Machine Learning & Artificial Intelligence for Data Scientists: Clustering (Part 1)

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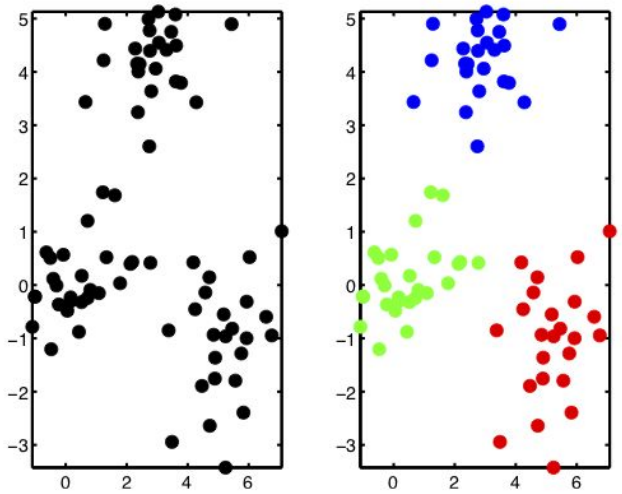
Unsupervised learning

- Everything we've seen so far has been *supervised*
- We were given a set of $\mathbf{x}_n$ **and** associated t_n.
- What if we just have $\mathbf{x}_n$?
- For example:
  - $\mathbf{x}_n$ is a binary vector indicating products customer n has bought.
  - Can group customers that buy similar products.
  - Can group products bought together.
- Known as **Clustering**
- And is an example of *unsupervised* learning.
- We'll also cover *projection* (next week)

Aims

- Understand what clustering is.
- Understand the K-means algorithm.
- Understand the idea of mixture models.

Clustering



- In this example each object has two attributes:

$$\mathbf{x}_n = [x_{n1}, x_{n2}]^{\mathsf{T}}$$

- Left: data.
- Right: data after clustering (points coloured according to cluster membership).

What we'll cover

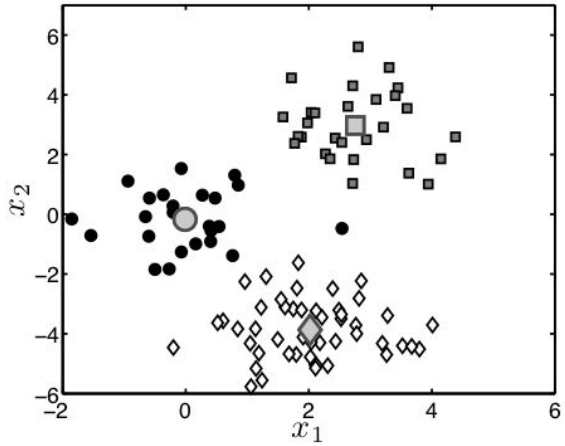
- 2 algorithms
  - K-means
  - Mixture models
- The two are related
- We'll also see how K-means can be kernelised

K-means

- Assume that there are K clusters.
- Each cluster is defined by a position in the input space:

$$\boldsymbol{\mu}_k = [\mu_{k1}, \mu_{k2}]^{\mathsf{T}}$$

- Each $\mathbf{x}_n$ is assigned to its closest cluster:



- Distance is normally Euclidean distance:

$$d_{nk} = (\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathsf{T}}(\mathbf{x}_n - \boldsymbol{\mu}_k)$$

How do we find the cluster means

- No analytical solution – we can't write down $\boldsymbol{\mu}_k$ as a function of $\mathbf{X}$.
- Use an iterative algorithm:
  1. Guss $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_K$
  2. Assign each $\mathbf{x}_n$ to its closest $\boldsymbol{\mu}_k$
  3. $z_{nk} = 1$ if $\mathbf{x}_n$ assigned to $\boldsymbol{\mu}_k$ (0 otherwise)
  4. Update $\boldsymbol{\mu}_k$ to average of $\mathbf{x}_n$s assigned to $\boldsymbol{\mu}_k$:

$$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} z_{nk}\mathbf{x}_n}{\sum_{n=1}^{N} z_{nk}}$$

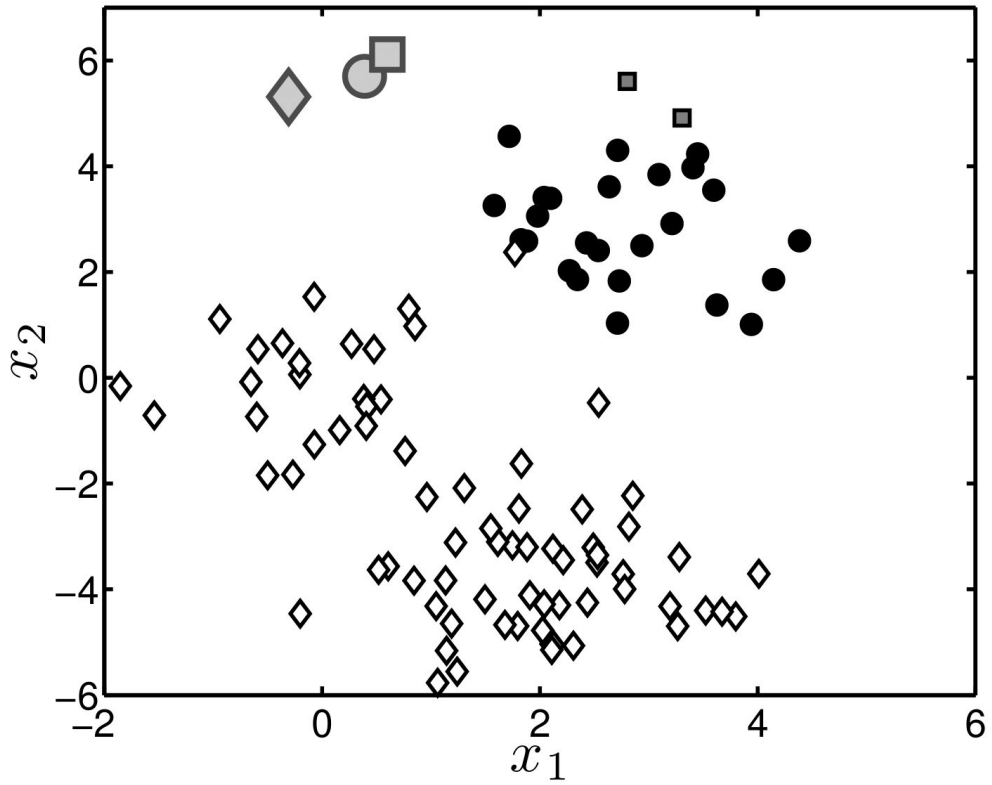
  5. Return to 2 until assignments do not change.
- Algorithm will converge....it will reach a point where the assignments don't change.

Let’s play a K-means game

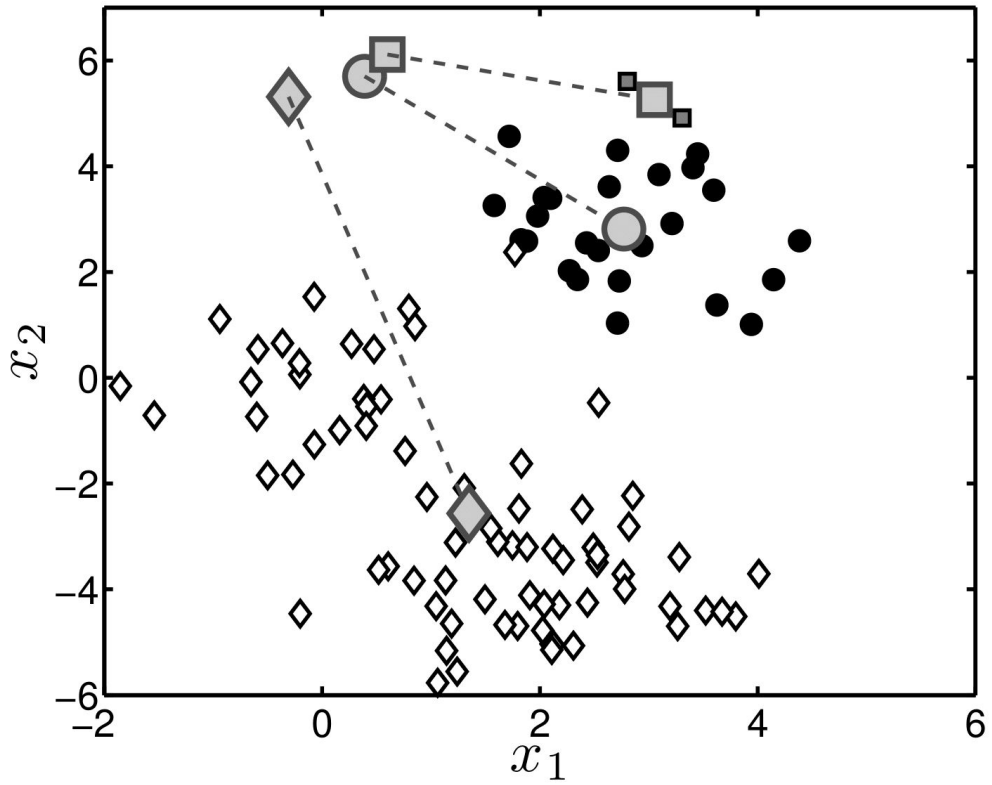
- Everyone comes to the front
- 3 volunteers act as 3 centroids
- All the rest as data points

Gather space: https://gather.town/i/Qw7GtyJN

K-means - example



K-means - example



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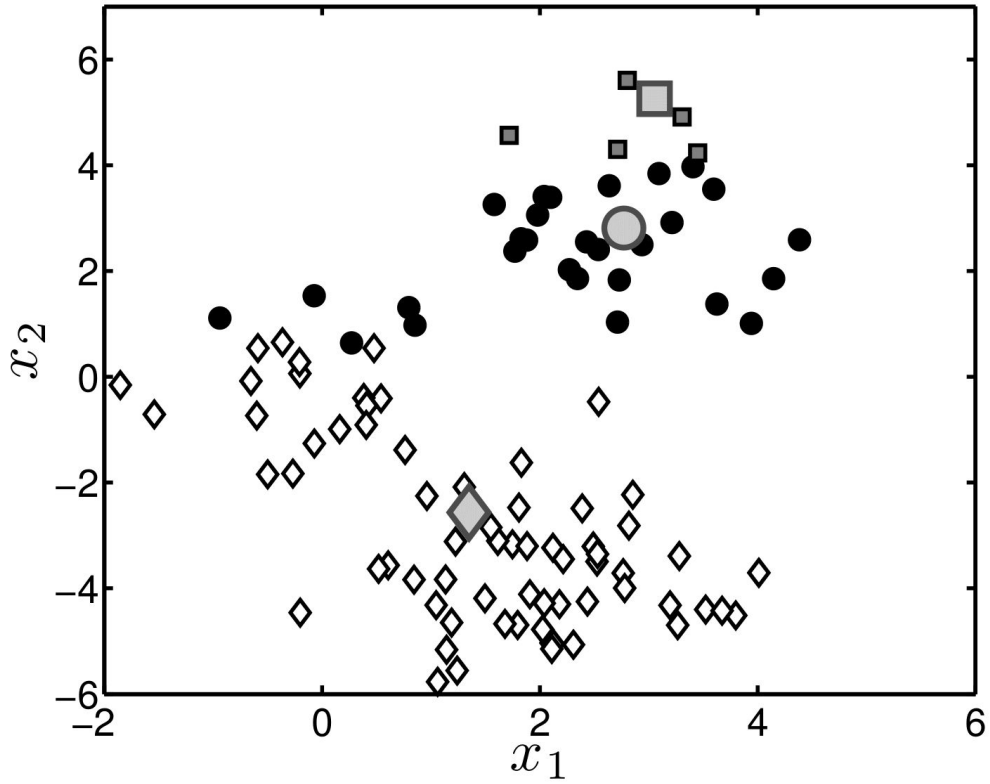

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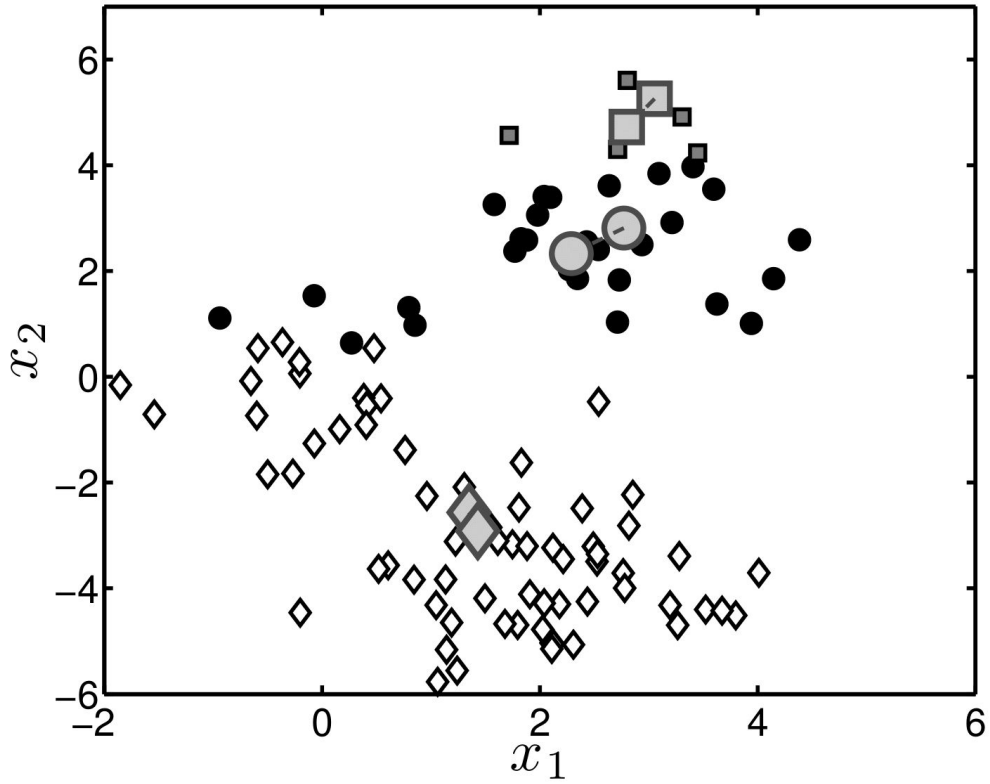

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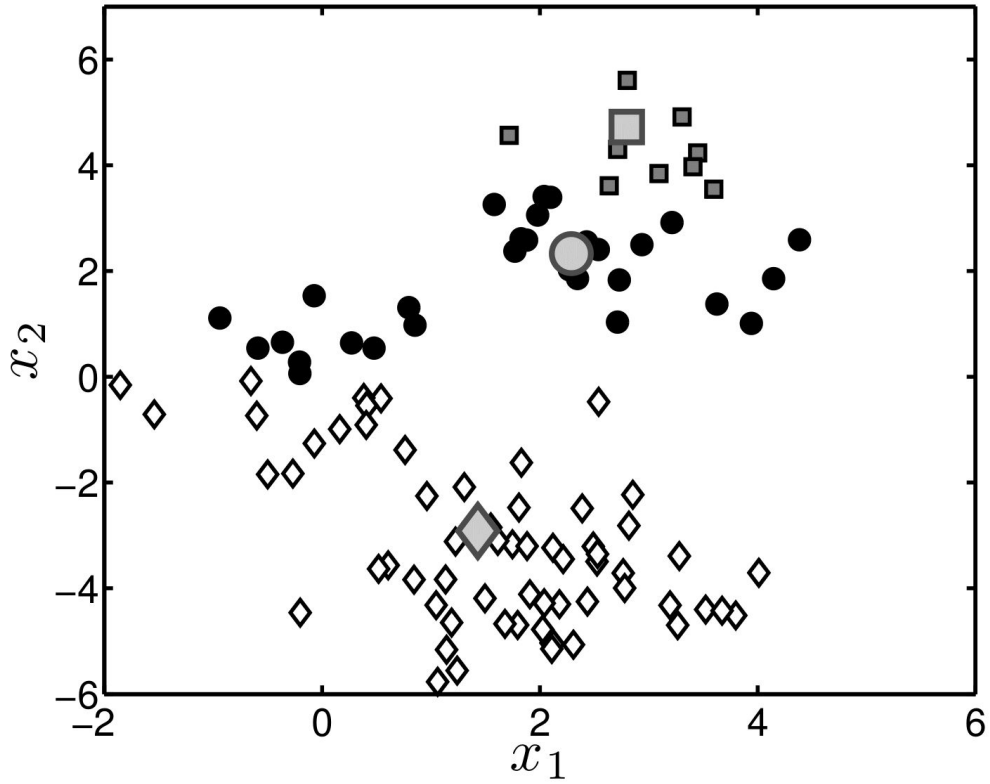

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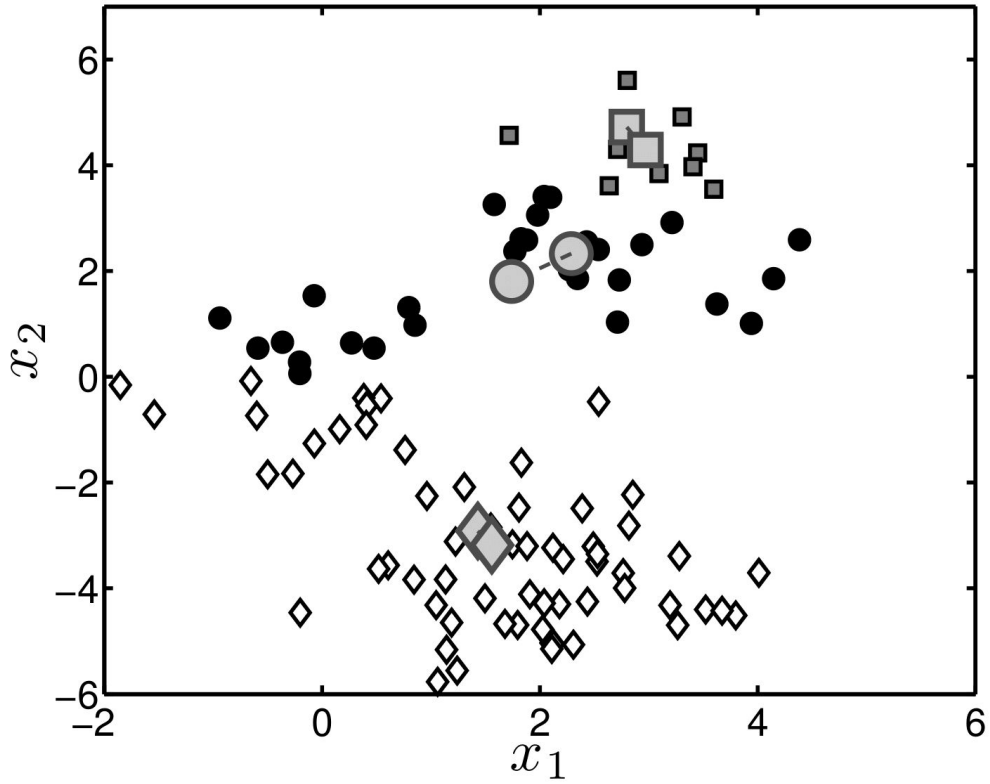
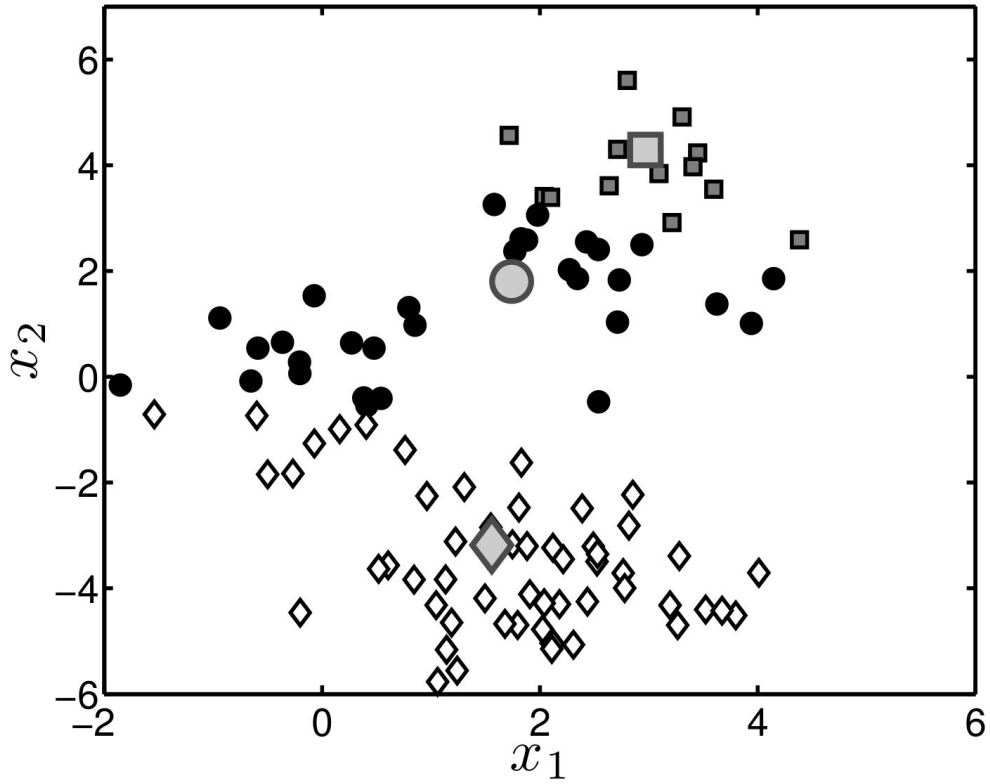


K-means - example



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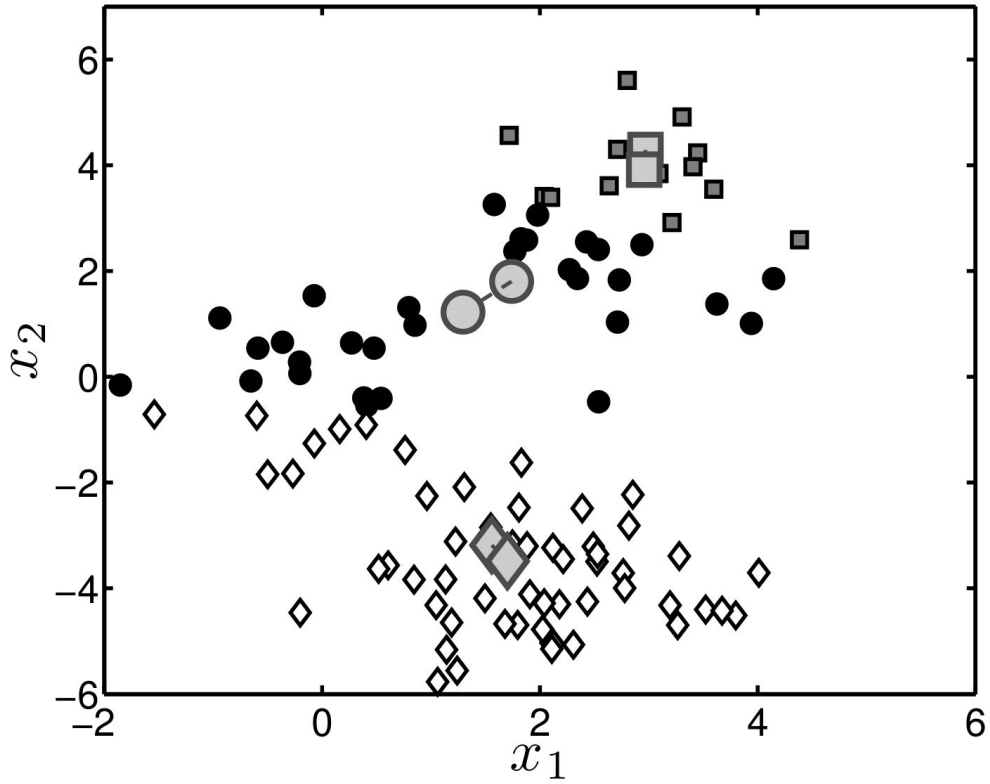

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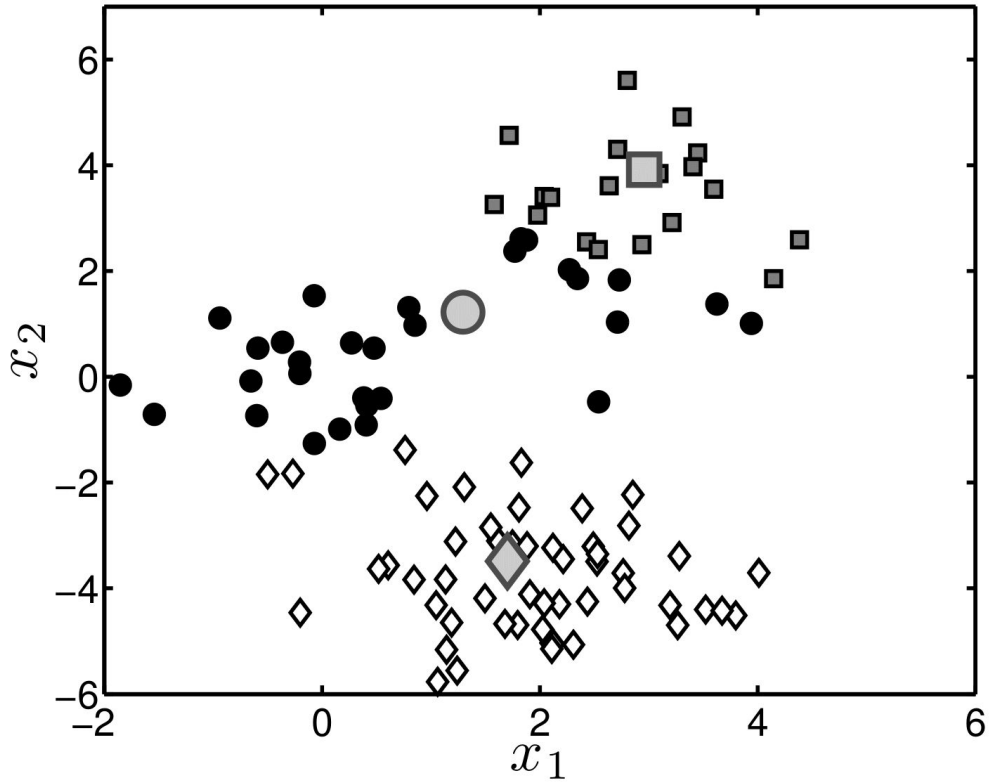
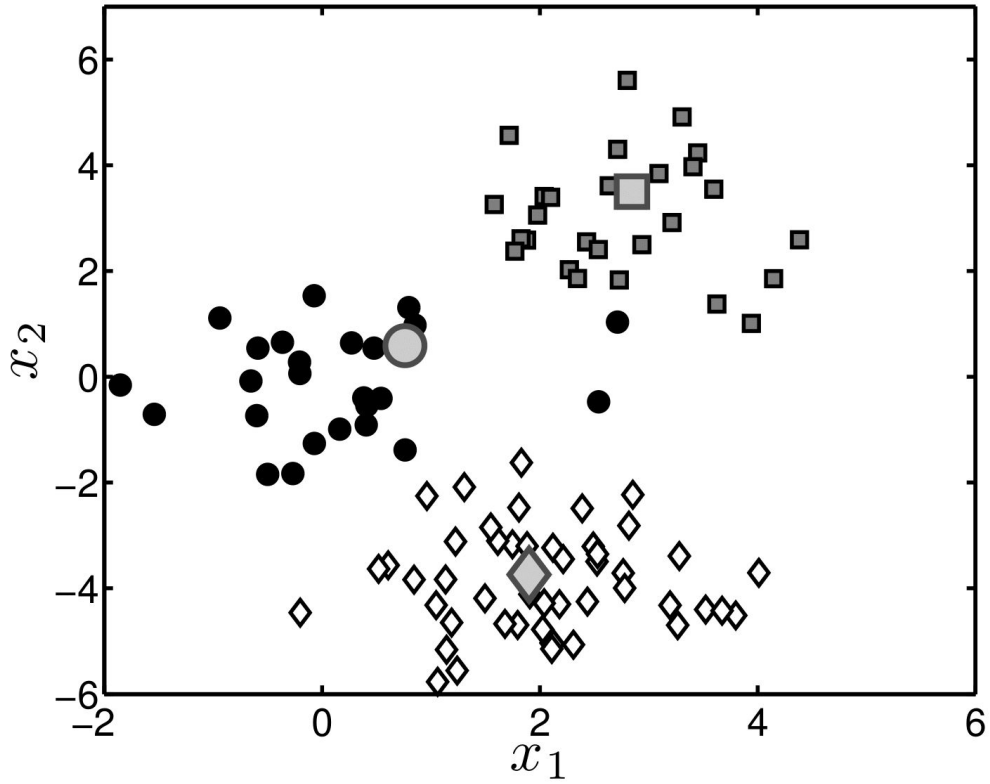
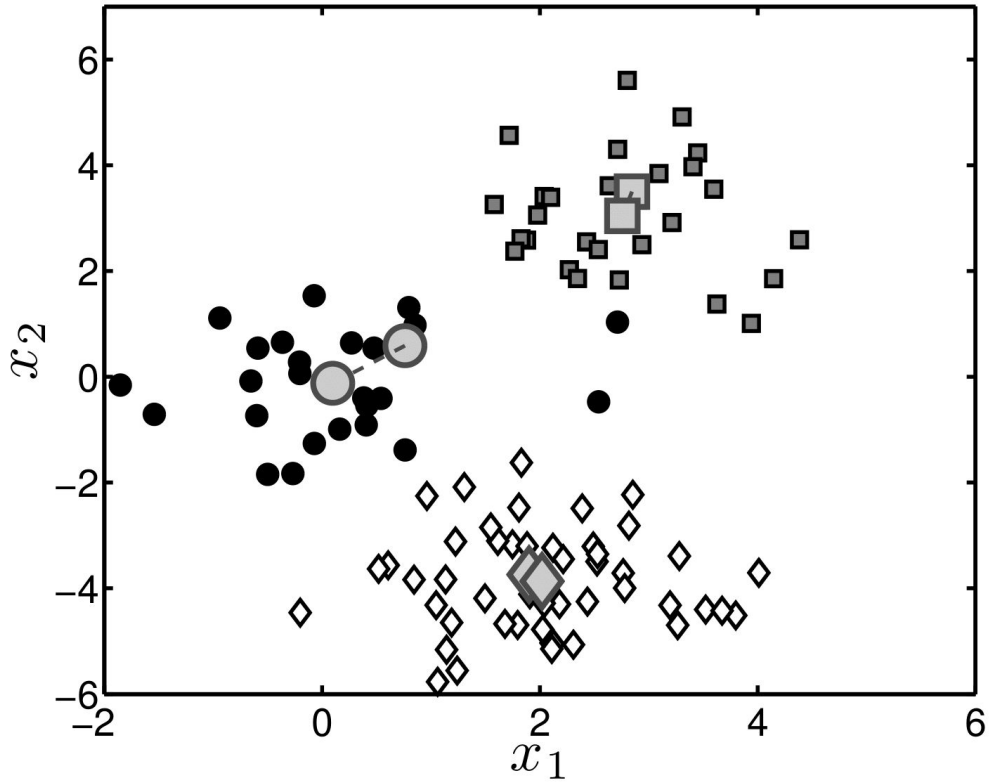


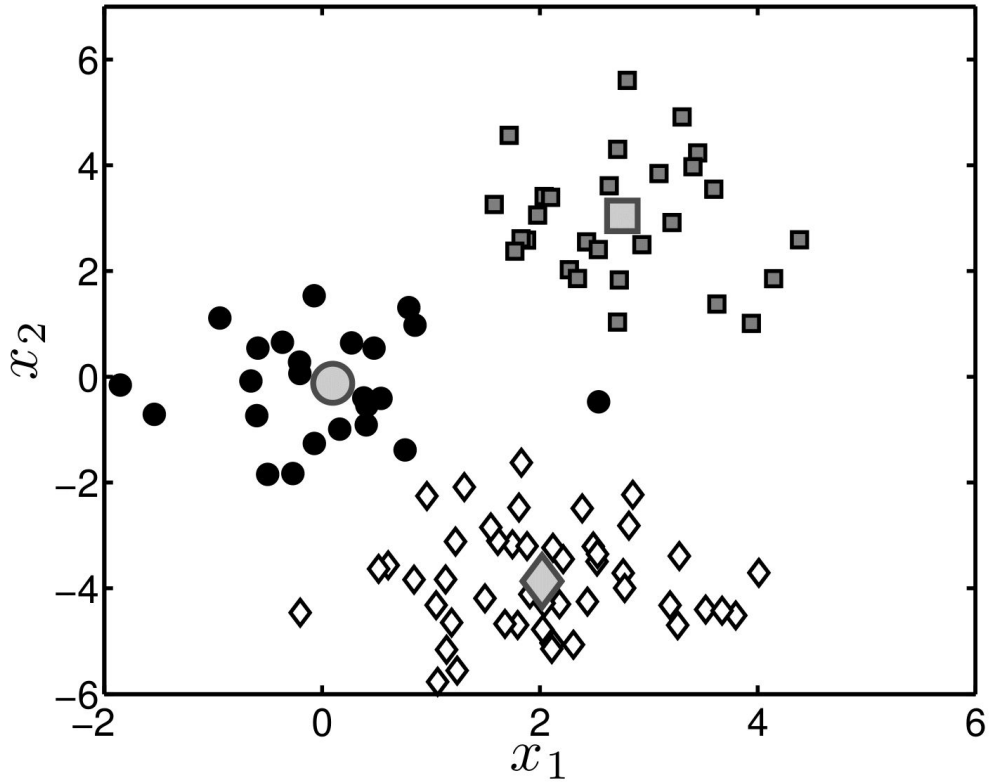
K-means - example



K-means - example



K-means - example



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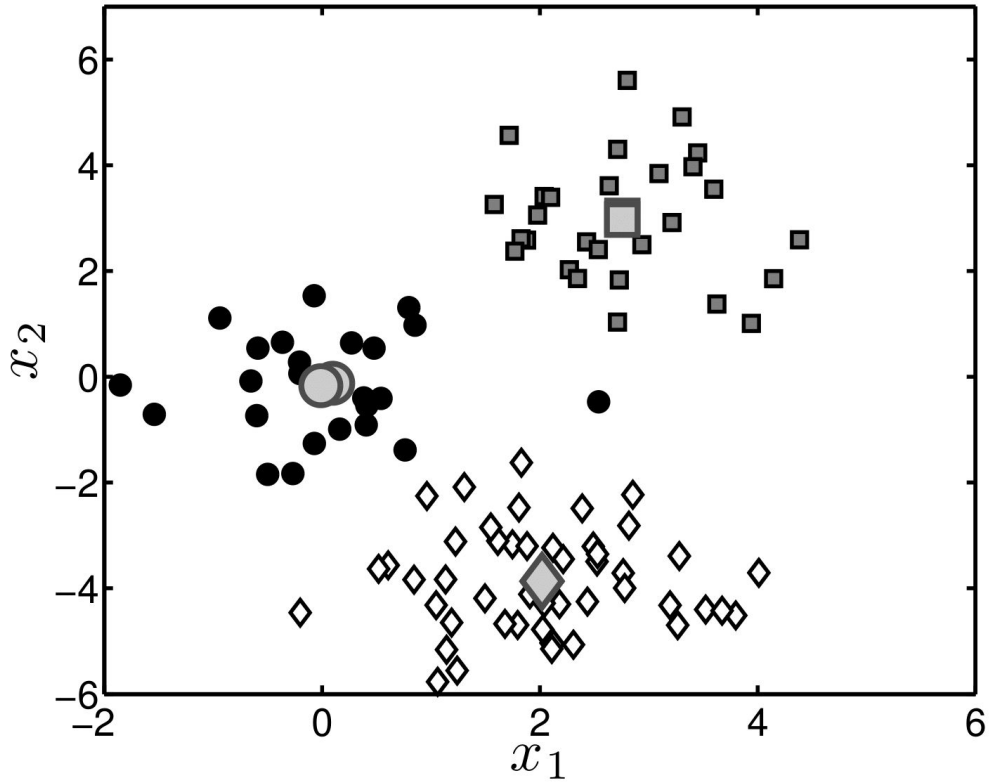
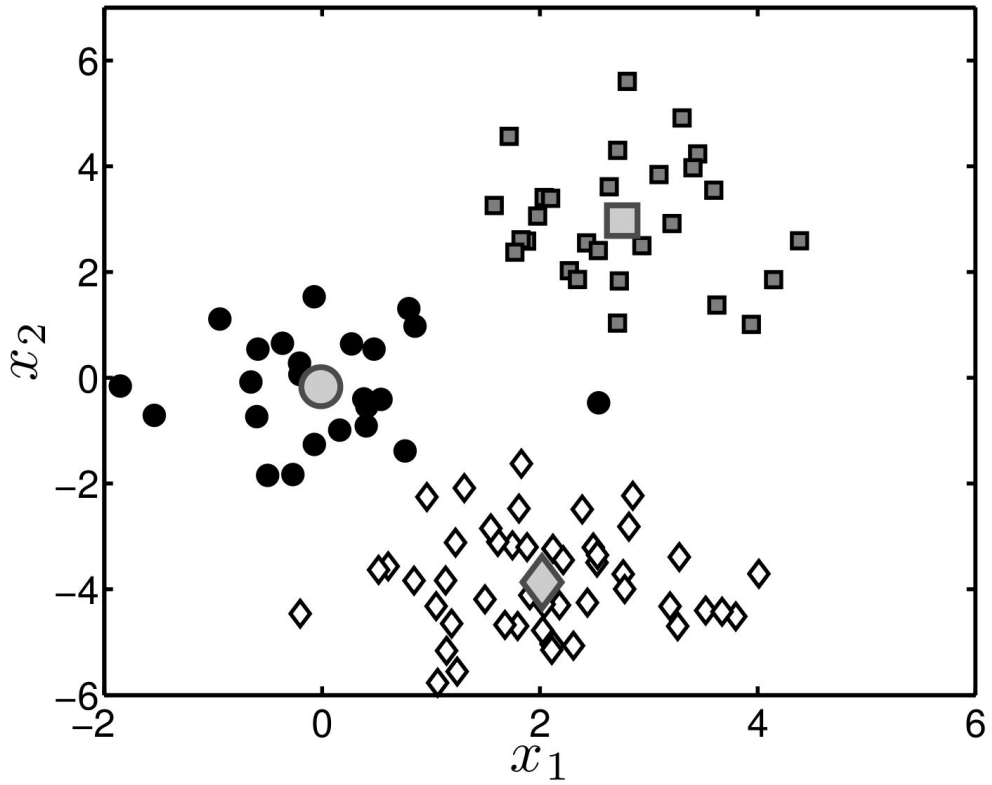
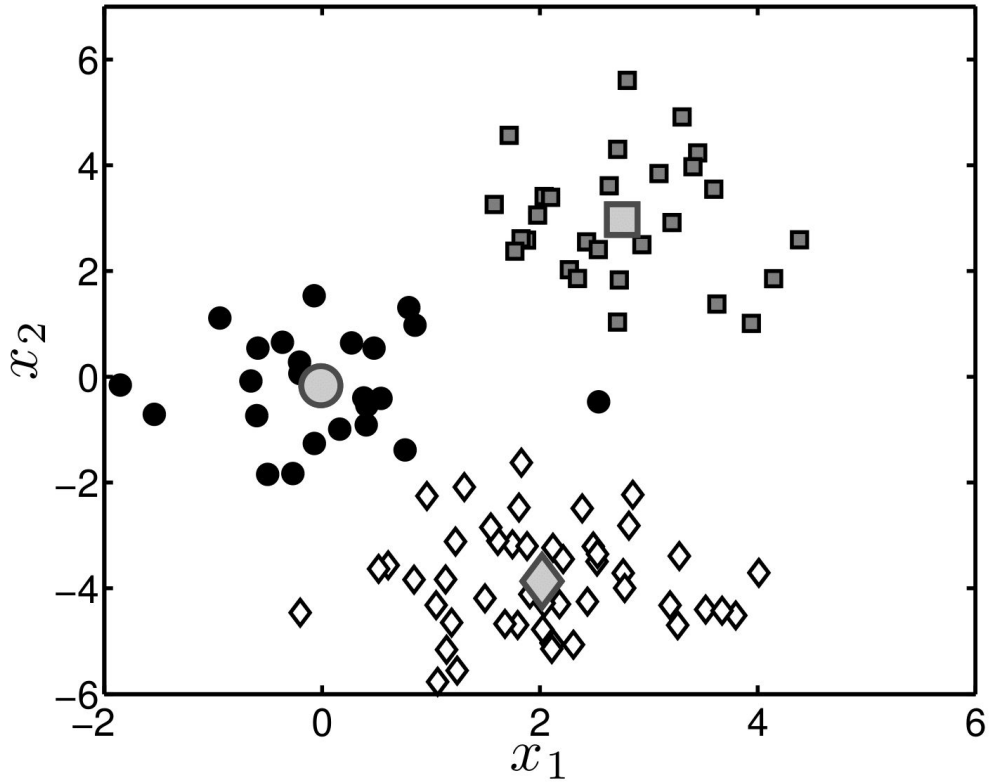


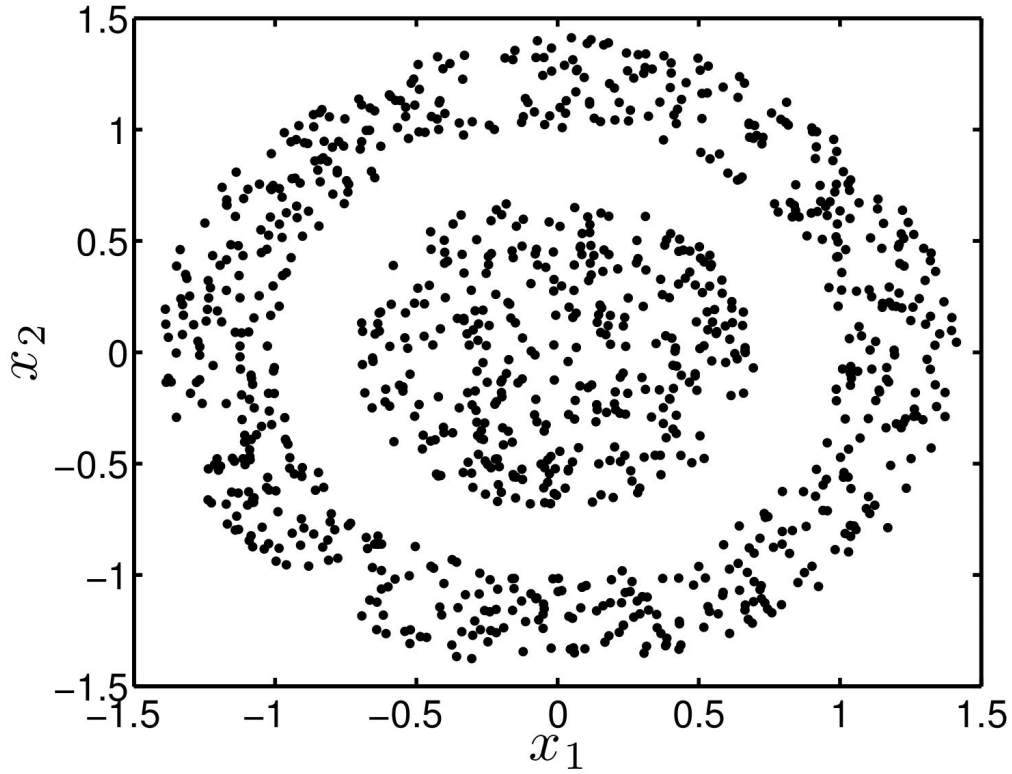
K-means - example



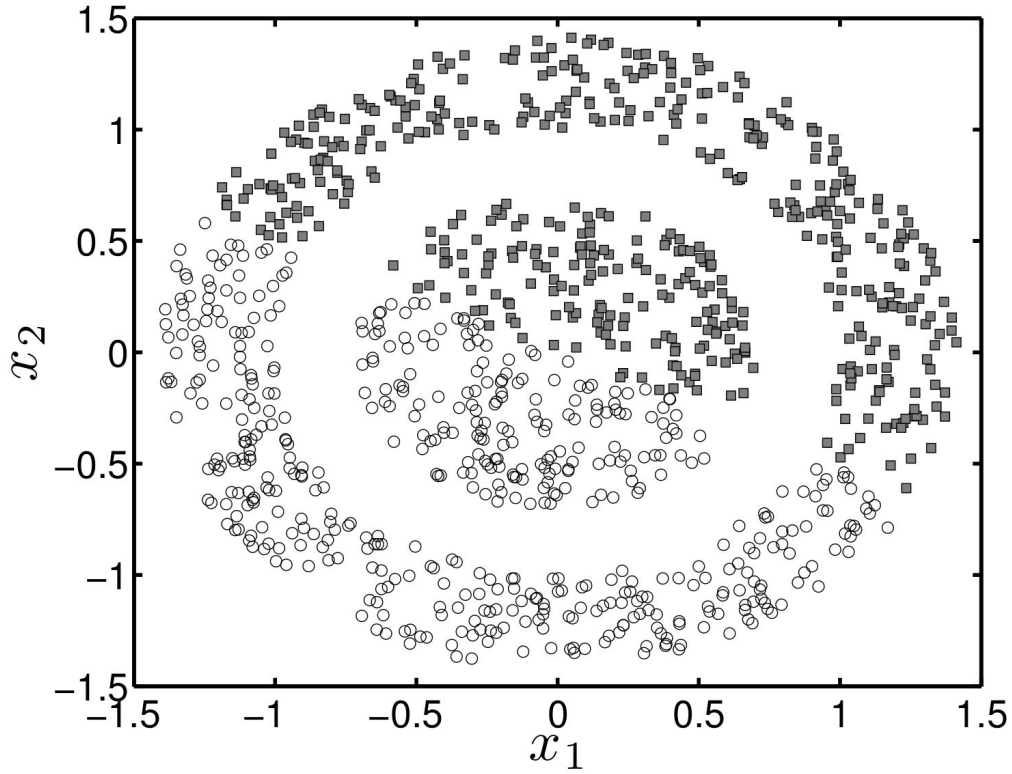
K-means - example - converged



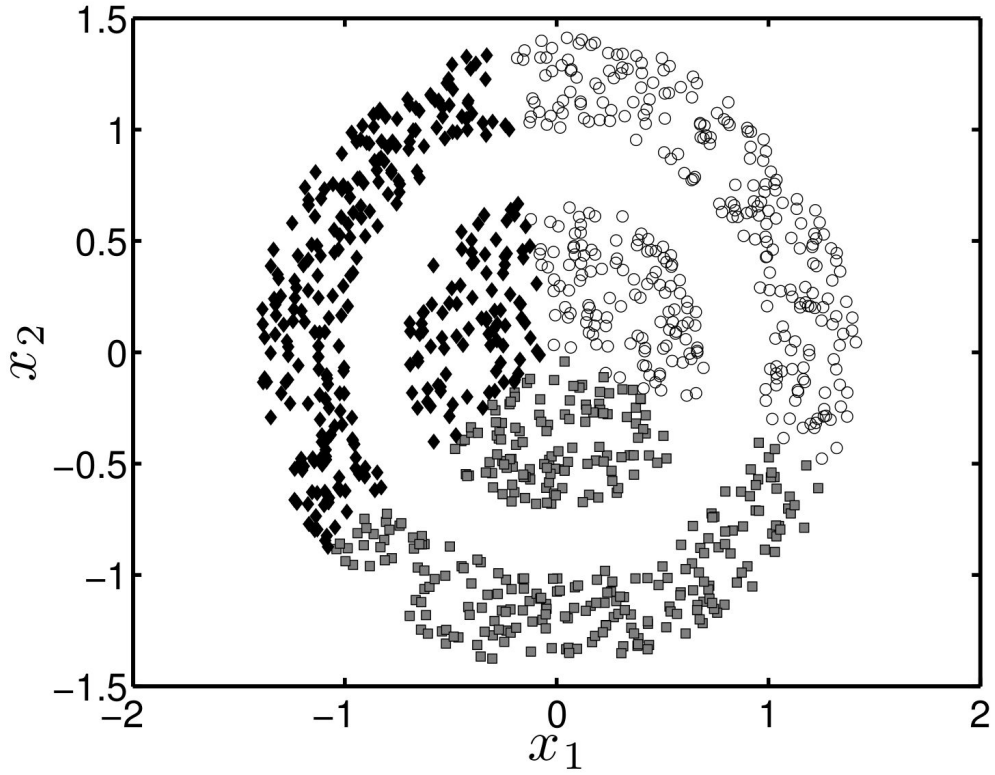
When does K-means break?



K-means with 2 clusters



K-means with 3 clusters



Kernelising K-means

$$d_{nk} = (\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathsf{T}}(\mathbf{x}_n - \boldsymbol{\mu}_k) \qquad \boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} z_{nk}\mathbf{x}_n}{\sum_{n=1}^{N} z_{nk}}$$

- Multiply out:

$$\mathbf{x}_n^{\mathsf{T}}\mathbf{x}_n - 2N_k^{-1}\sum_{m=1}^{N} z_{mk}\mathbf{x}_m^{\mathsf{T}}\mathbf{x}_n + N_k^{-2}\sum_{m,l} z_{mk}z_{lk}\mathbf{x}_m^{\mathsf{T}}\mathbf{x}_l$$

- Kernel substitution:

$$k(\mathbf{x}_n,\mathbf{x}_n) - 2N_k^{-1}\sum_{m=1}^{N} z_{mk}k(\mathbf{x}_n,\mathbf{x}_m) + N_k^{-2}\sum_{m,l=1}^{N} z_{mk}z_{lk}k(\mathbf{x}_m,\mathbf{x}_l)$$

Kernel K-means

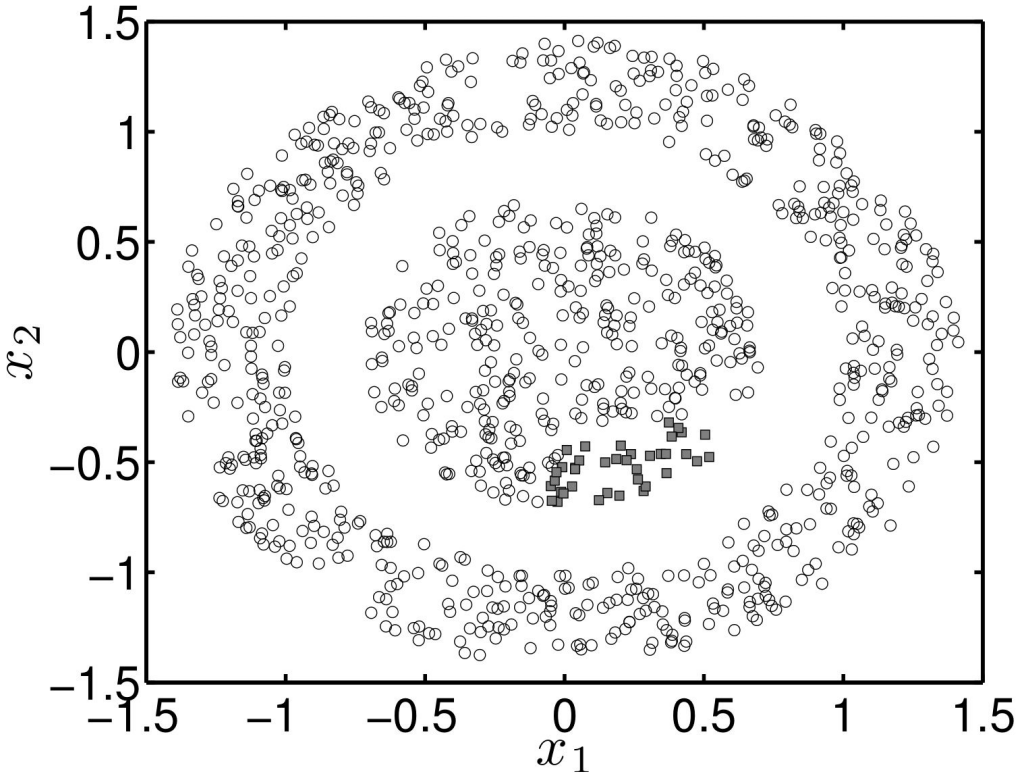
- Algorithm:
  1. Choose a kernel and any necessary parameters.
  2. Start with random assignments z_{nk}.
  3. For each $\mathbf{x}_n$ assign it to the nearest 'center' where distance is defined as:

$$k(\mathbf{x}_n, \mathbf{x}_n) - 2N_k^{-1} \sum_{m=1}^{N} z_{mk} k(\mathbf{x}_n, \mathbf{x}_m) + N_k^{-2} \sum_{m,l=1}^{N} z_{mk} z_{lk} k(\mathbf{x}_m, \mathbf{x}_l)$$

  4. If assignments have changed, return to 3.

- Note – no $\boldsymbol{\mu}_k$. This would be $N_k^{-1} \sum_n z_{nk} \phi(\mathbf{x}_n)$ but we don't know $\phi(\mathbf{x}_n)$ for kernels. We only know $\phi(\mathbf{x}_n)^{\mathsf{T}} \phi(\mathbf{x}_m)$ (last week)...

Kernel K-means - example



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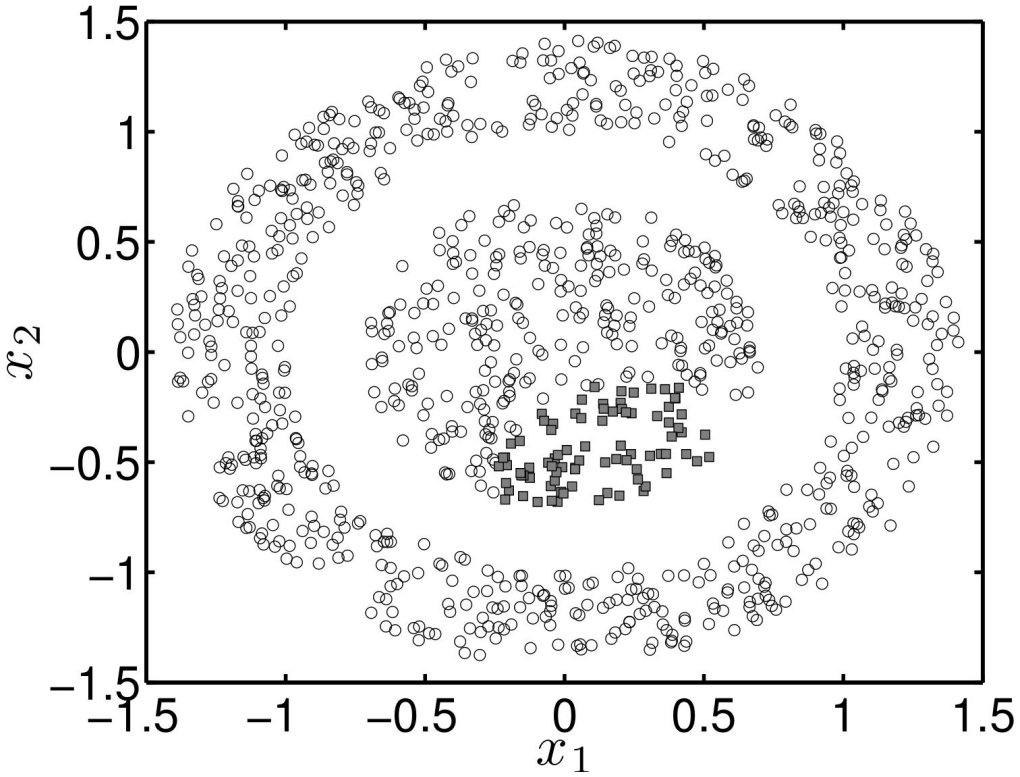

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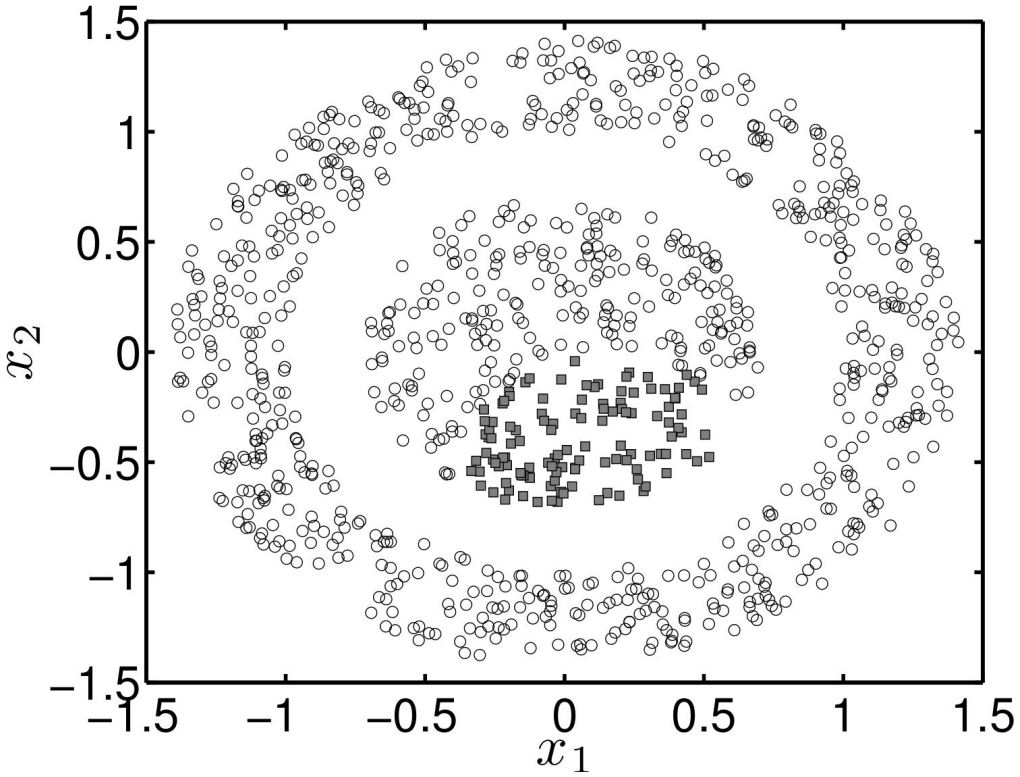

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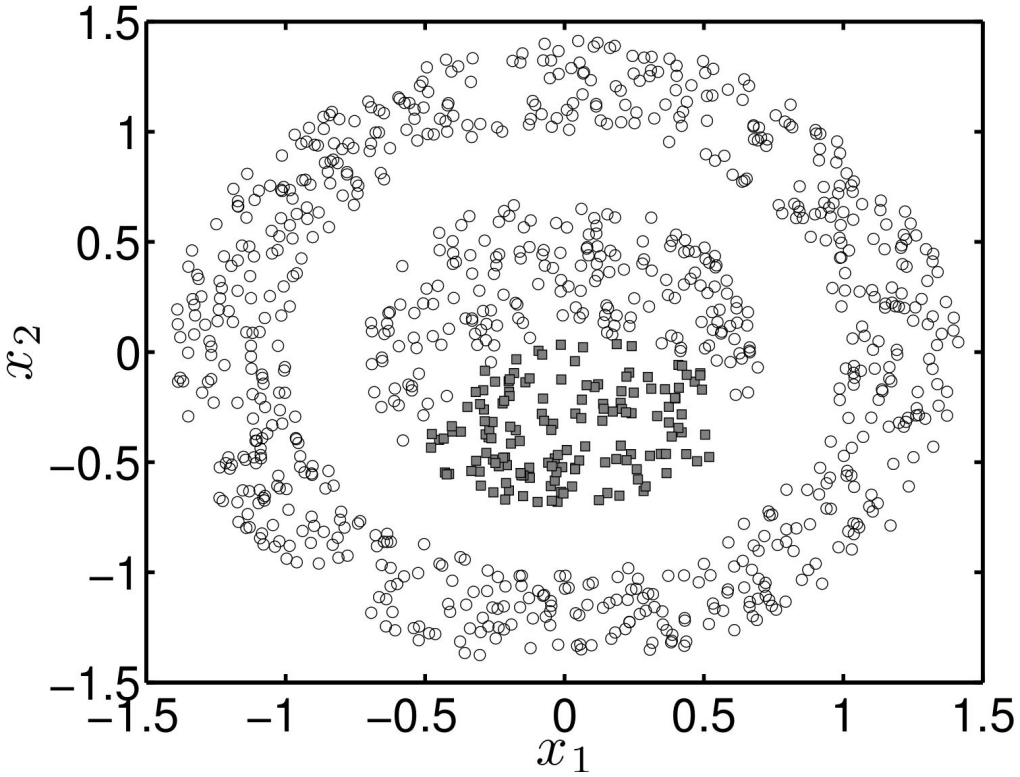

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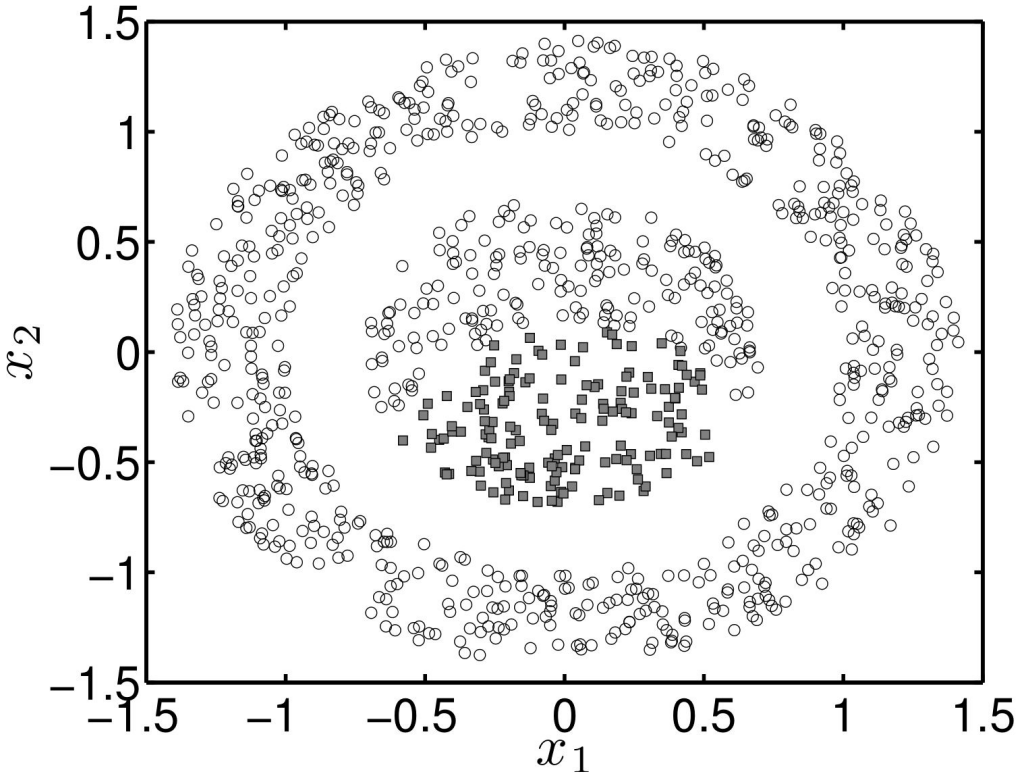

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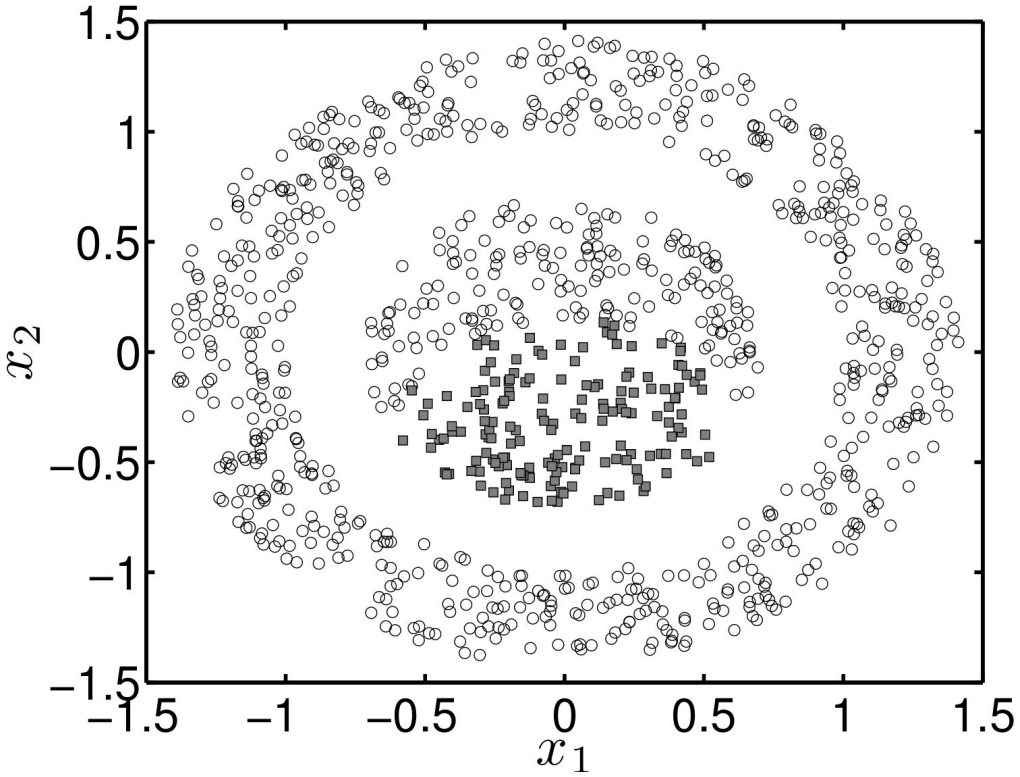

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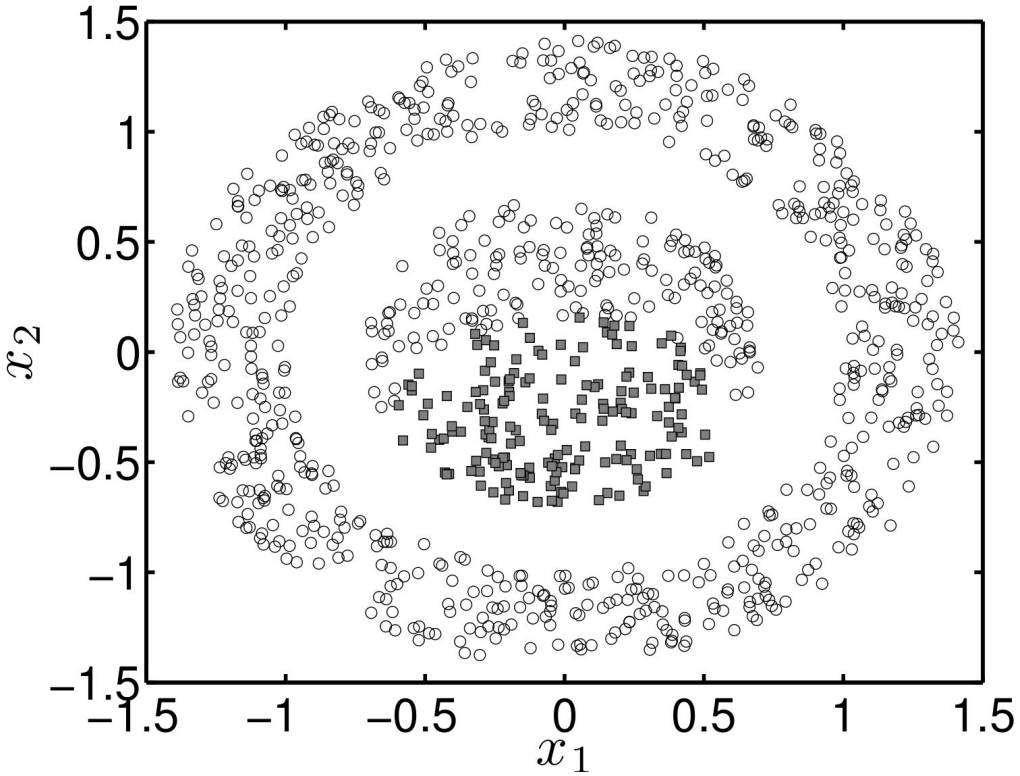

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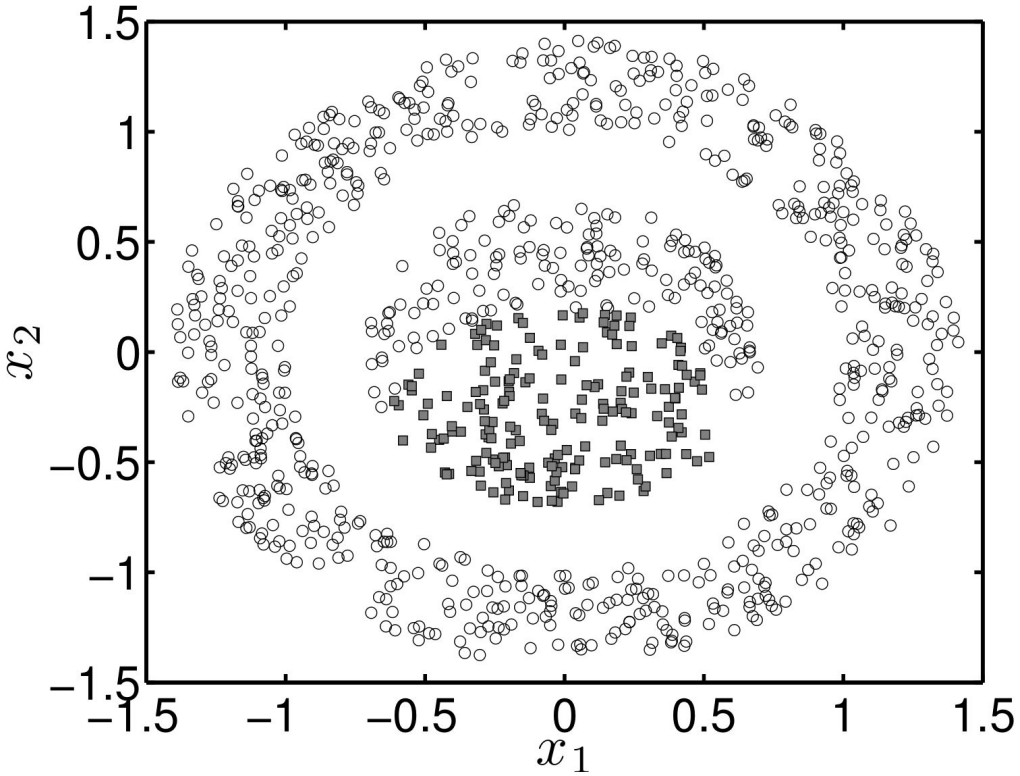

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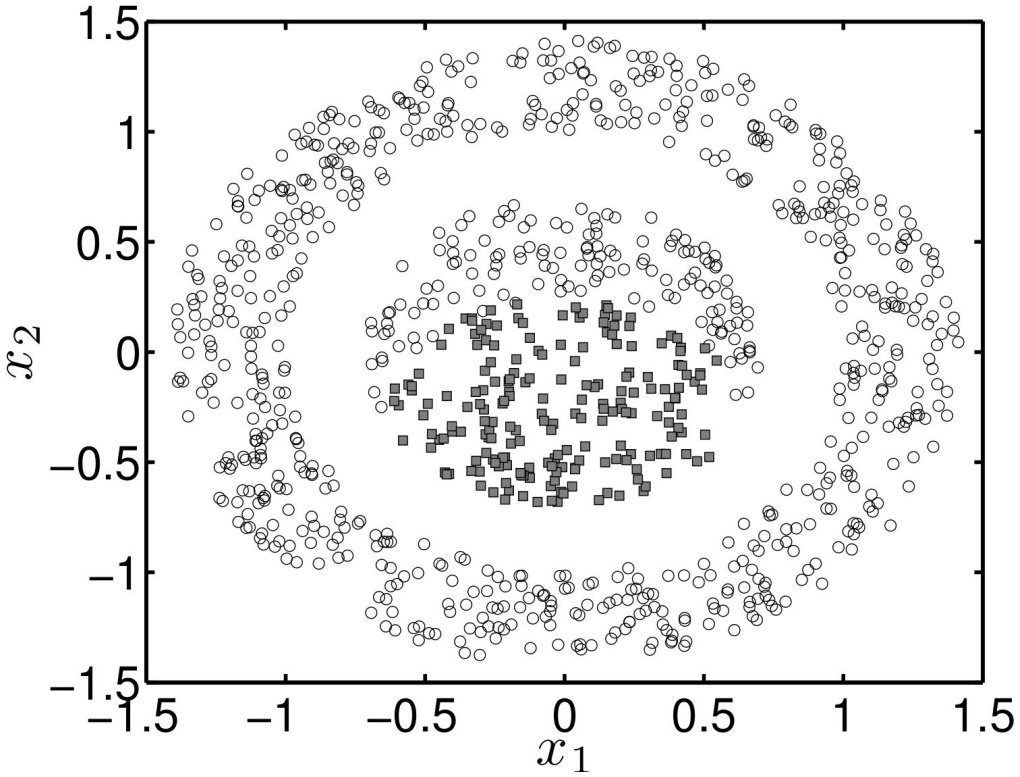

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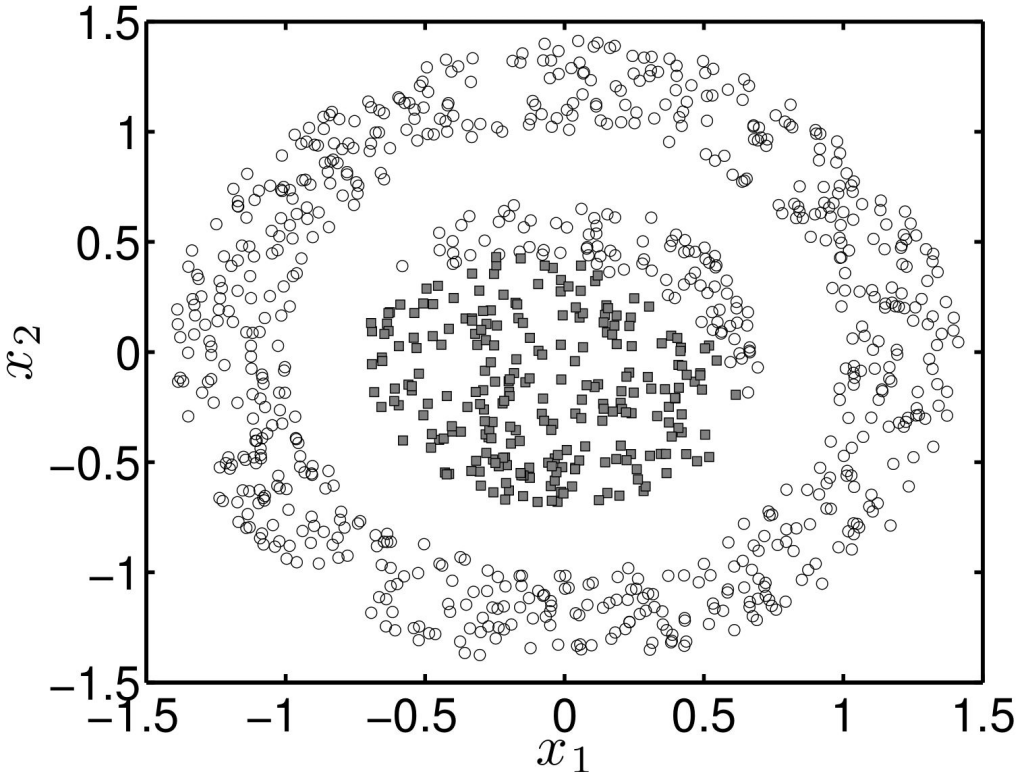

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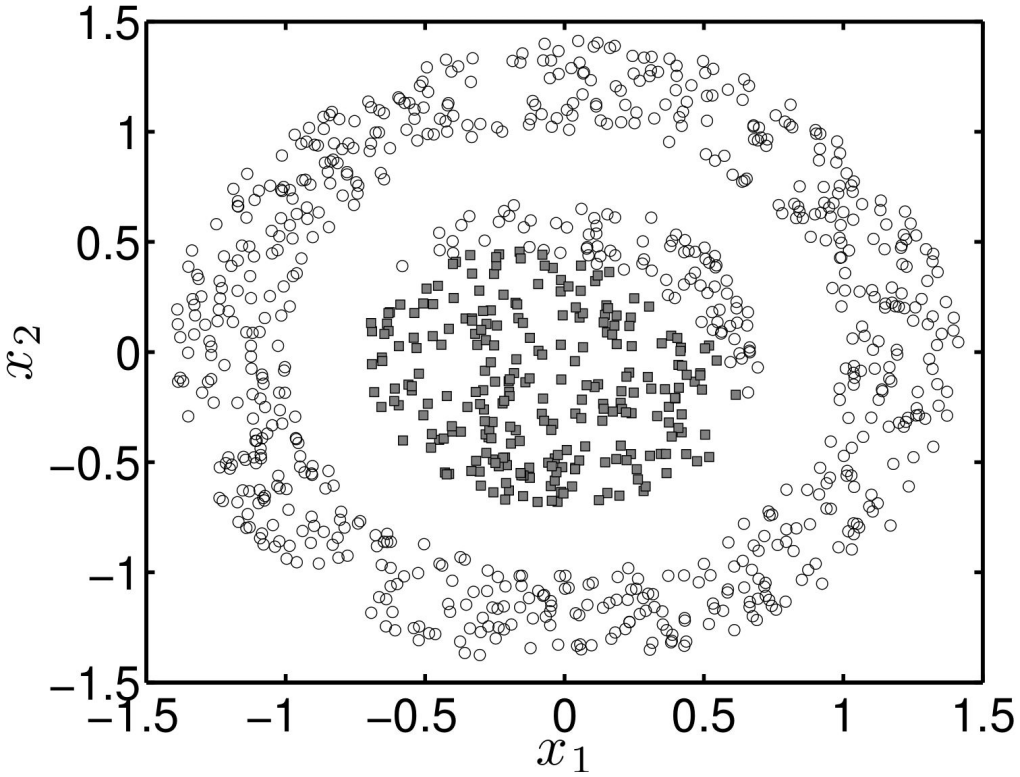

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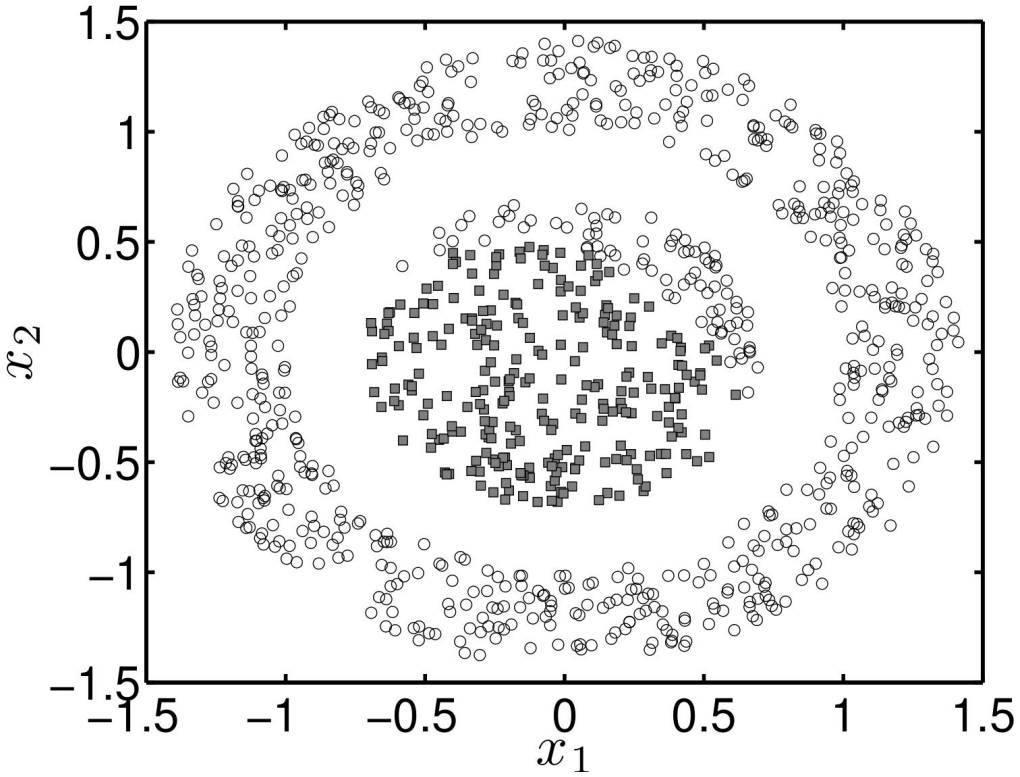

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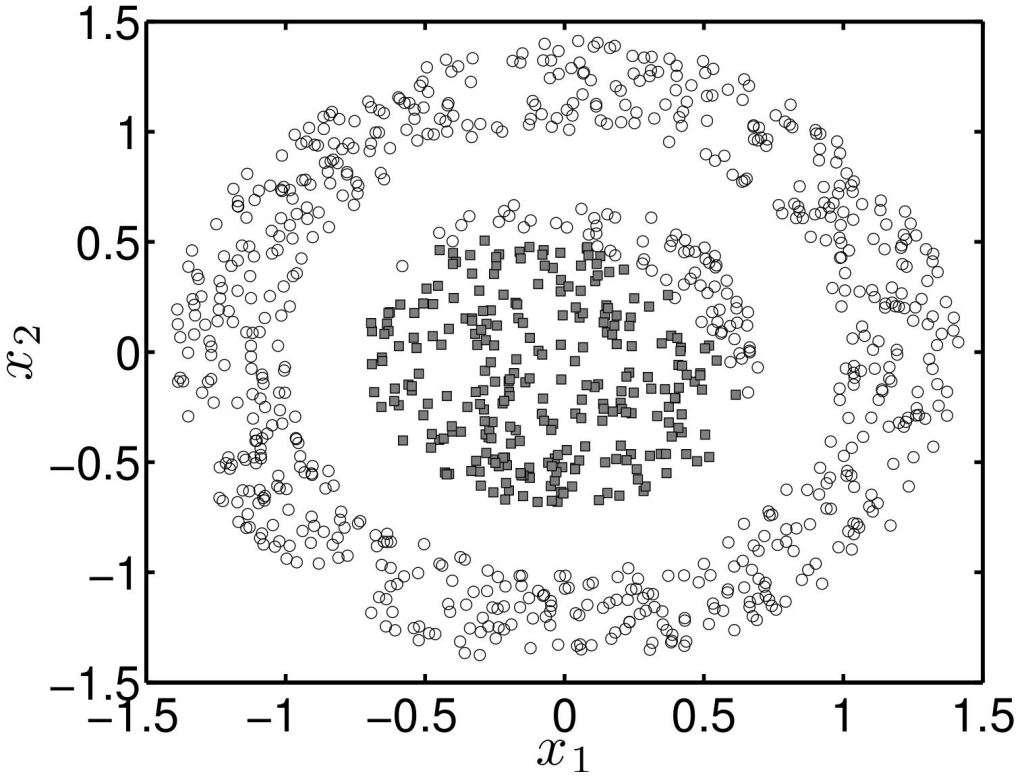

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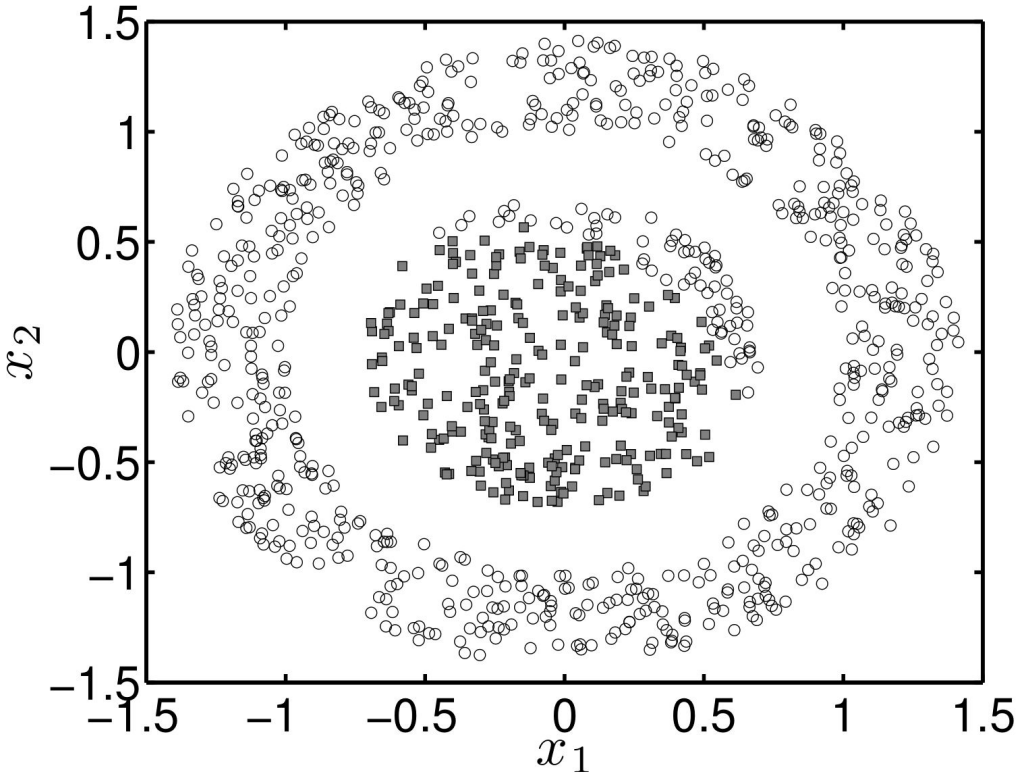

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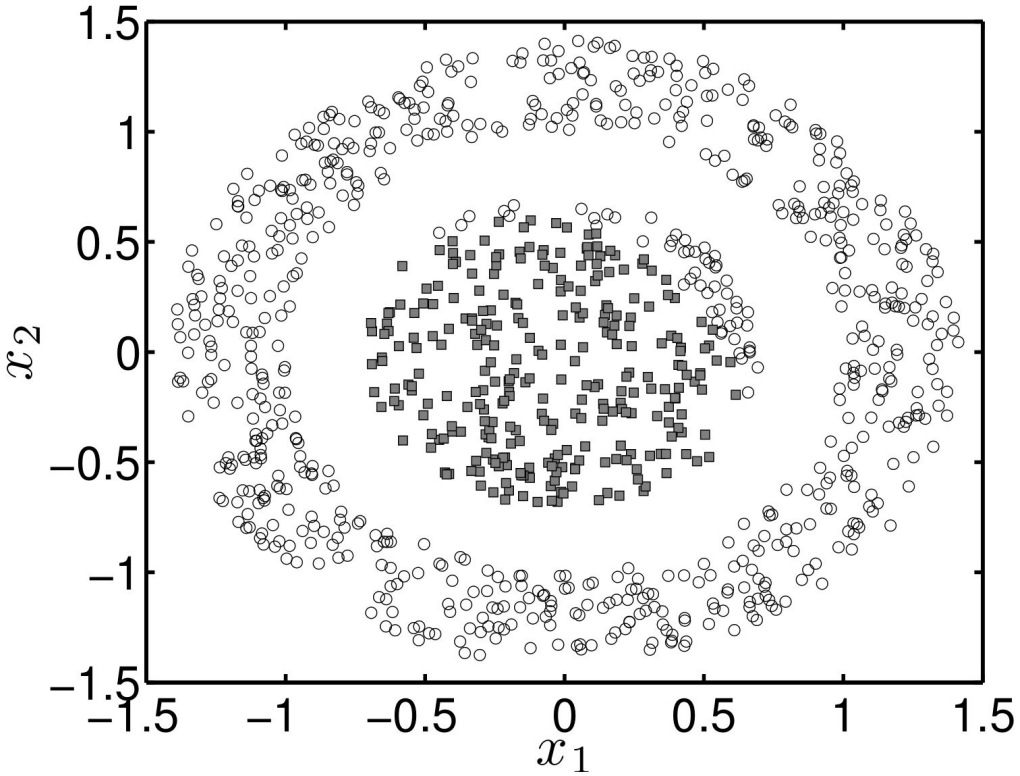

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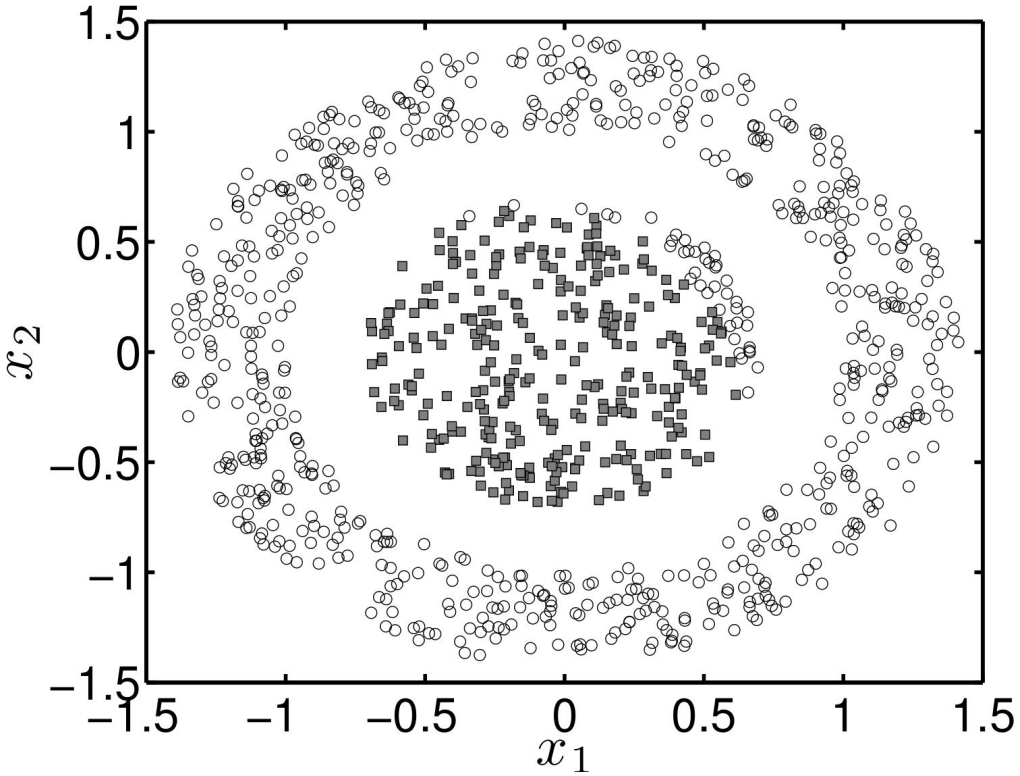

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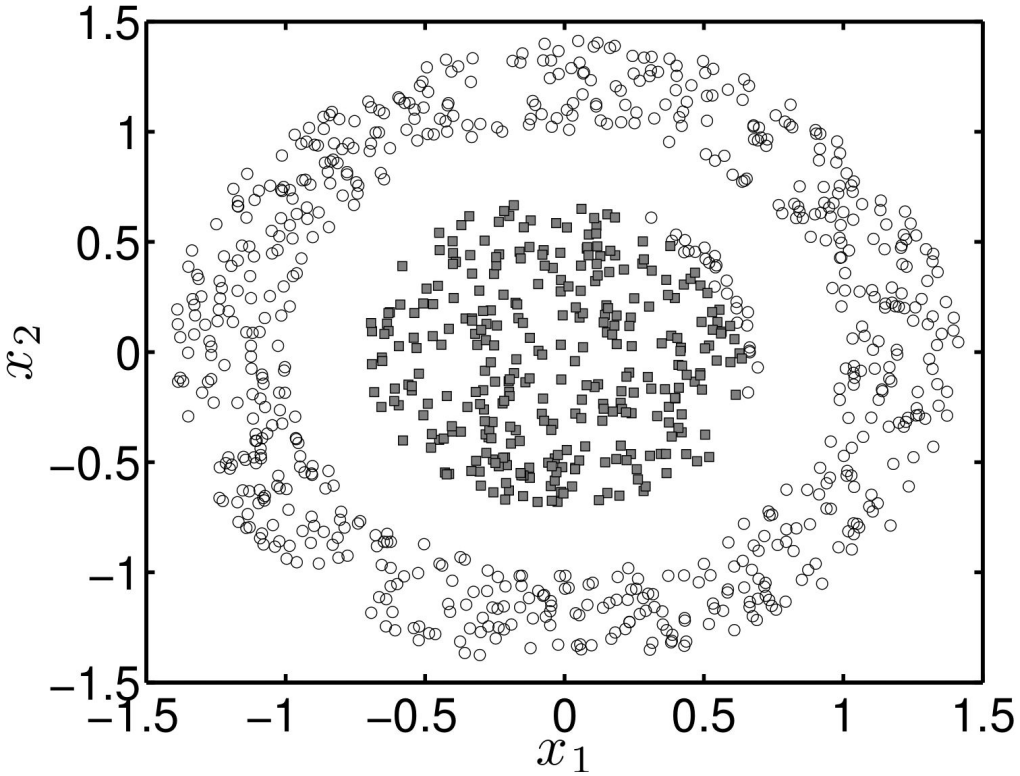

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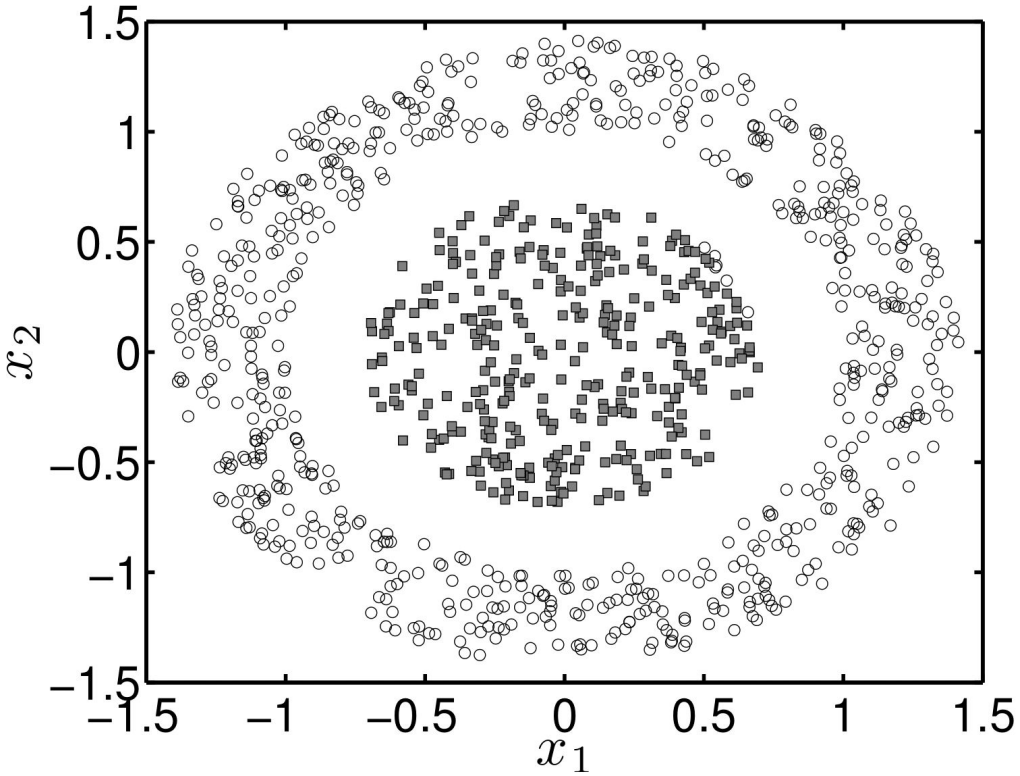

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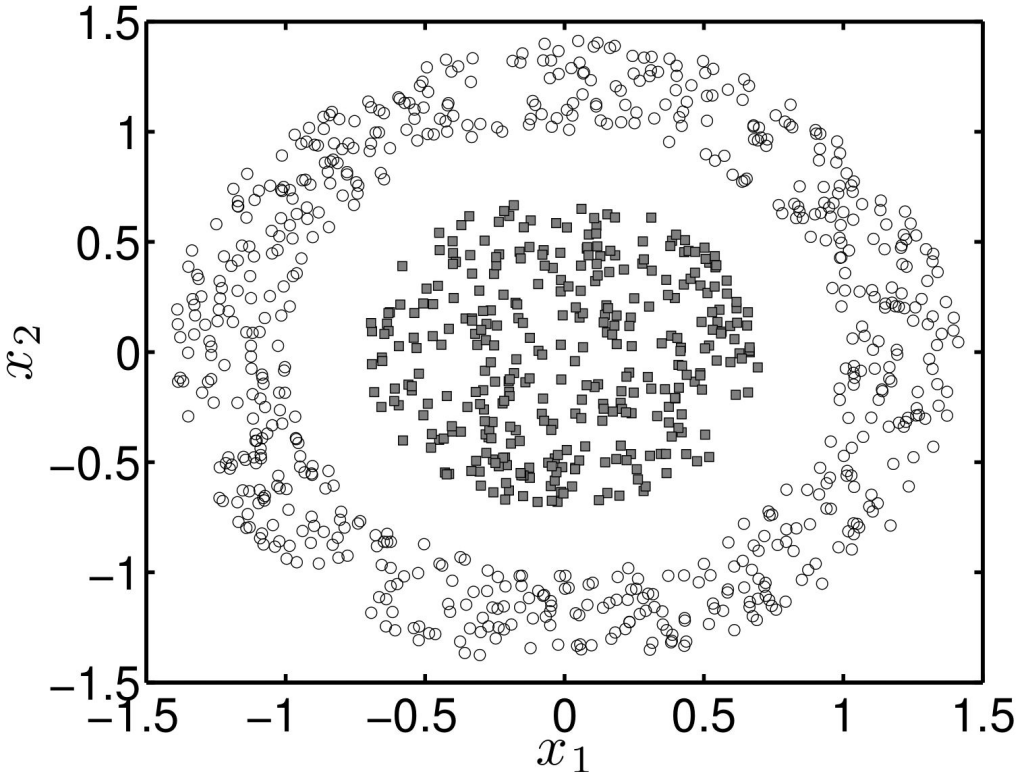

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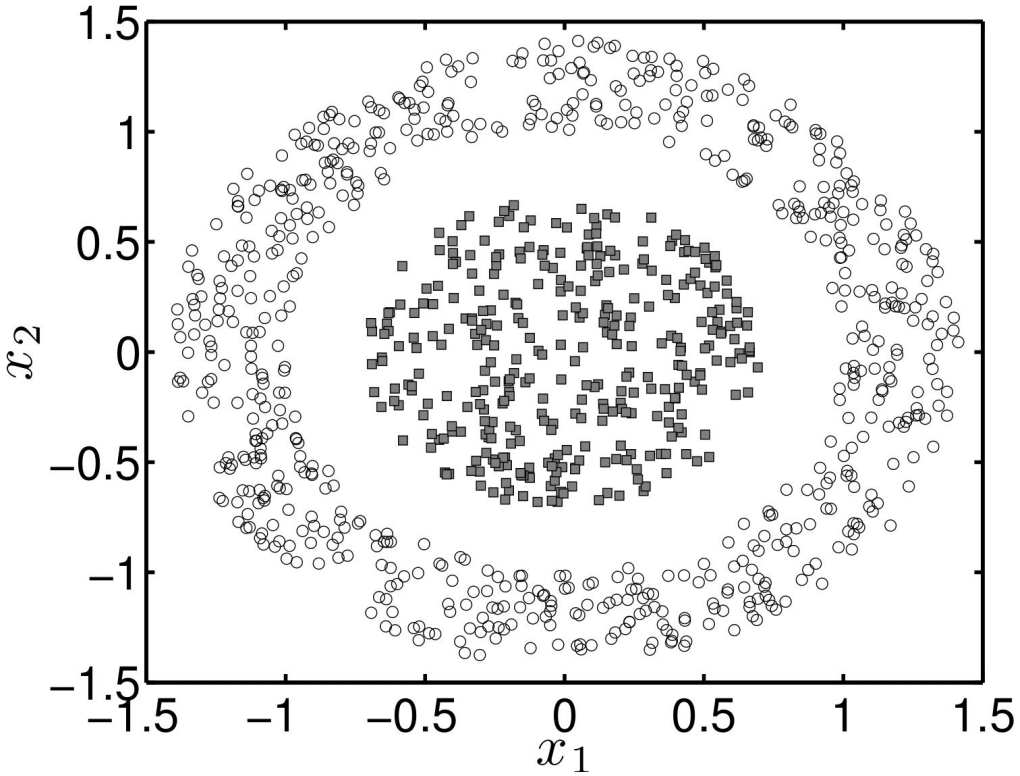

Kernel K-means

- Makes simple K-means algorithm more flexible.
- But, have to now set additional parameters.
- Very sensitive to initial conditions – lots of local optima.

K-means - summary

- Simple (and effective) clustering strategy.
- Converges to (local) minima of:

$$\sum_n \sum_k z_{nk} (\mathbf{x}_n - \boldsymbol{\mu}_k)^\mathsf{T} (\mathbf{x}_n - \boldsymbol{\mu}_k)$$

- Sensitive to initialisation.
- How do we choose K?
  - Tricky: Quantity above always decreases as K increases.
  - Can use CV if we have a measure of 'goodness'.
  - For clustering these will be application specific.