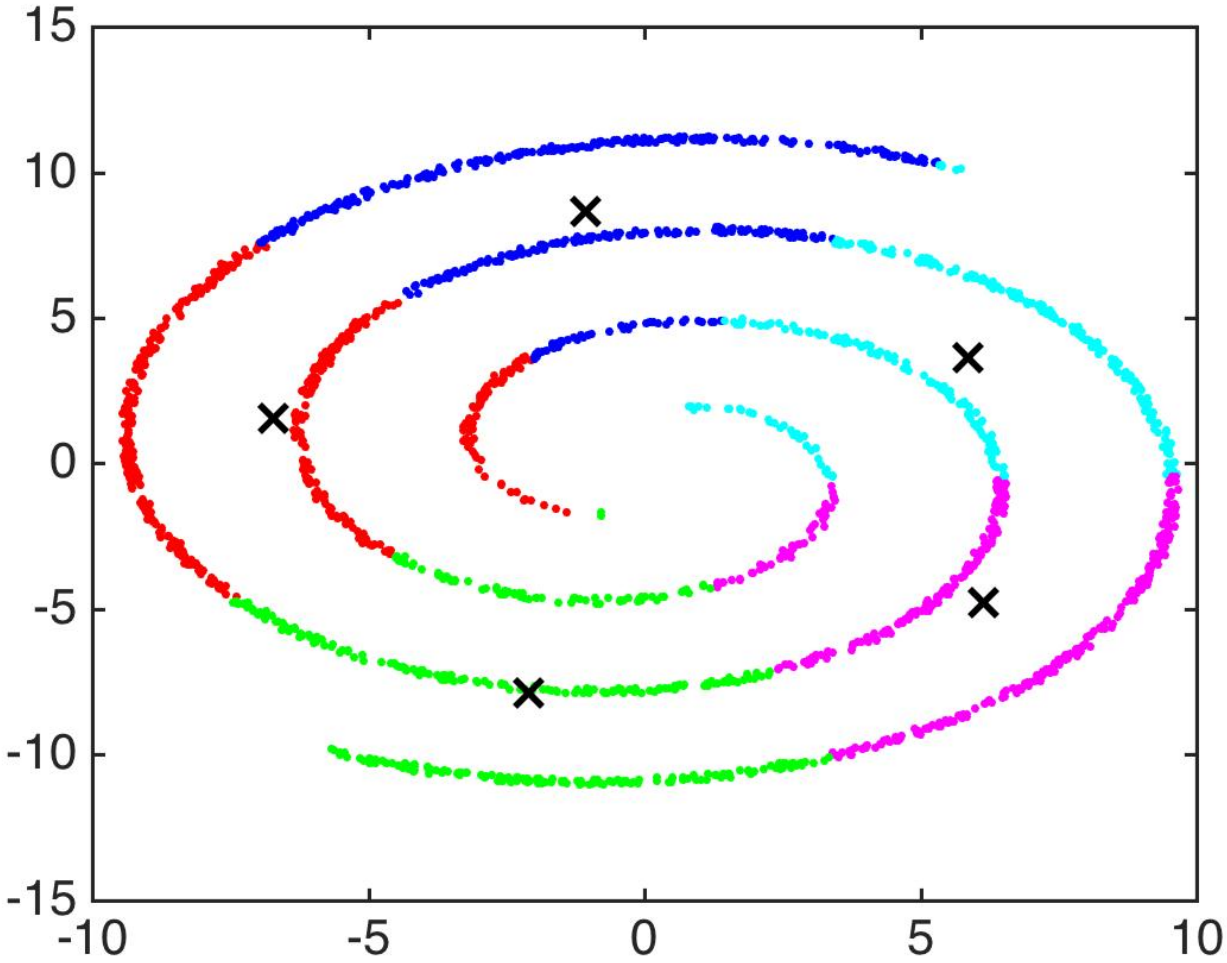
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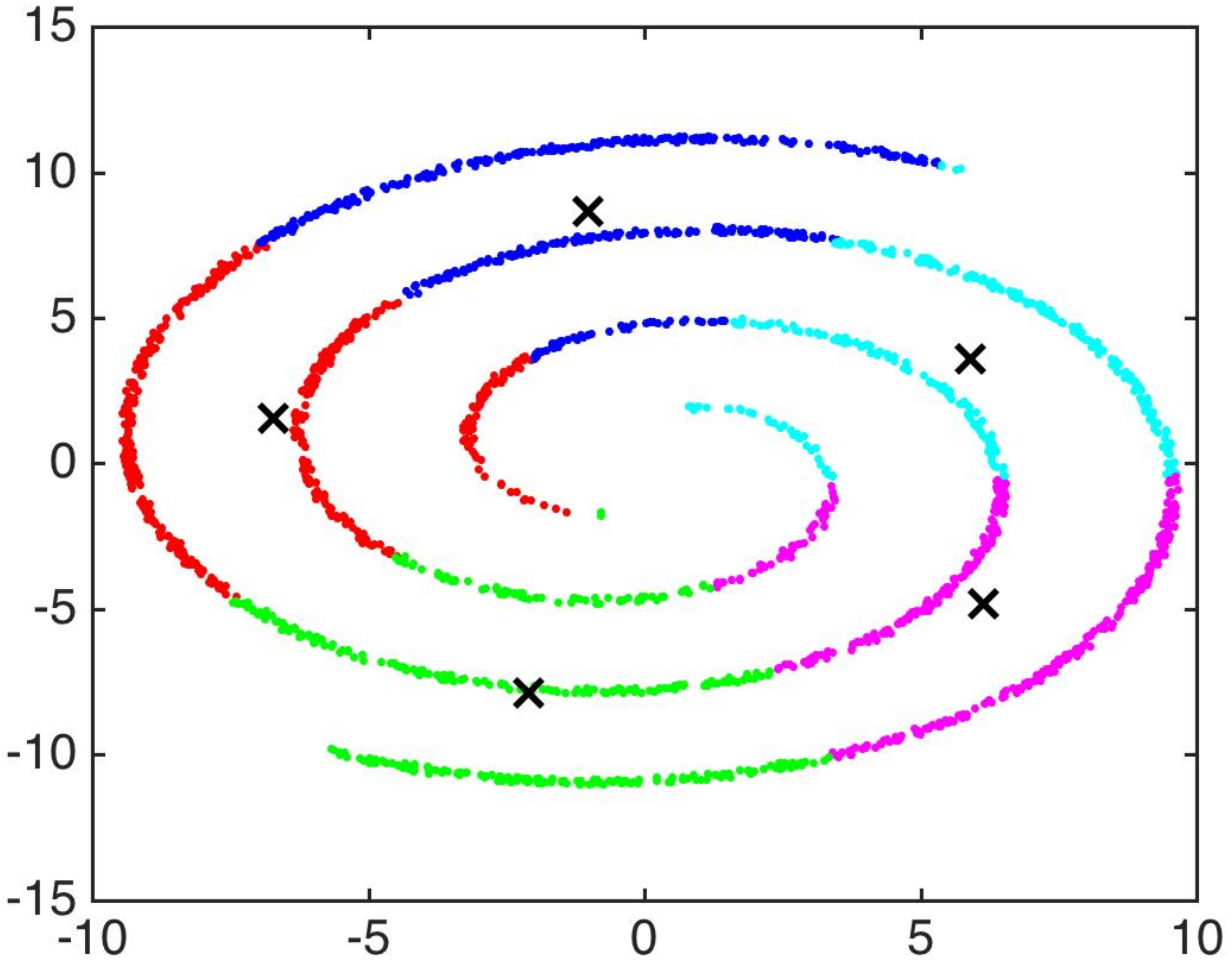
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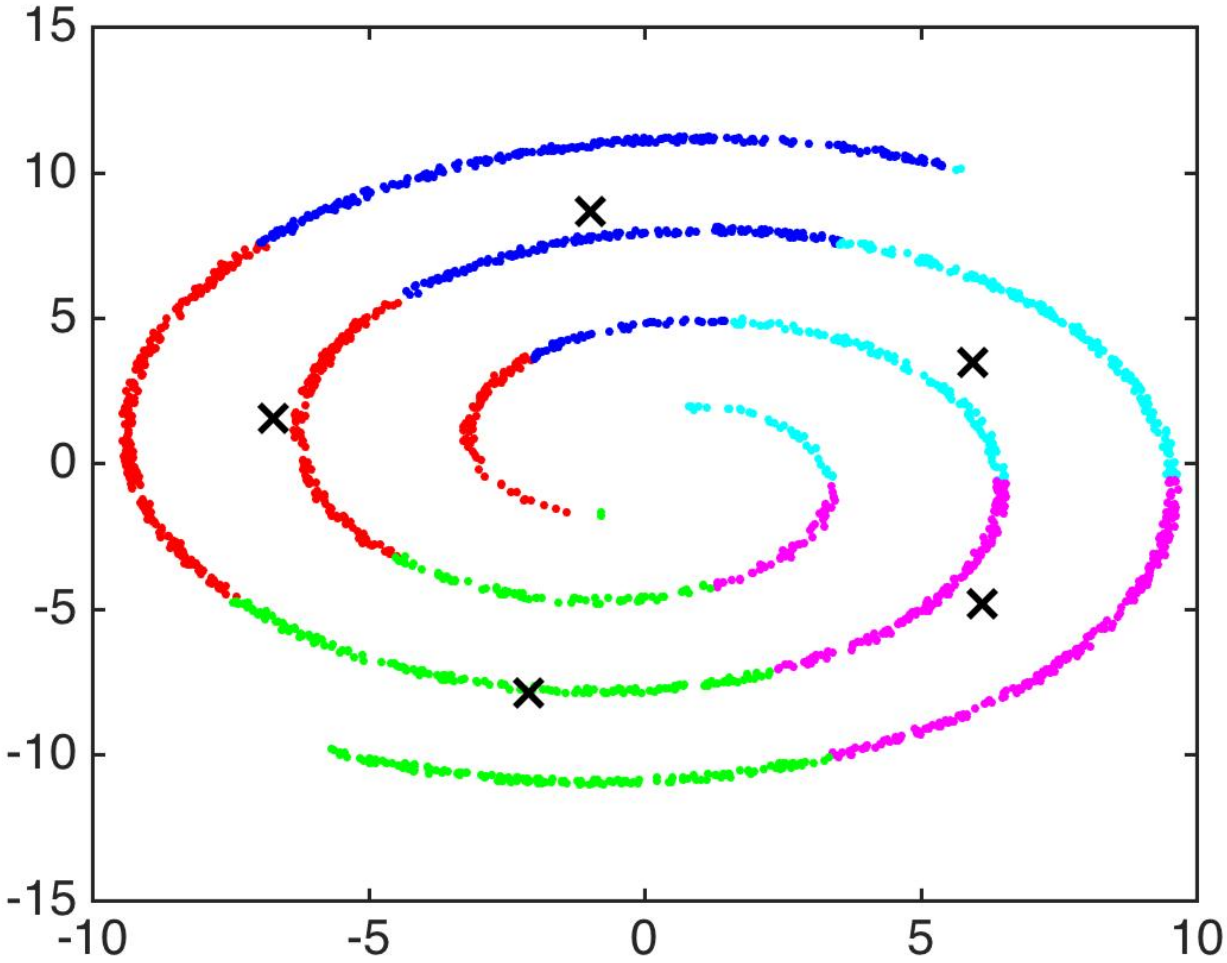
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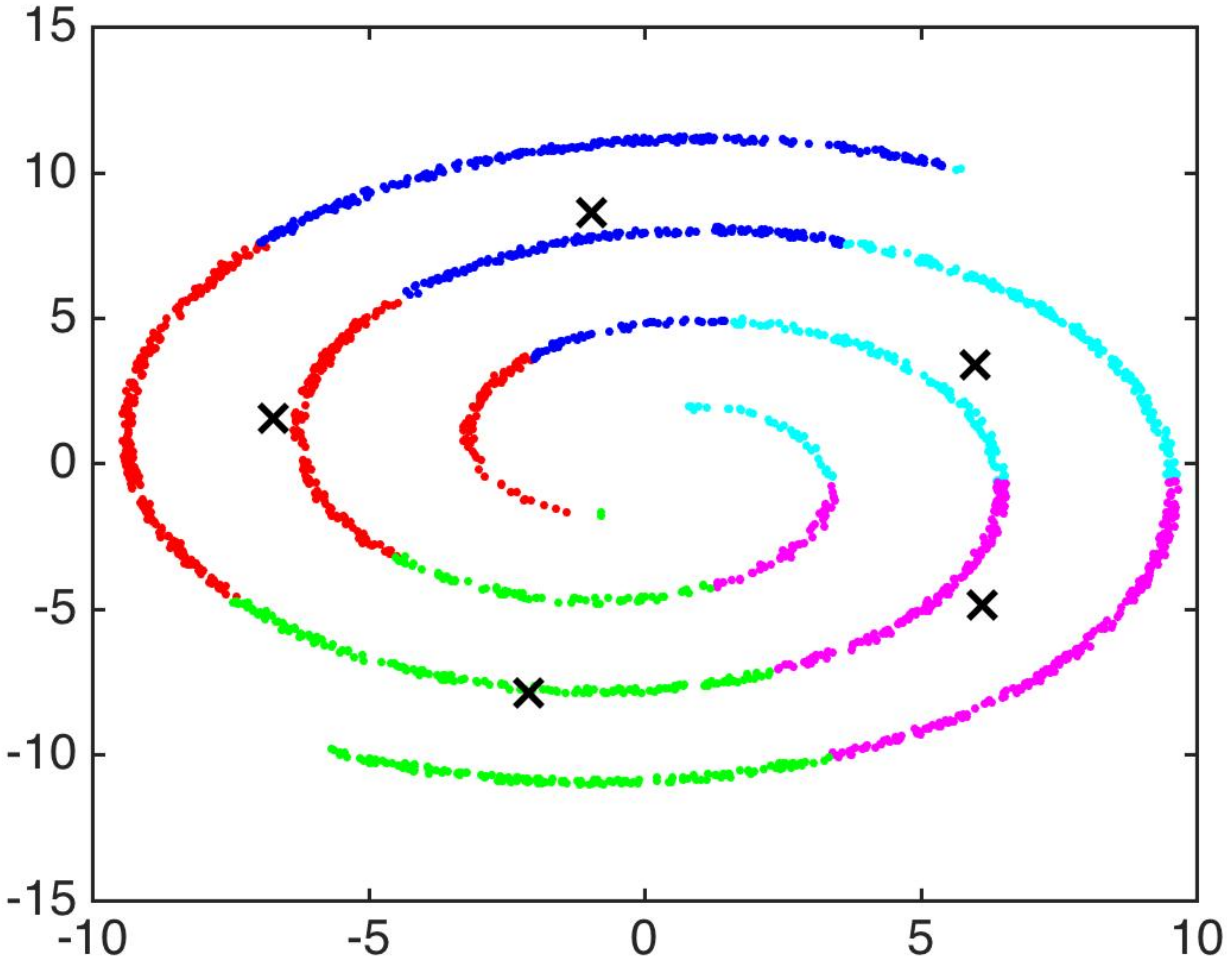
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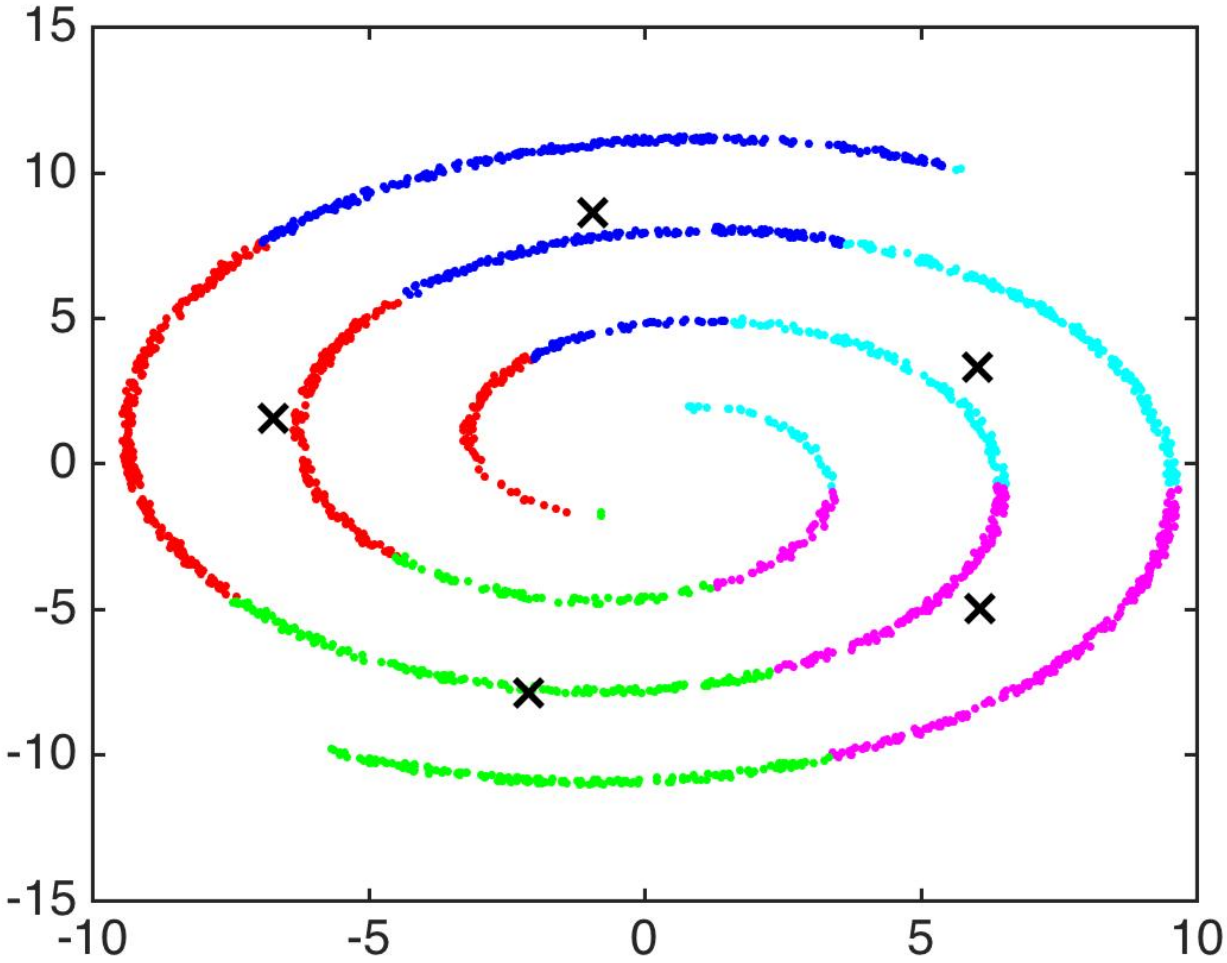
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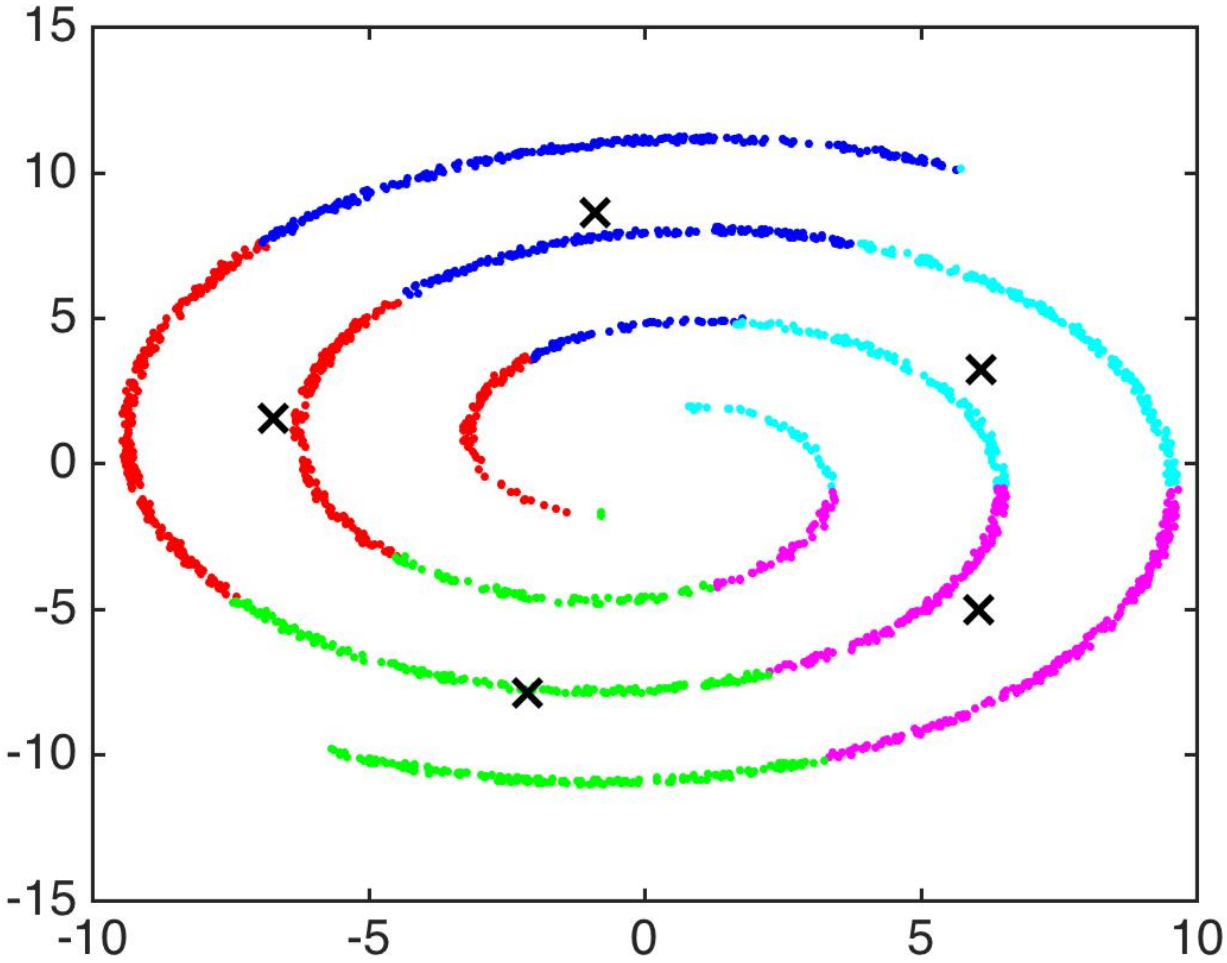
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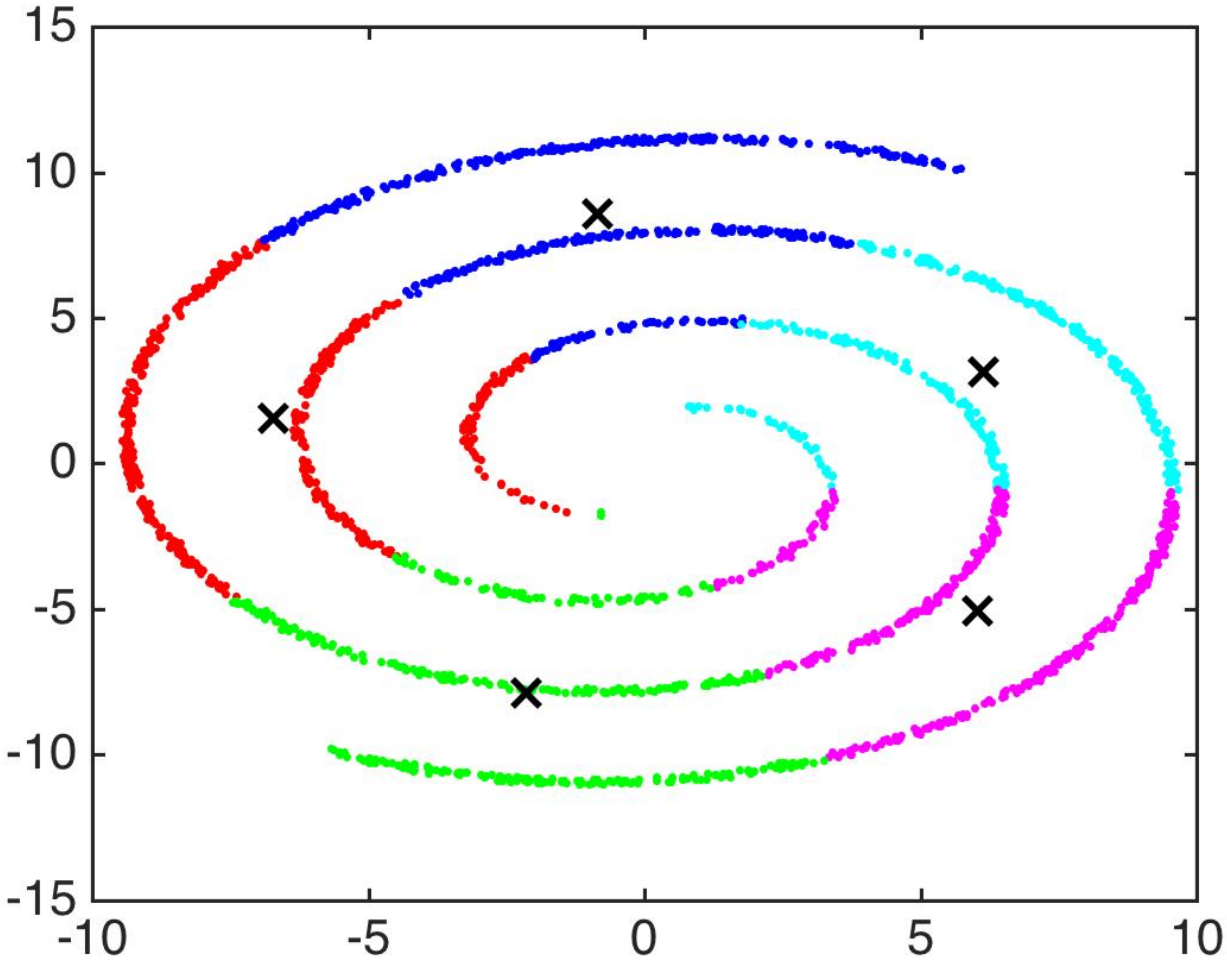
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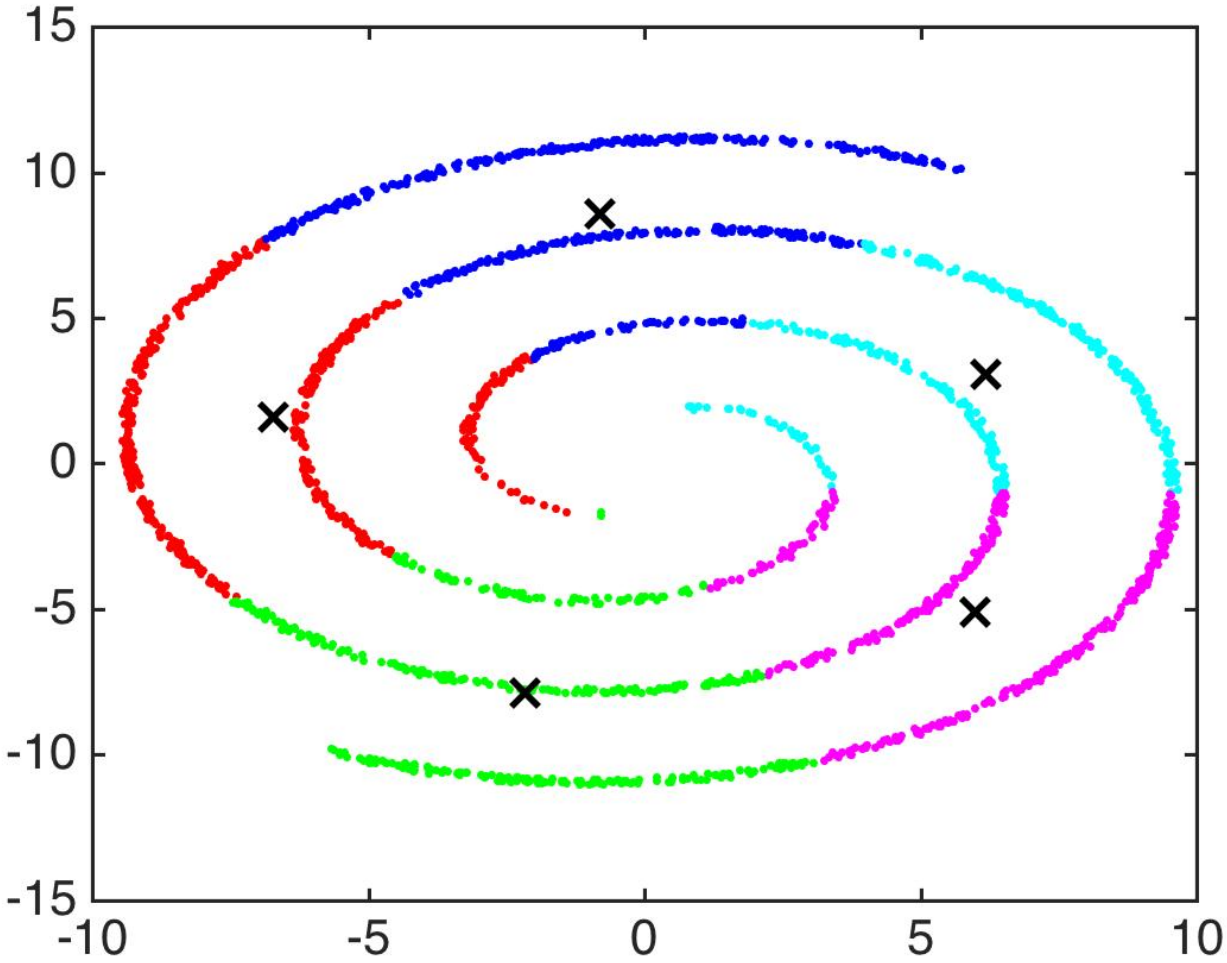
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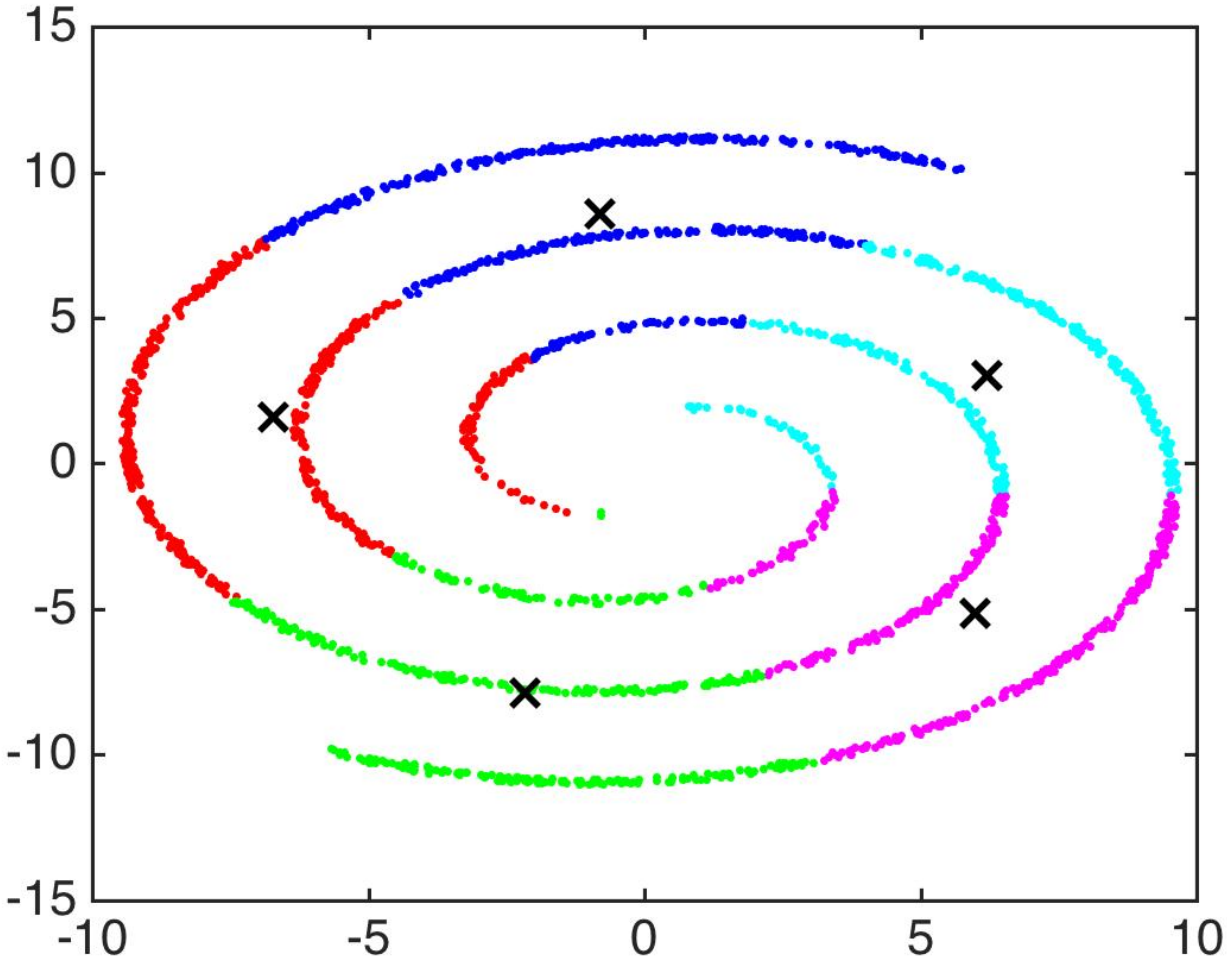
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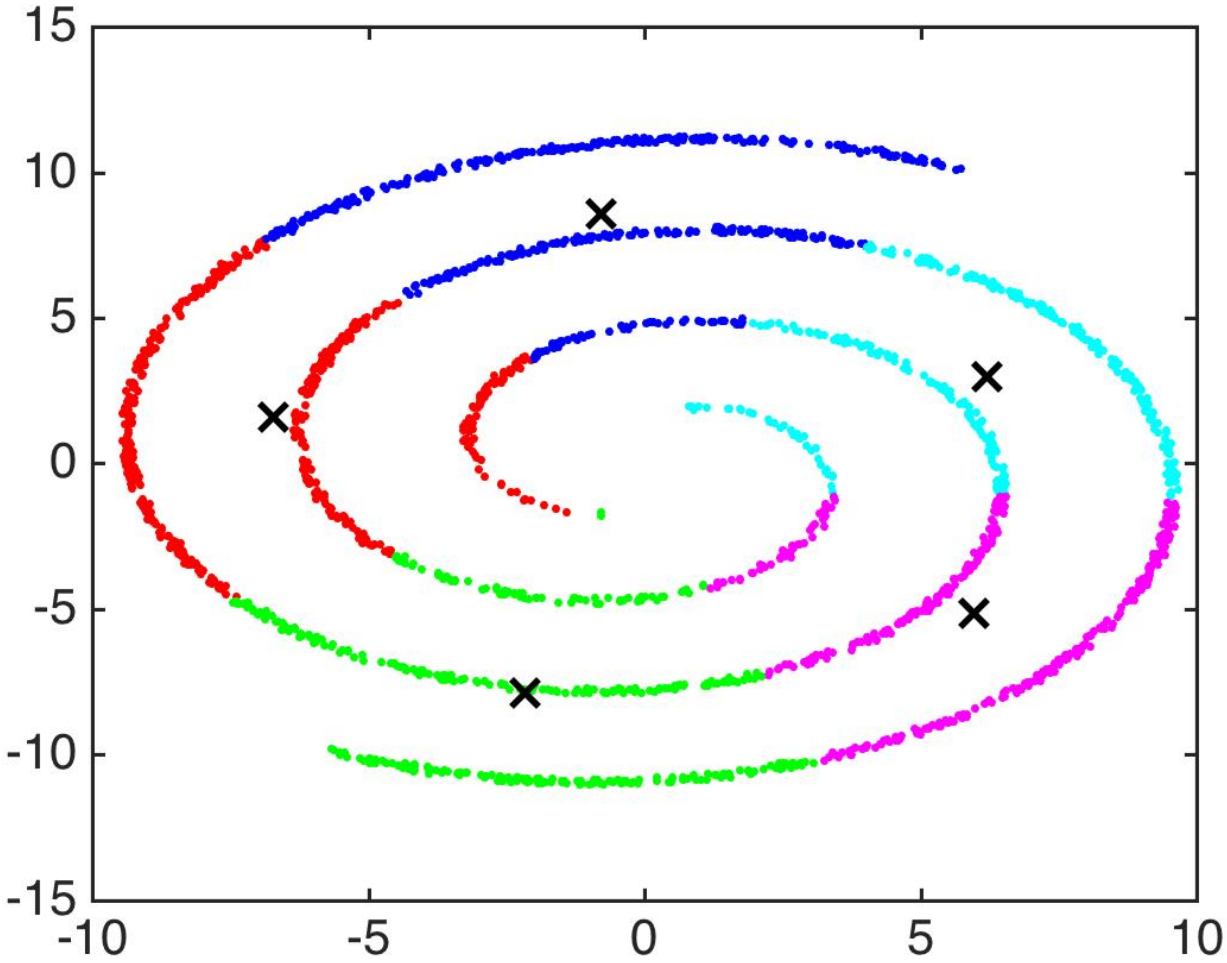
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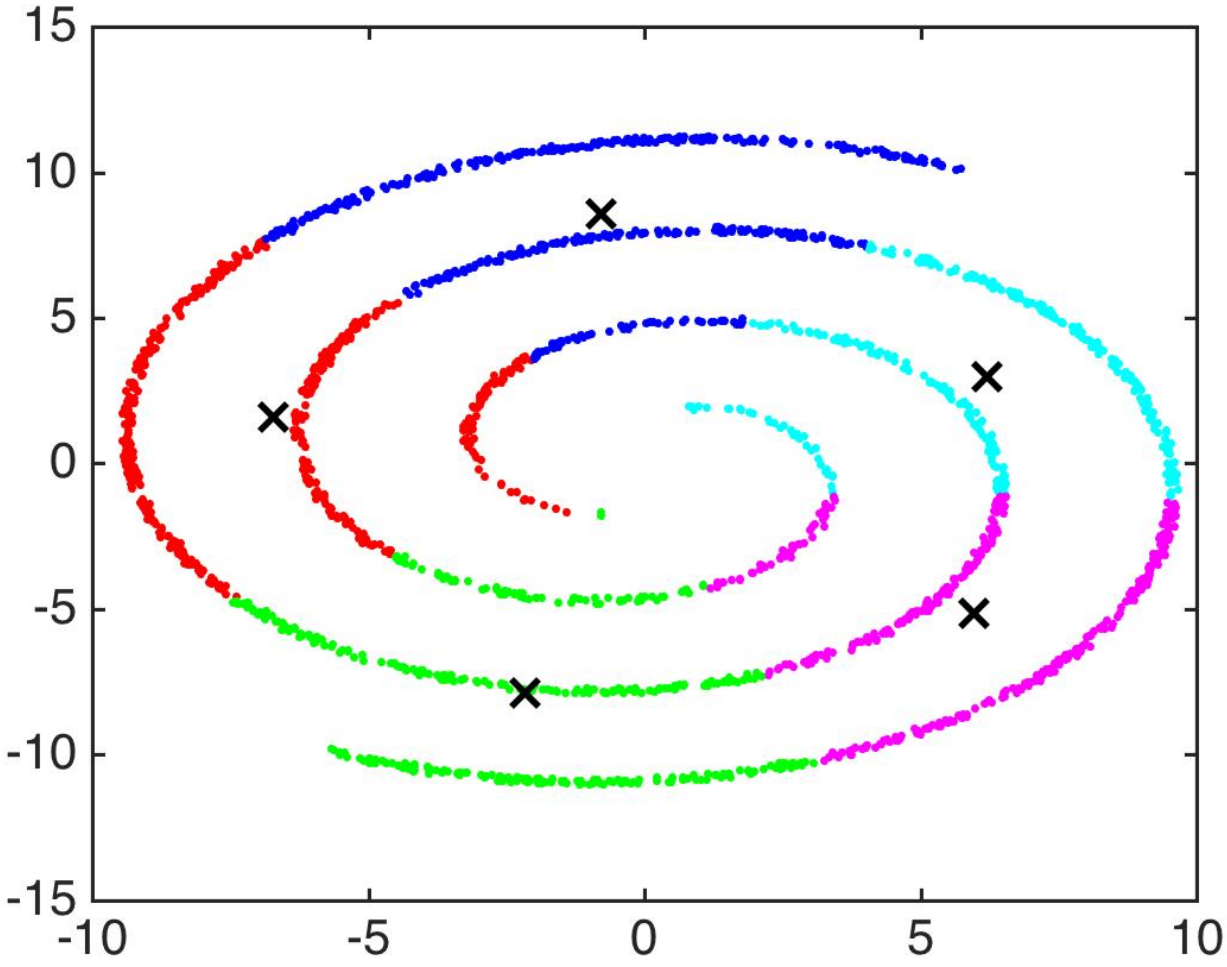
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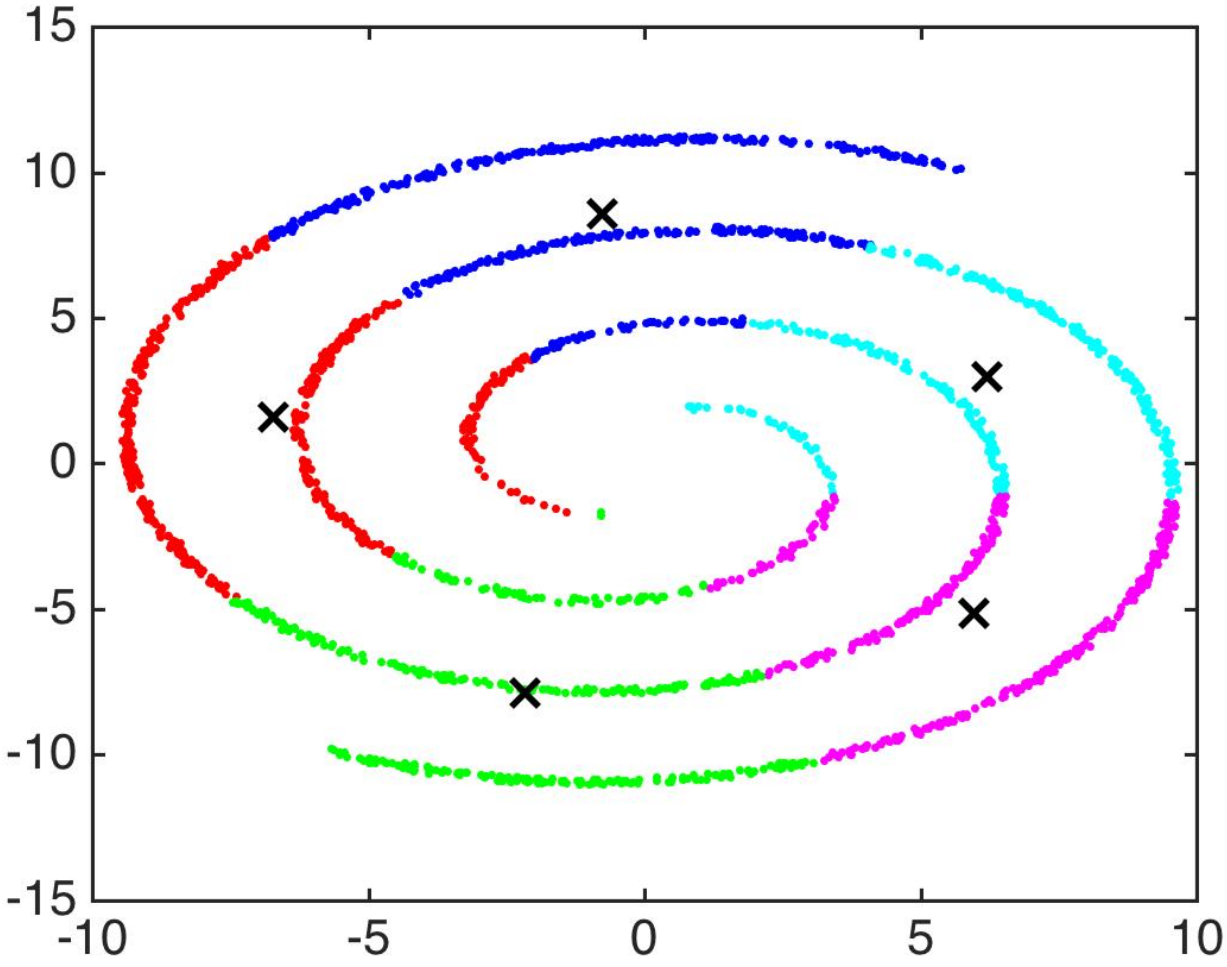
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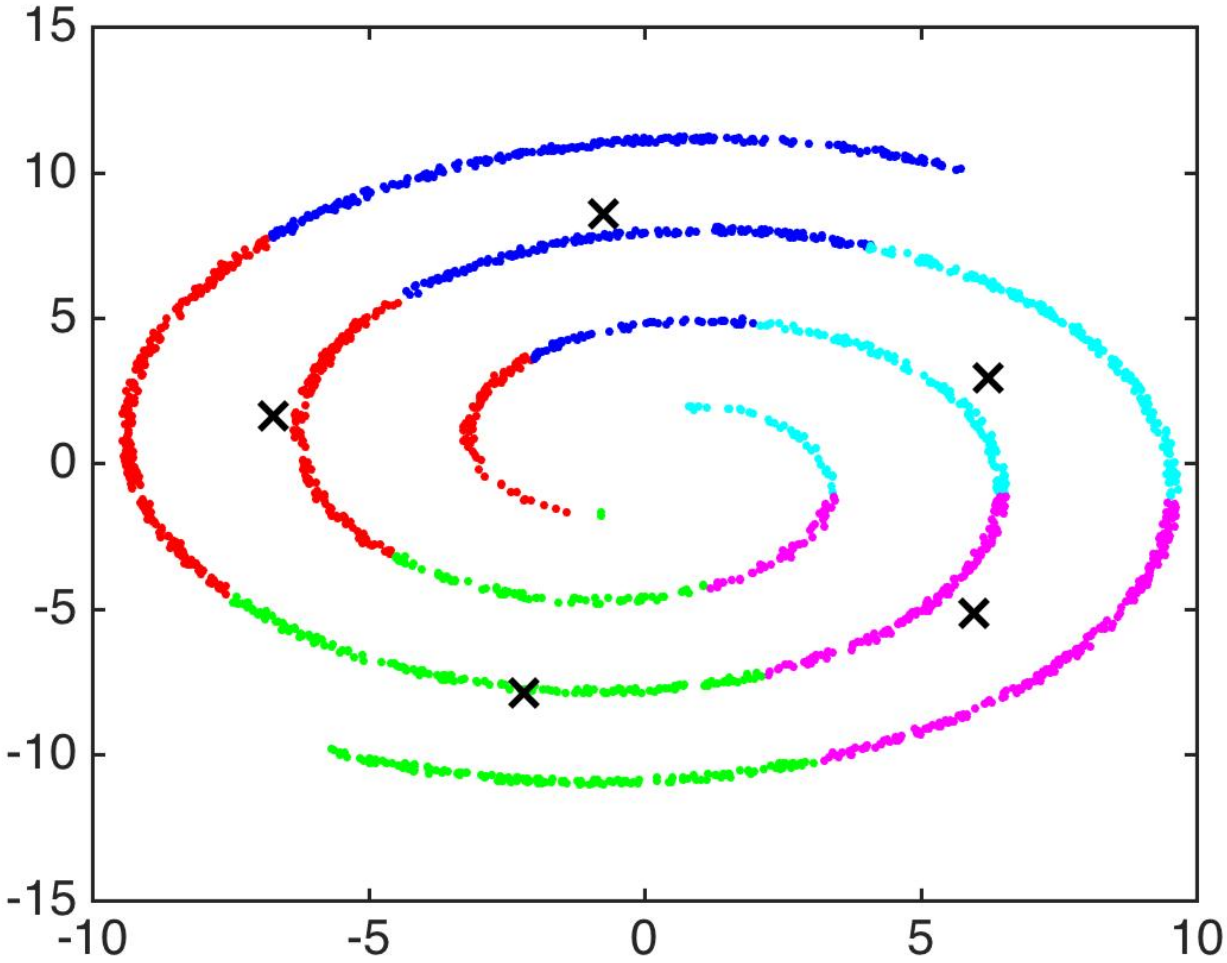
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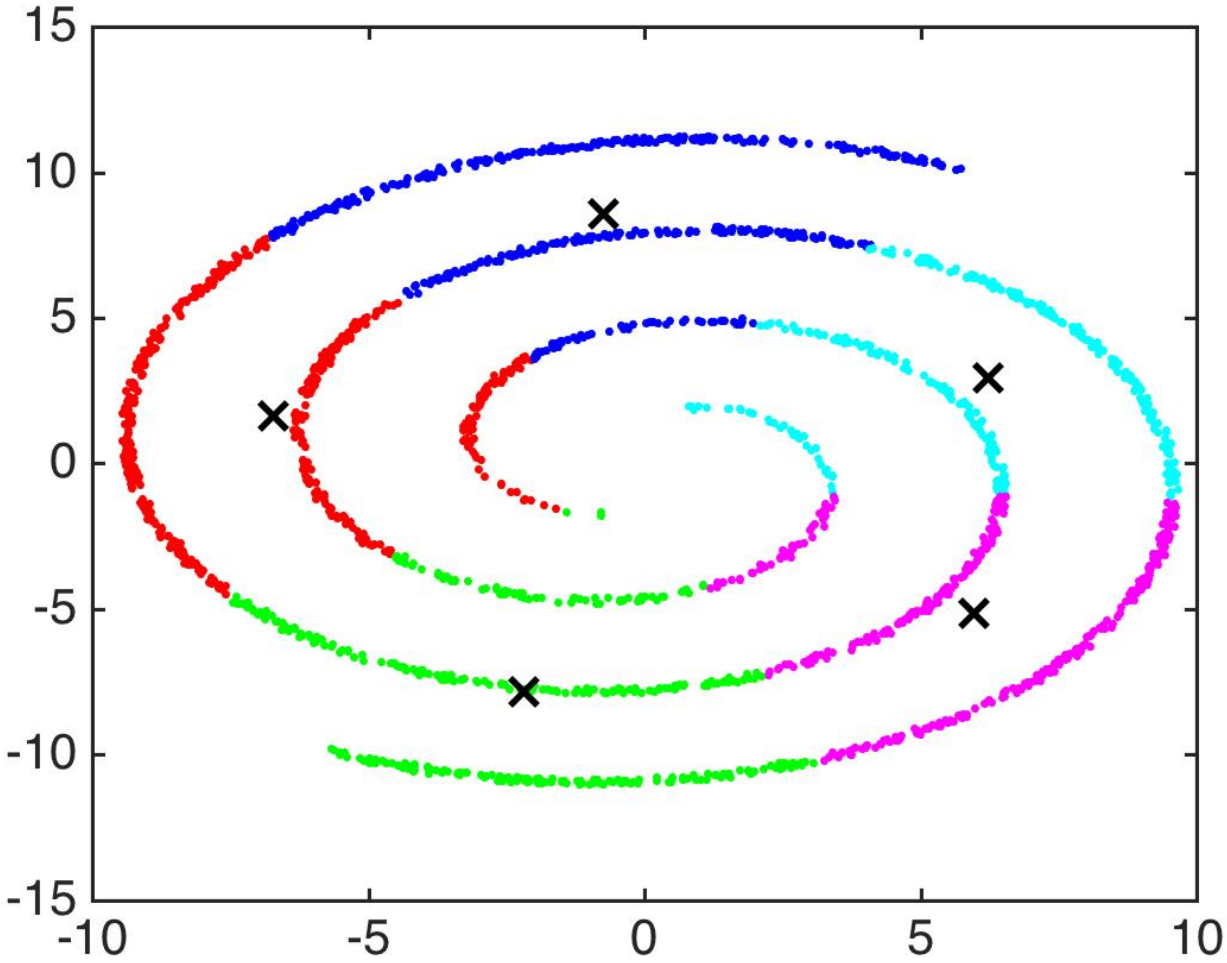
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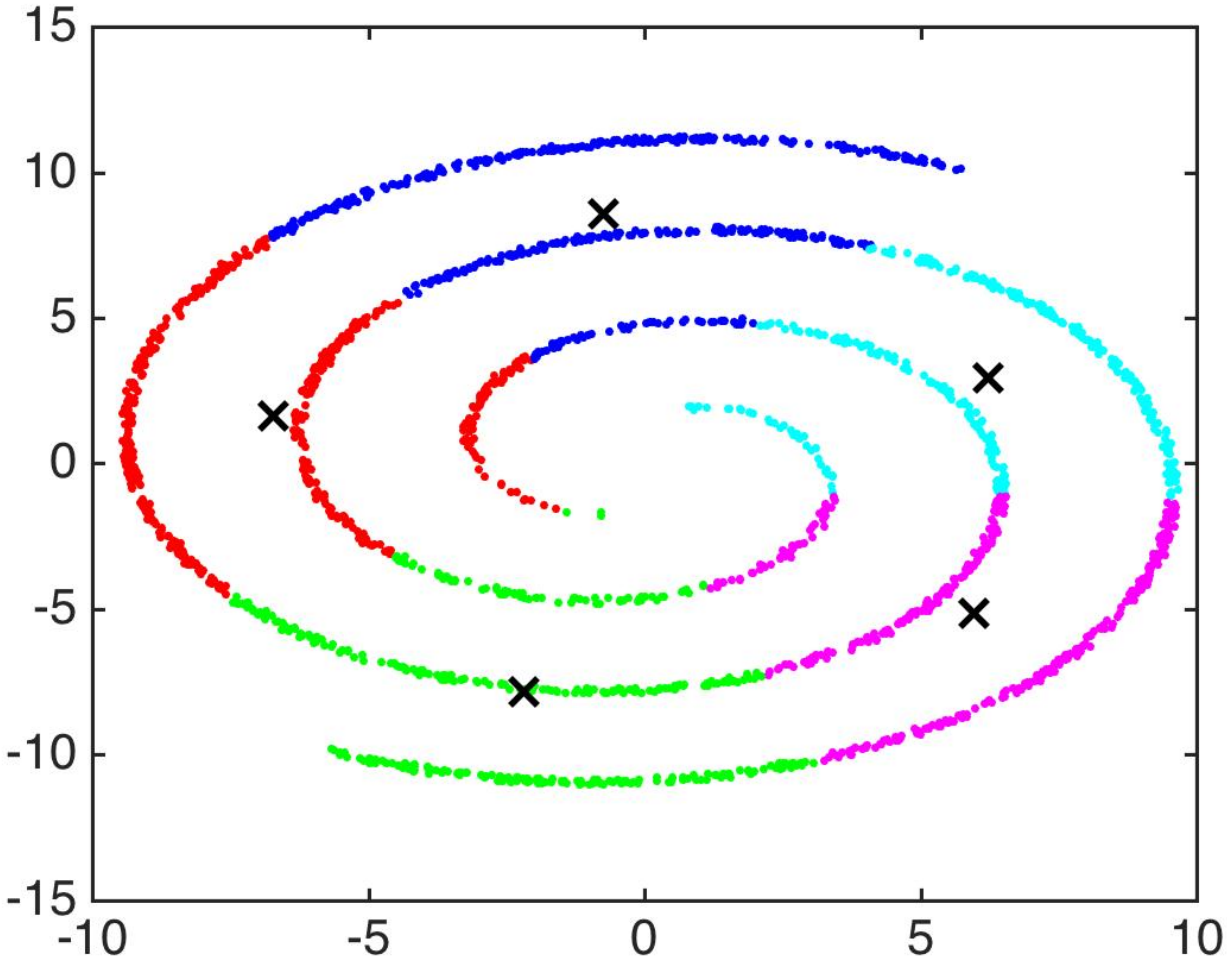
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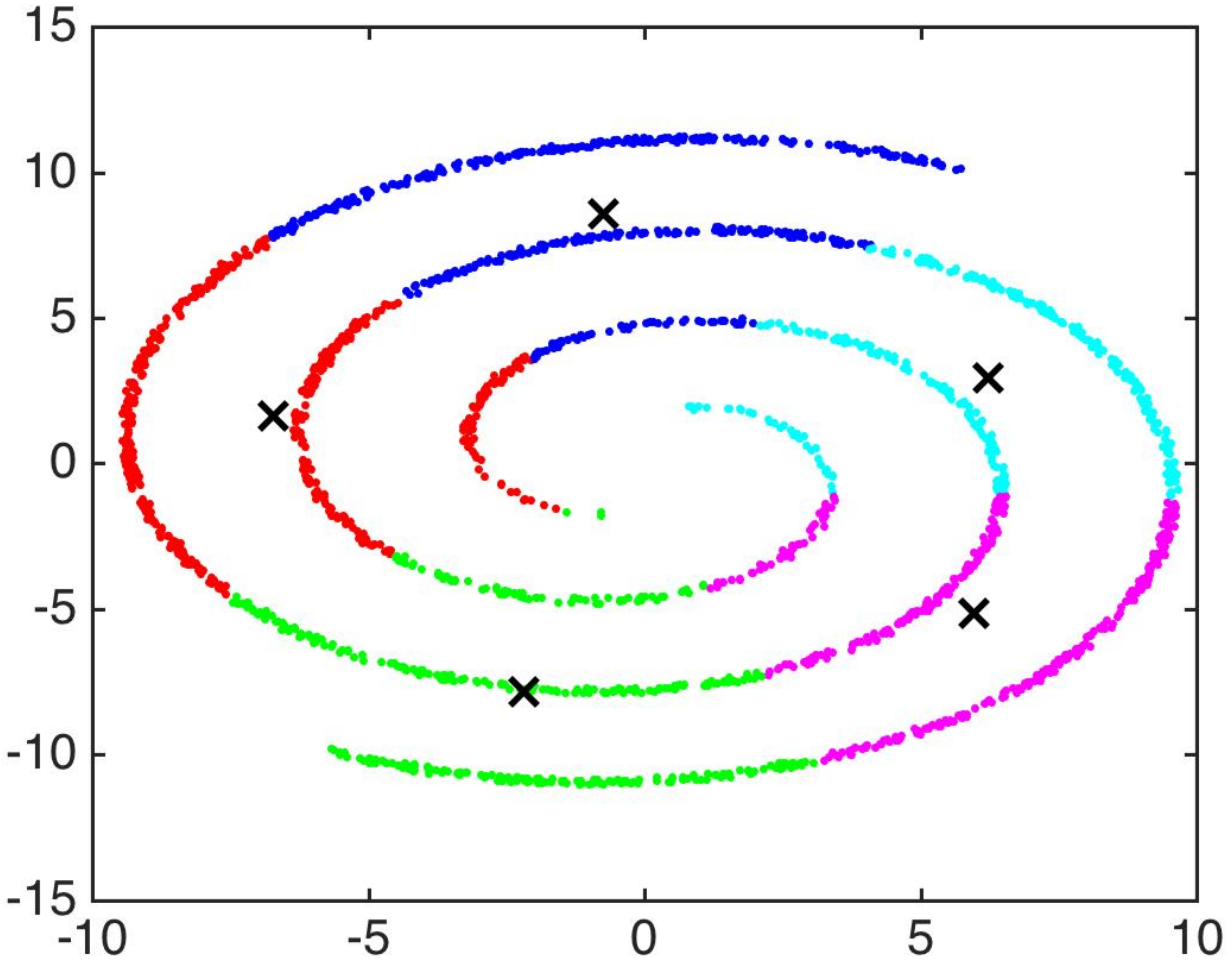
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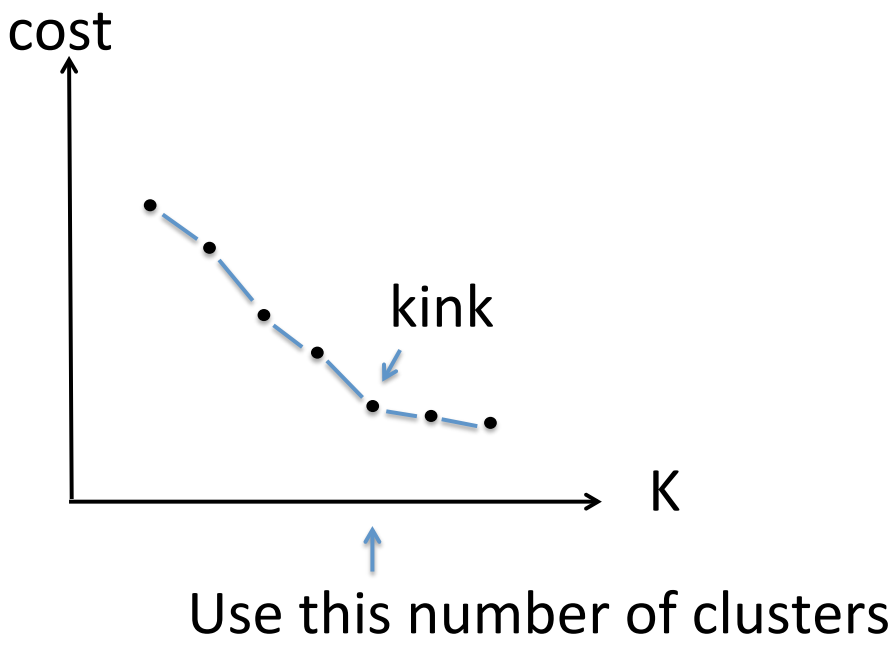
How to Choose K for K-Means

How to Choose K for K-Means



- Look for the point of diminishing returns.

K-Means

- Popular clustering algorithm, computationally efficient
- Performs alternating minimization on a cost function
- Does not always fully minimize that cost function (multiple replicates might be needed for a good solution)
- Can use the cost function to evaluate whether one replicate is better than another
- Can use cost function to help choose the number of clusters
- Doesn’t work well for highly non-spherical clusters

Note: I used Euclidean distance, but can use other distances.

Hierarchical Agglomerative Clustering

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- Start with each point in its own cluster
- Repeatedly merge the clusters of the closest two points

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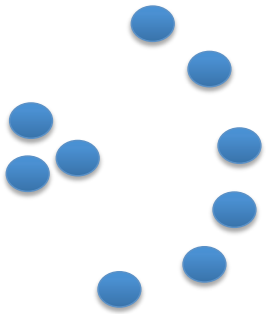

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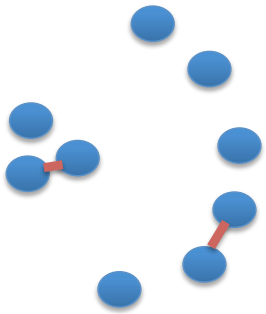

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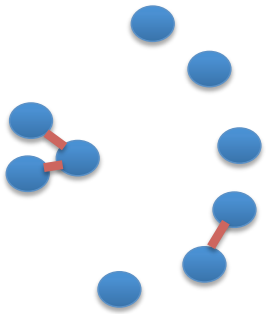

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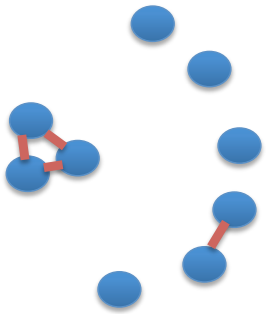

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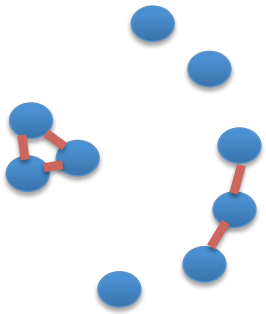

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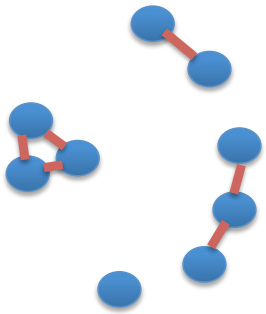

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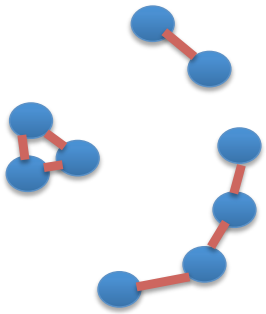

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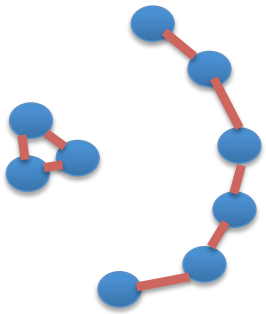

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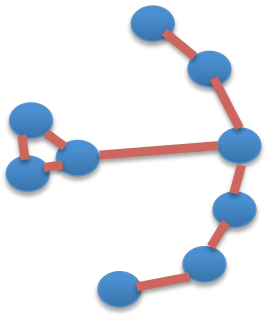

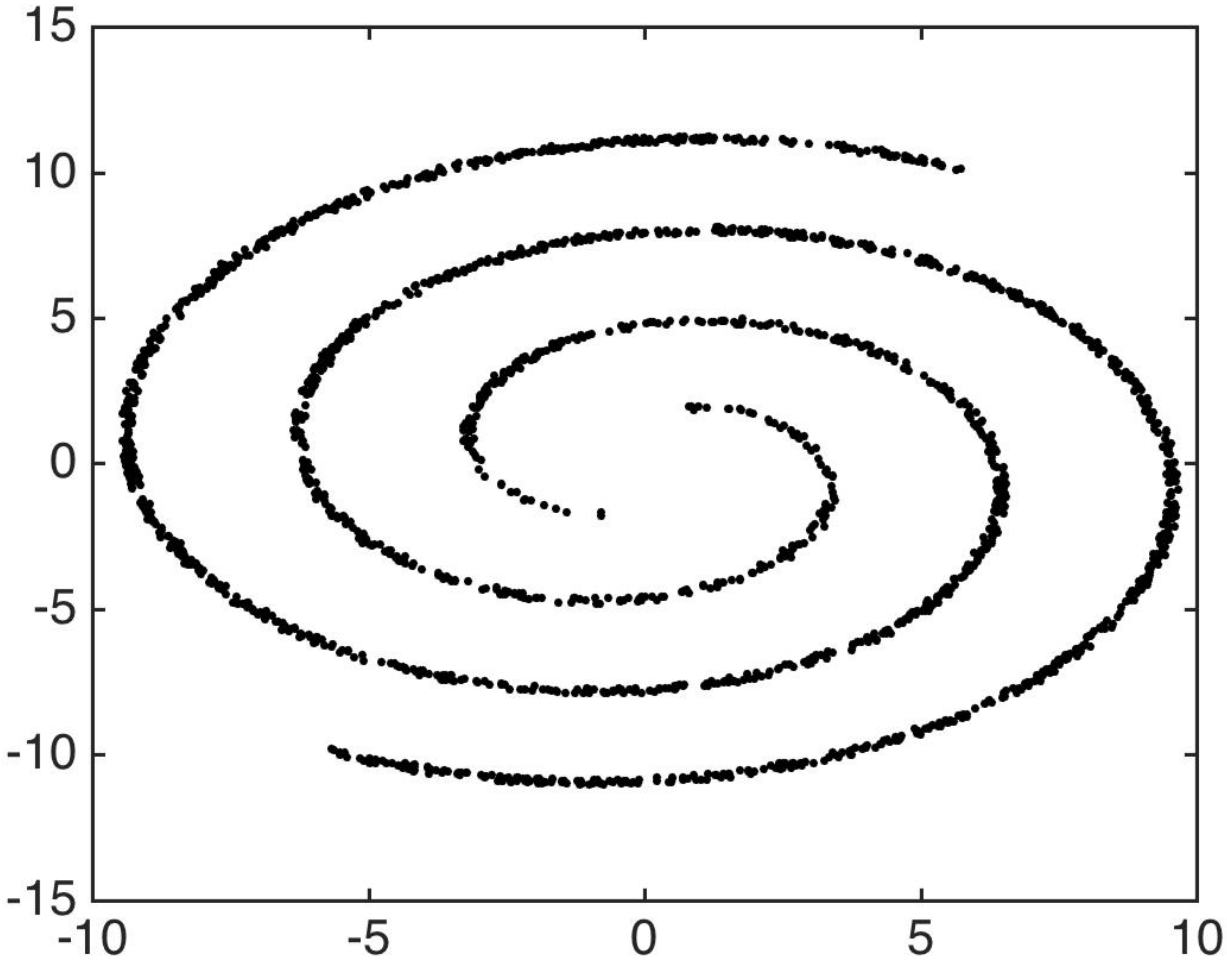
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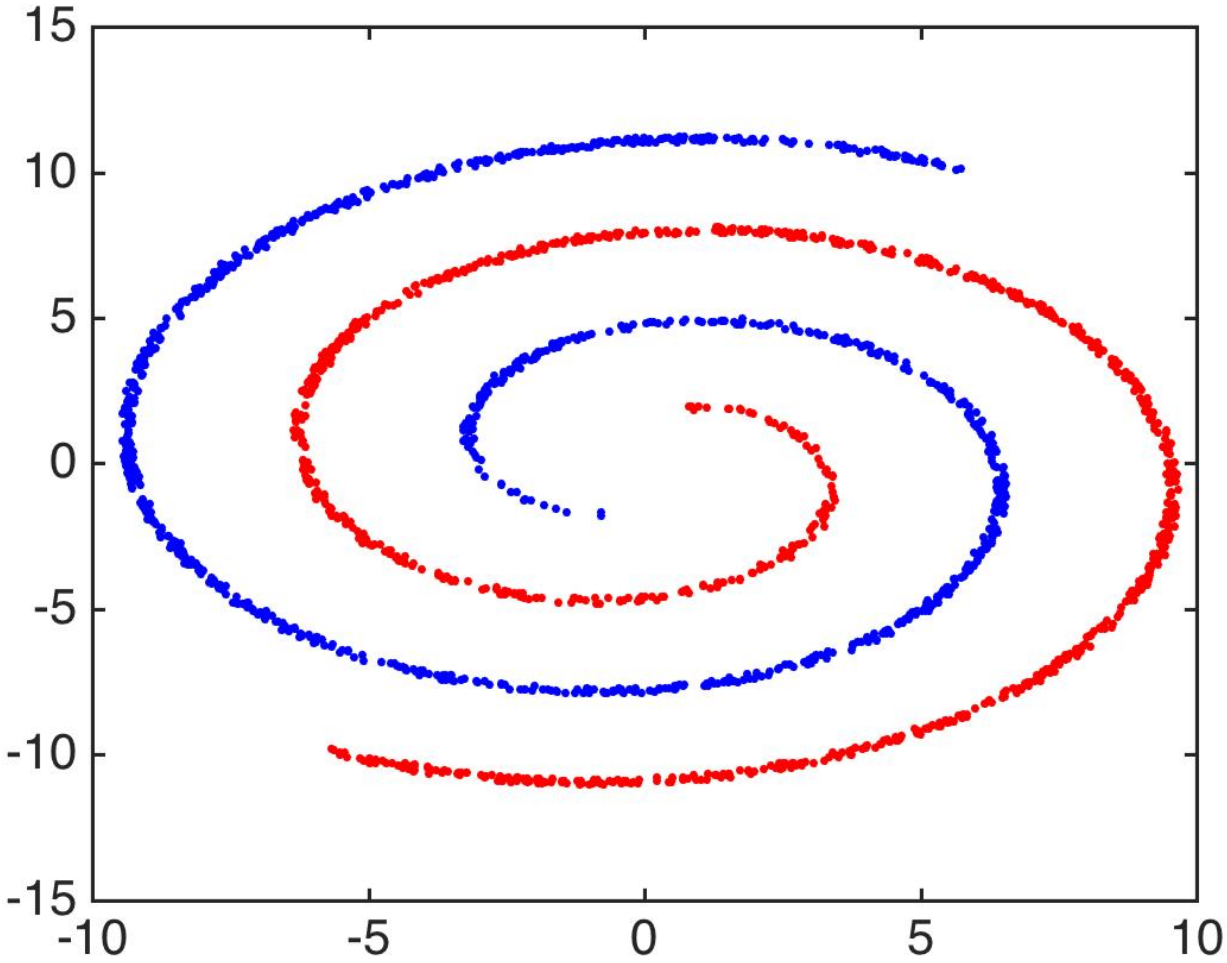
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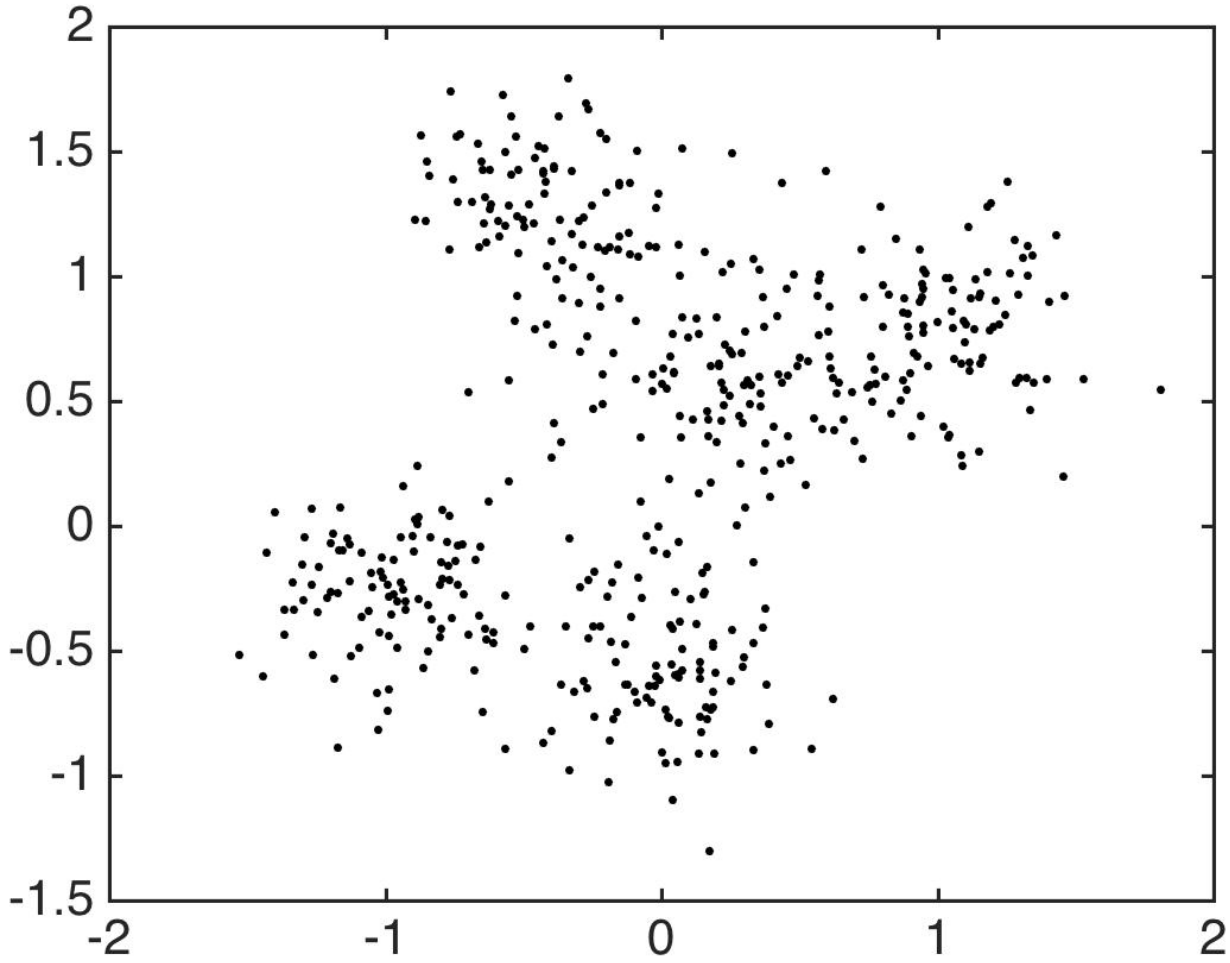
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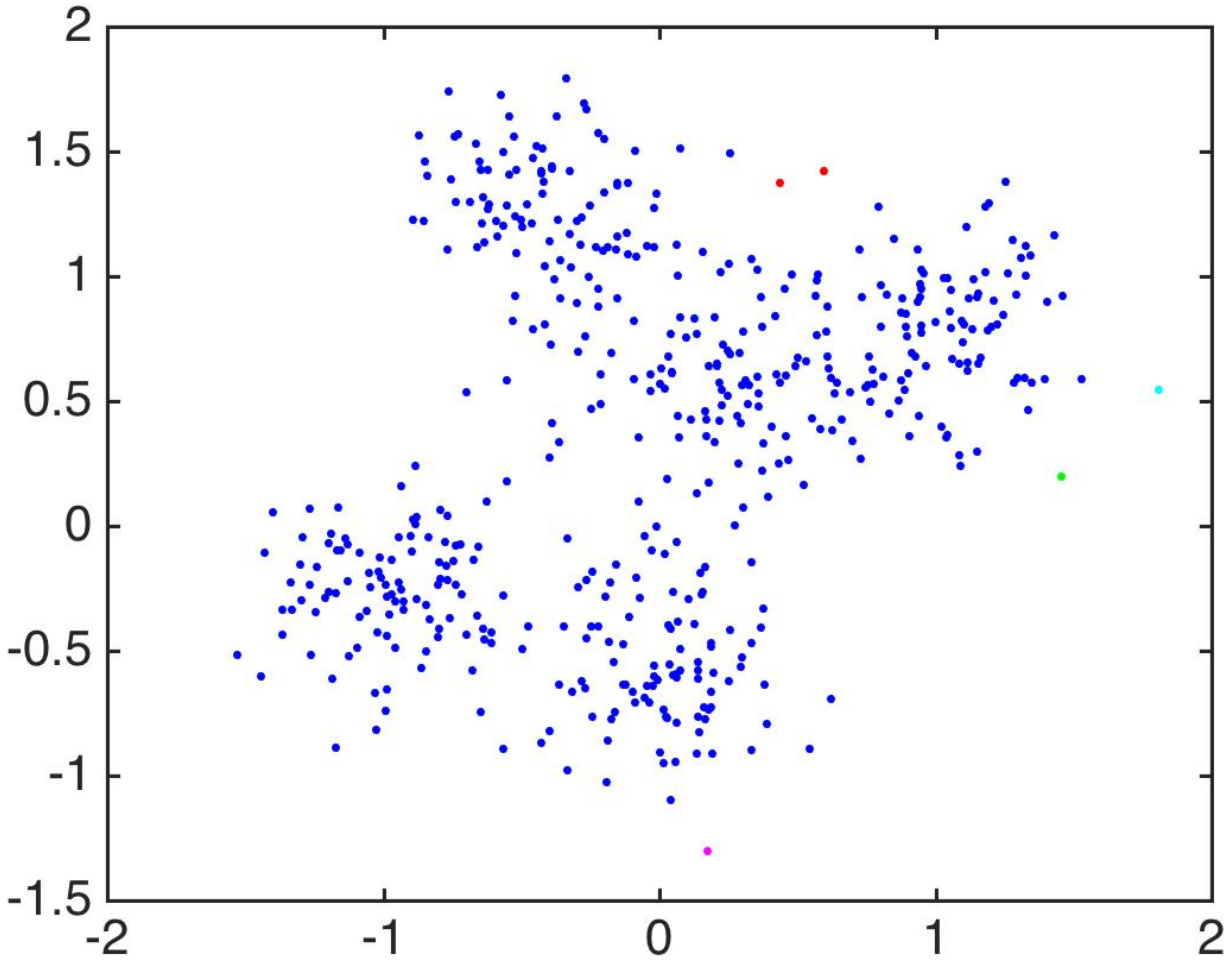
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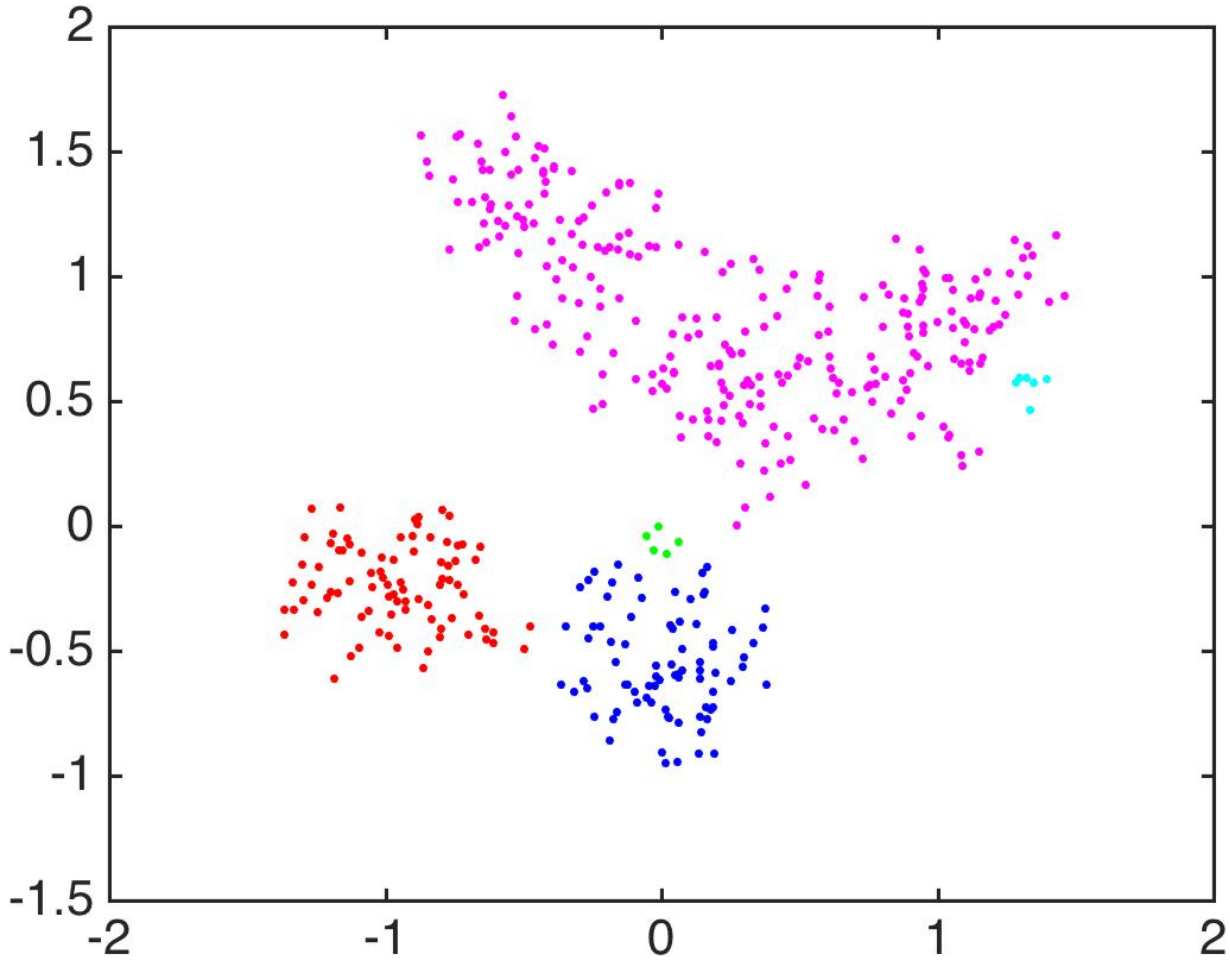
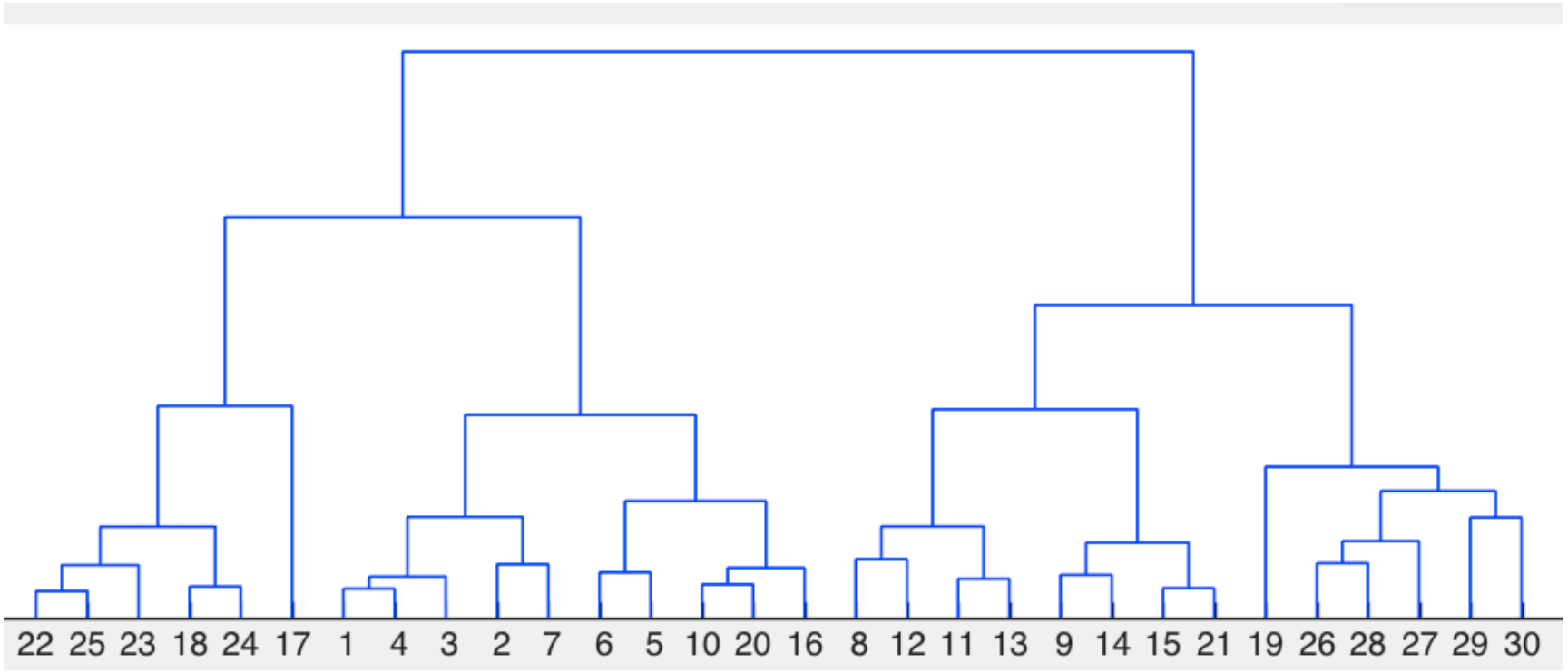
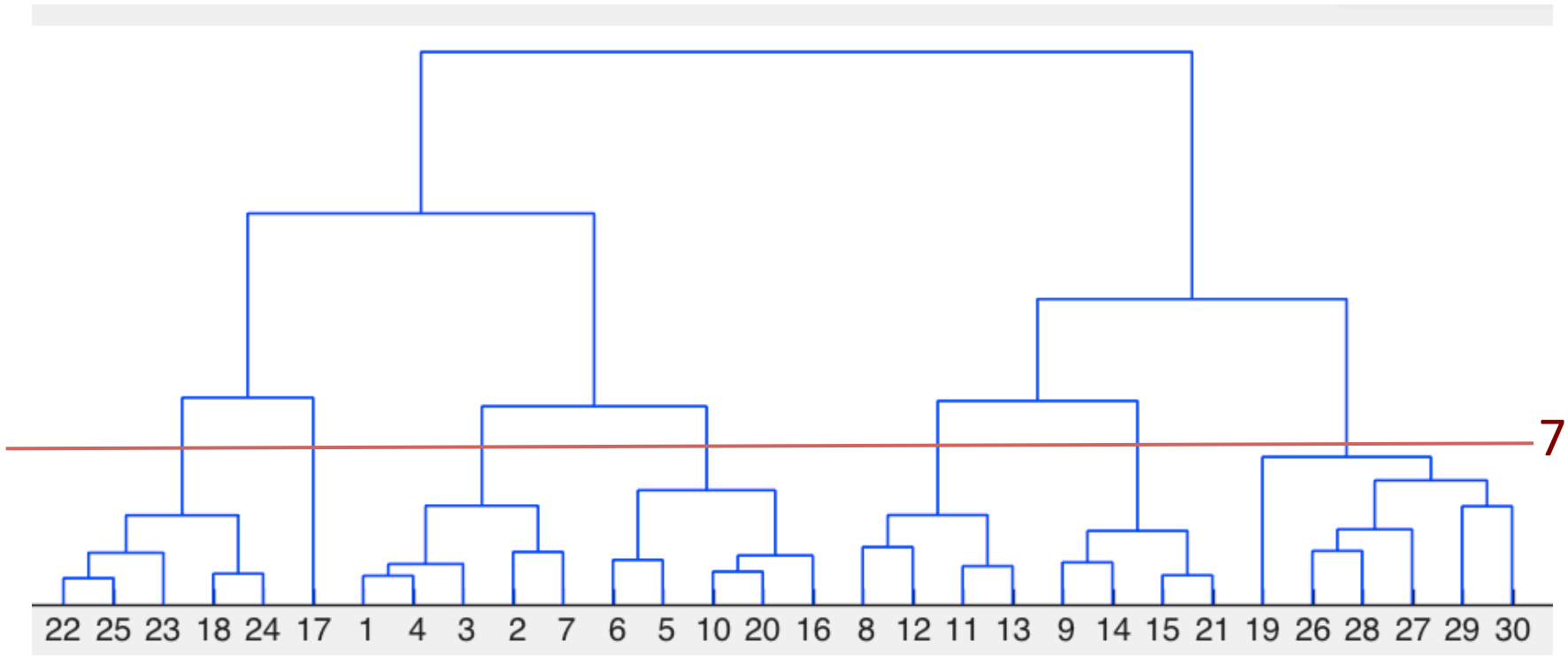

2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-1
0
1
2

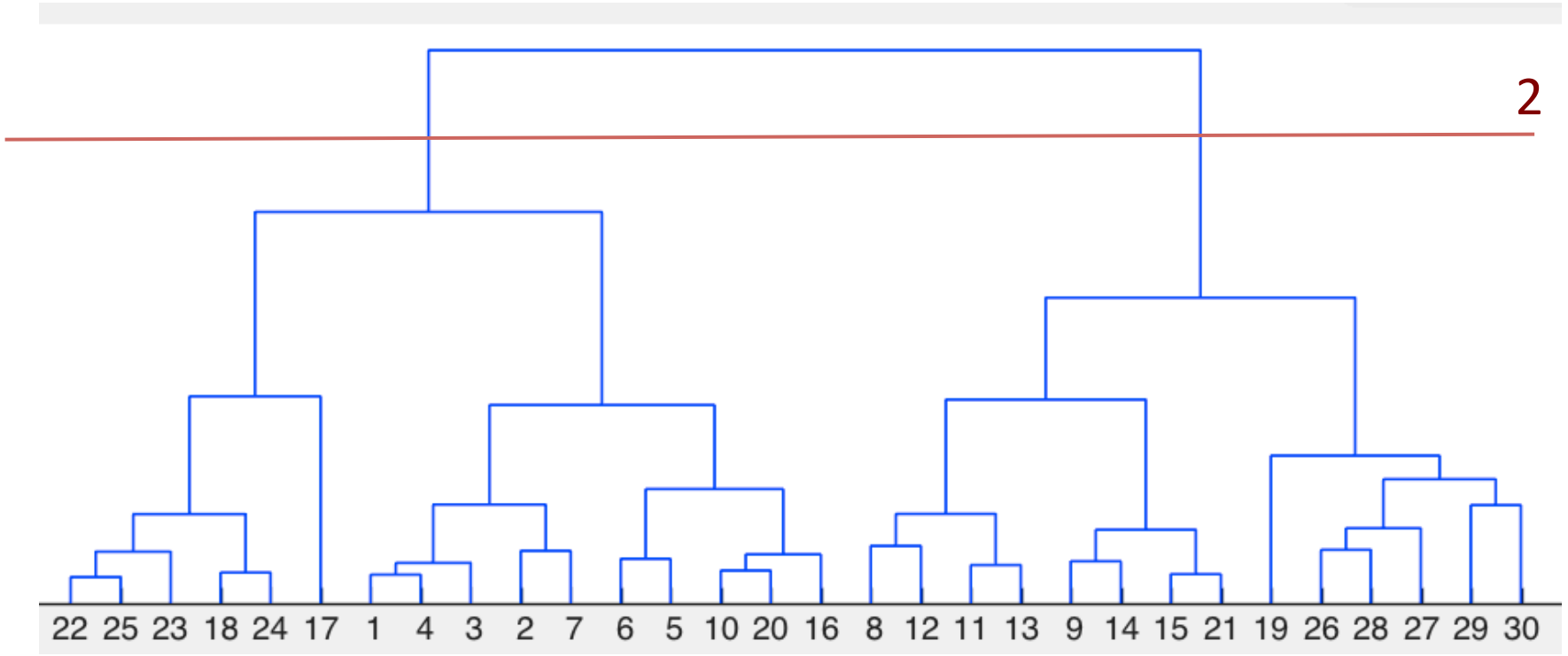
Dendrogram for Hierarchical Agglomerative Clustering



Dendrogram for Hierarchical Agglomerative Clustering



Dendrogram for Hierarchical Agglomerative Clustering



K-Means vs Hierarchical Agglomerative Clustering

- Both are useful for different sorts of problems. K-Means works well for spherical data.
- Hierarchical Agglomerative Clustering is useful when clusters are well-separated. (This means data that are close together should be in the same cluster.)
- For K-means, one needs to choose the number of clusters (try a few different ones). For hierarchical clustering, one chooses when to stop merging clusters.
- The distance metric is important. Can have a large impact on the solution.