

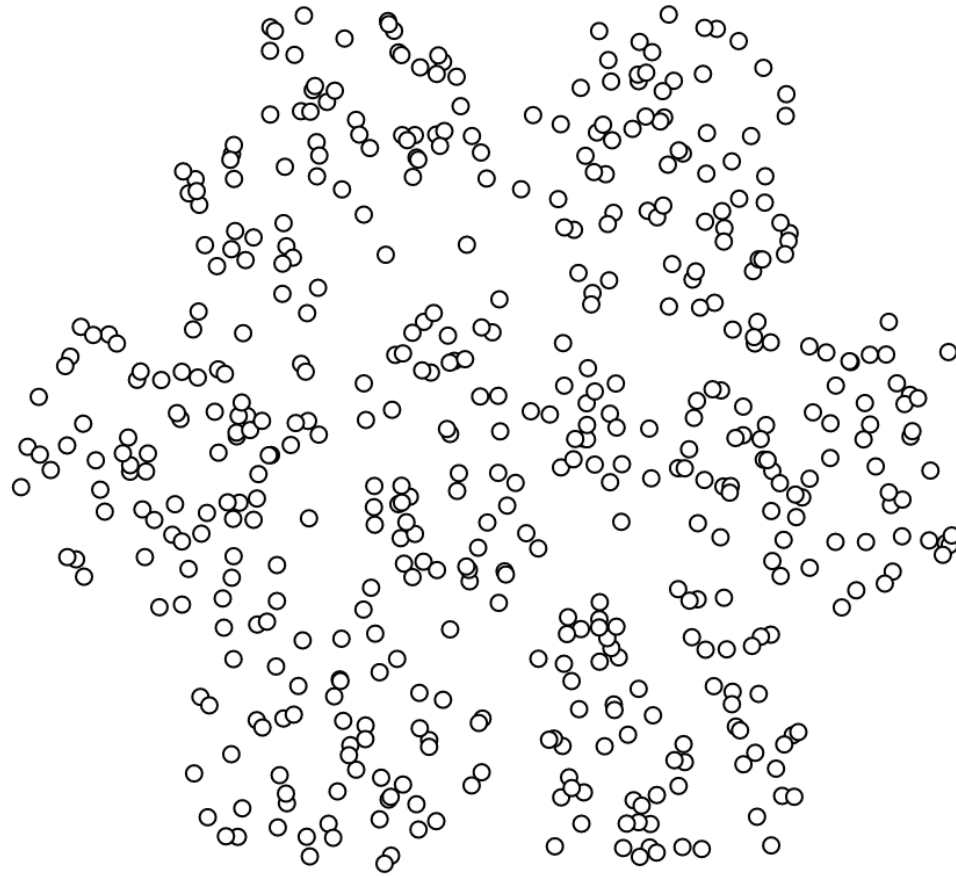
Machine learning

- Unsupervised learning
 - dimension reduction, clustering
- Supervised learning
 - classification, regression

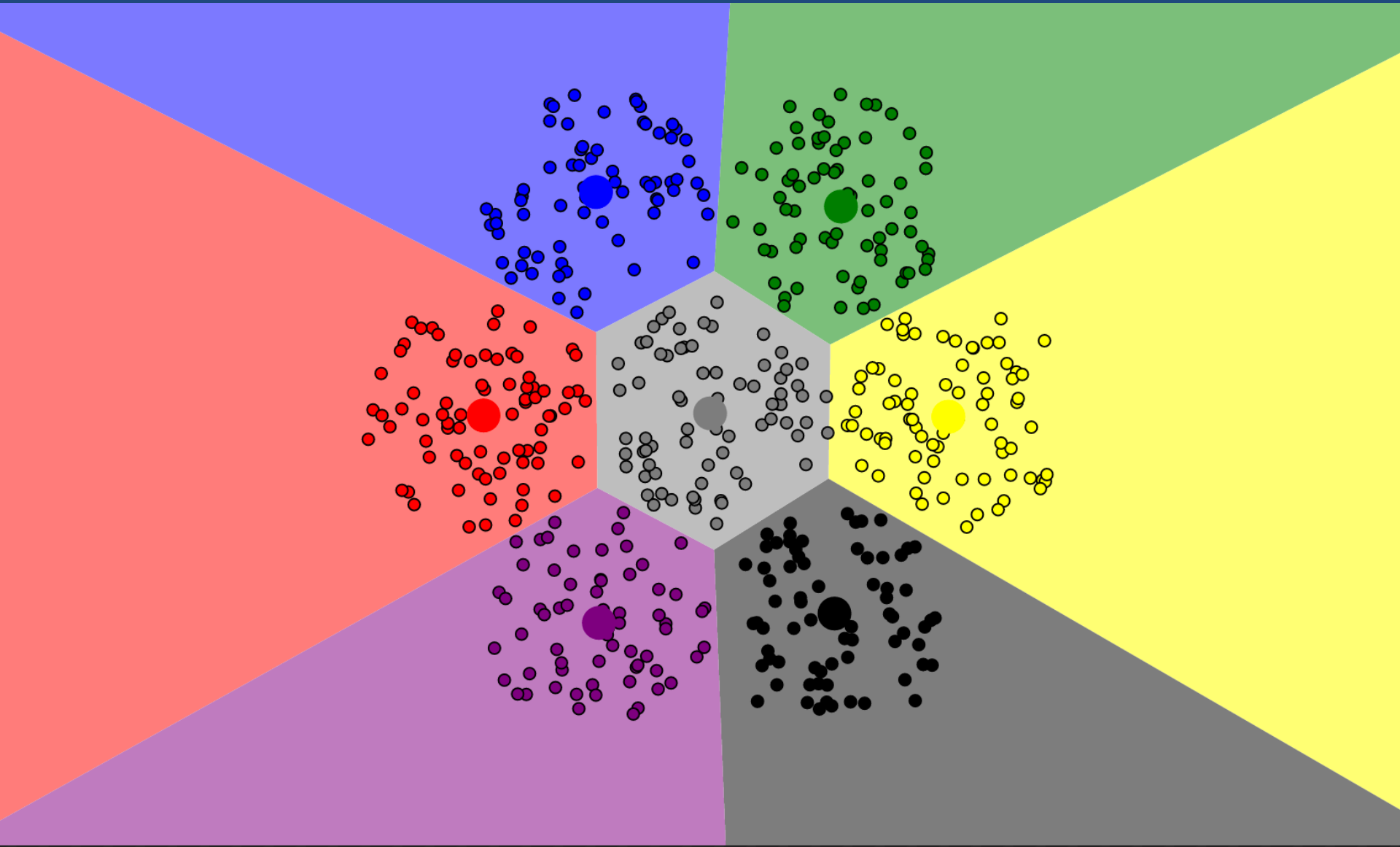
k-means clustering

Method to automatically separate data sets into distinct groups.

Clustering example



Clustering example

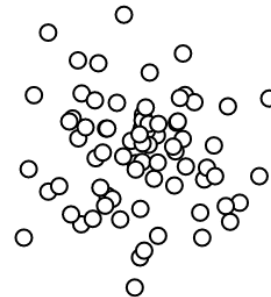
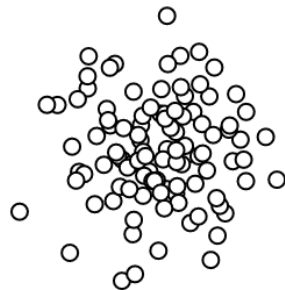
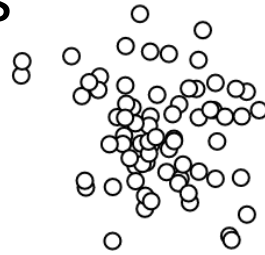


k -means clustering algorithm

1. Start with k randomly chosen means
2. Color data points by the shortest distance to any mean
3. Move means to centroid position of each group of points
4. Repeat from step 2 until convergence

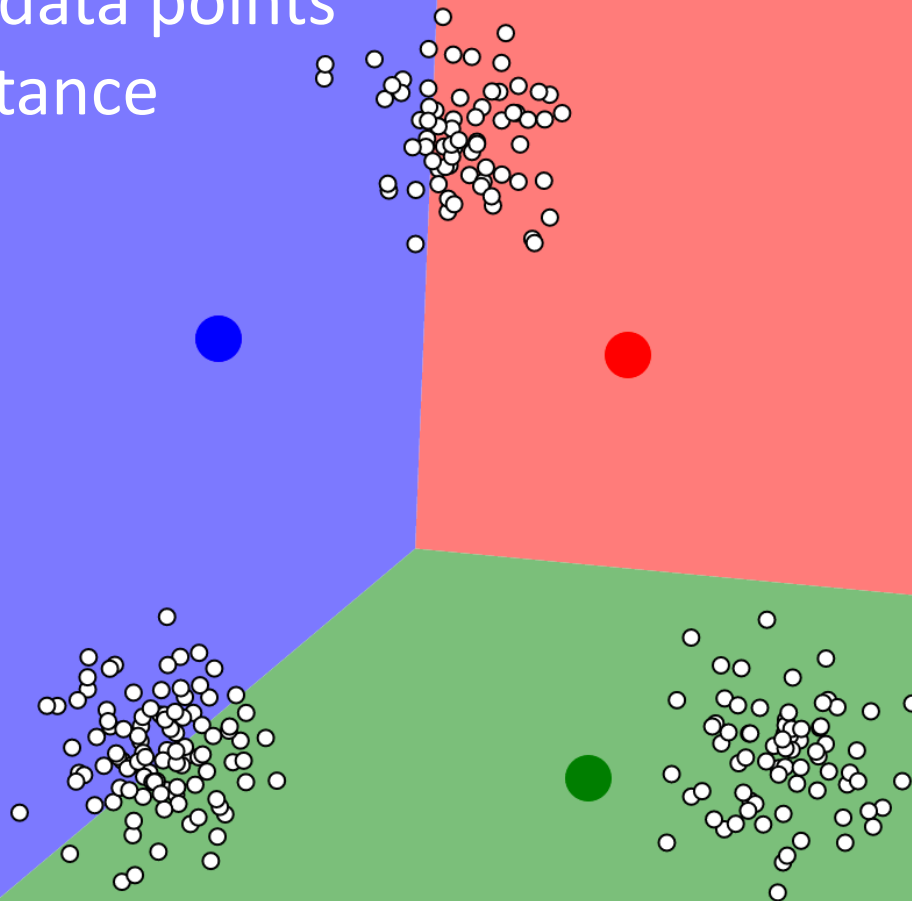
Algorithm example ($k = 3$)

Step 1: Choose 3 means
at random



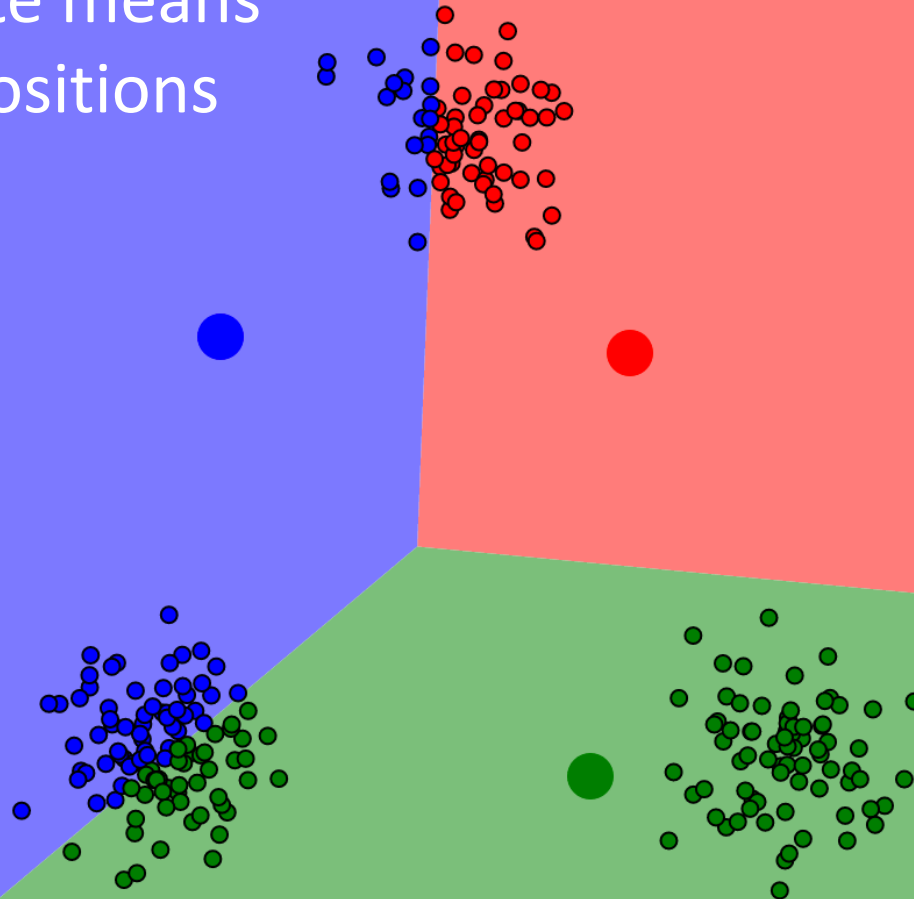
Algorithm example ($k = 3$)

Step 2: Color data points
by closest distance
to any mean



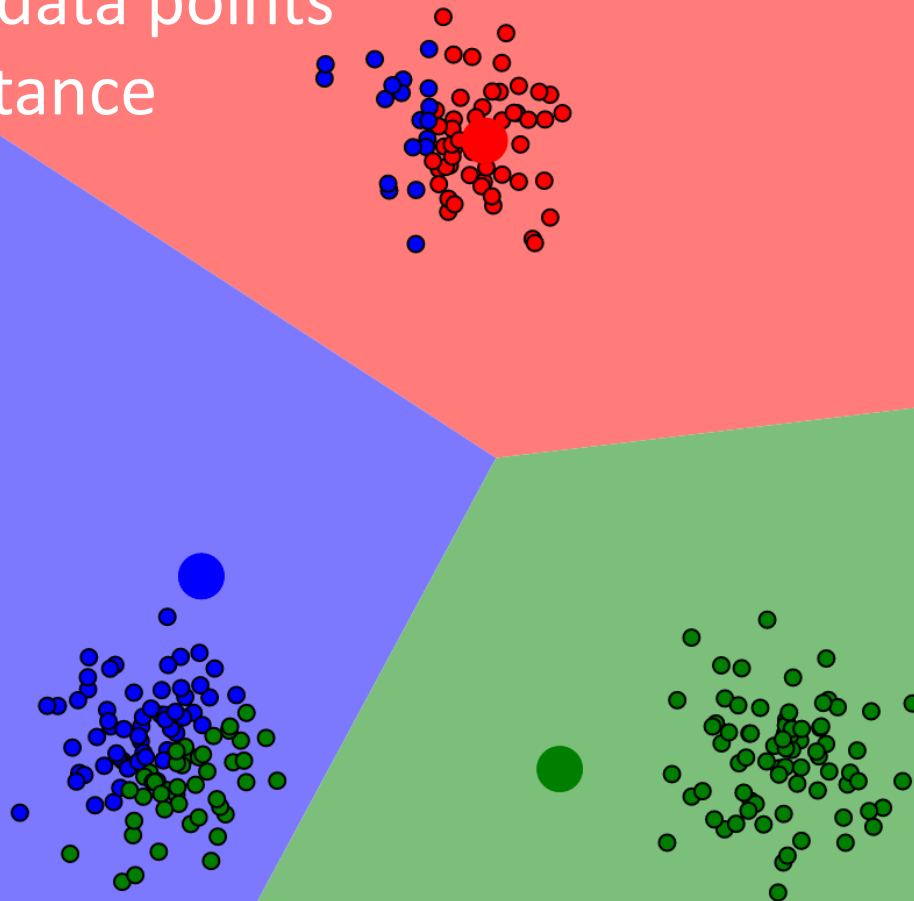
Algorithm example ($k = 3$)

Step 3: Update means to centroid positions



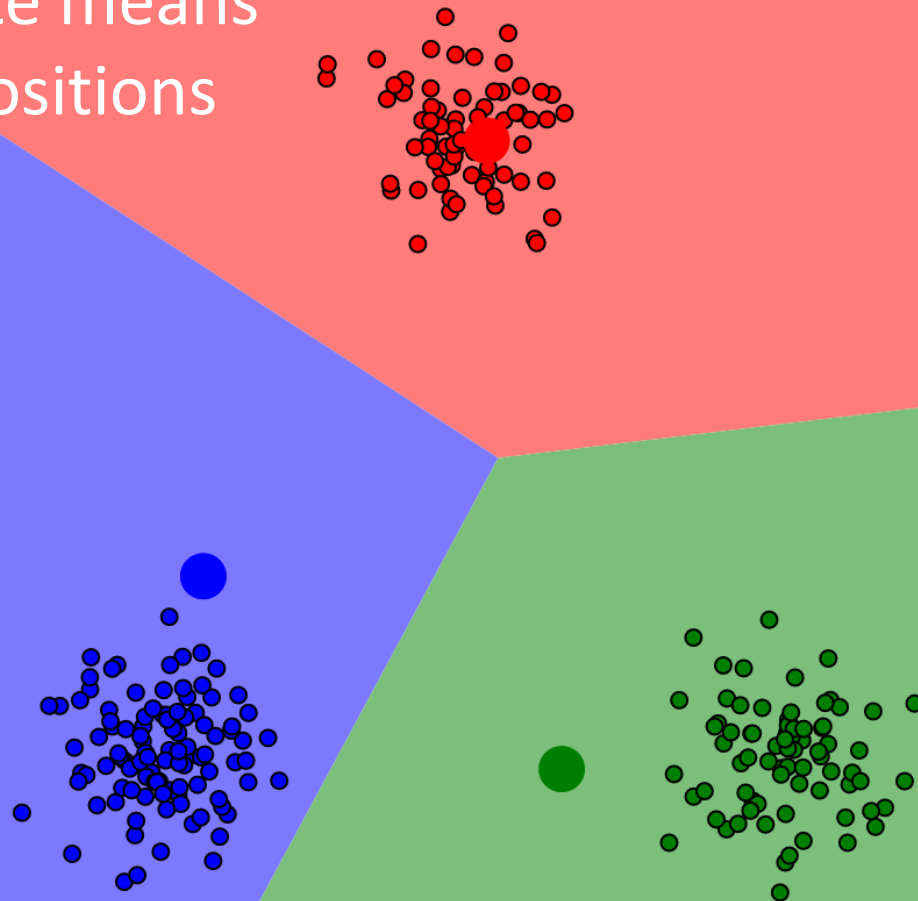
Algorithm example ($k = 3$)

Step 2: Color data points
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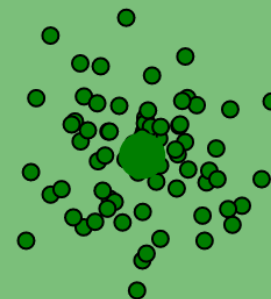
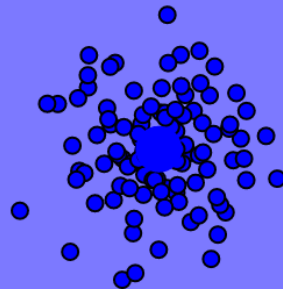
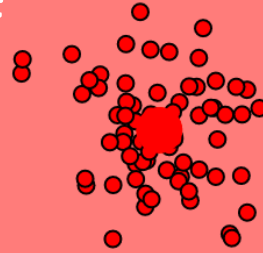
Algorithm example ($k = 3$)

Step 3: Update means
to centroid positions



Algorithm example ($k = 3$)

Stop: no further change occurs



Now try it yourself

<http://www.naftaliharris.com/blog/visualizing-k-means-clustering/>

k-means in R

(example: iris data set)

```
iris %>%  
  select(-Species) %>%      # remove Species column  
  kmeans(centers=3) ->      # do k-means clustering  
                               # with 3 centers  
km                           # store result as "km"
```

k-means in R (example: iris data set)

> km

K-means clustering with 3 clusters of sizes 38, 62, 50

Cluster means:

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width
1	6.850000	3.073684	5.742105	2.071053
2	5.901613	2.748387	4.393548	1.433871
3	5.006000	3.428000	1.462000	0.246000

Clustering vector:

[1]	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	
[38]	3	3	3	3	3	3	3	3	3	3	3	3	2	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
[75]	2	2	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	2	1	1	1	1	2
[112]	1	1	2	2	1	1	1	1	2	1	2	1	2	1	1	2	2	1	1	1	1	1	2	1	1	1	1	2	1	1
[149]	1	2																												

Within cluster sum of squares by cluster:

```
[1] 23.87947 39.82097 15.15100
```

(between SS / total SS = 88.4 %)

k-means in R (example: iris data set)

> km

K-means clustering with 3 clusters of sizes 38, 62, 50

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	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width
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Cluster means:
the location of the
final centroids

Clustering vector:

[1]	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	
[38]	3	3	3	3	3	3	3	3	3	3	3	3	2	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
[75]	2	2	2	1	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	1	2	1	1	1	1	2	1
[112]	1	1	2	2	1	1	1	1	2	1	2	1	2	1	1	2	2	1	1	1	1	1	2	1	1	1	1	2	1	1
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(between_SS / total_SS = 88.4 %)
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k-means in R (example: iris data set)

> km

K-means clustering with 3 clusters of sizes 38, 62, 50

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Clustering vector:

[1]	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	
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[112]	1	1	2	2	1	1	1	1	2	1	2	1	2	1	1	2	2	1	1	1	1	2	1	1	1	1	2	1	1	2
[149]	1	2																												

Clustering vector: provides the cluster to which each

Within cluster sum of squares by cluster:

```
[1] 23.87947 39.82097 15.15100
```

(between SS / total SS = 88.4 %)

cluster to which each
observation belongs

k-means in R (example: iris data set)

> km

K-means clustering with 3 clusters of sizes 38, 62, 50

Cluster means:

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width
1	6.850000	3.073684	5.742105	2.071053
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Clustering vector:

[1]	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3			
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[112]	1	1	2	2	1	1	1	1	2	1	2	1	2	1	1	2	2	1	1	1	1	1	2	1	1	1	2	1	1	1	2	1	1	2	1
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Within cluster sum of squares: measures quality of

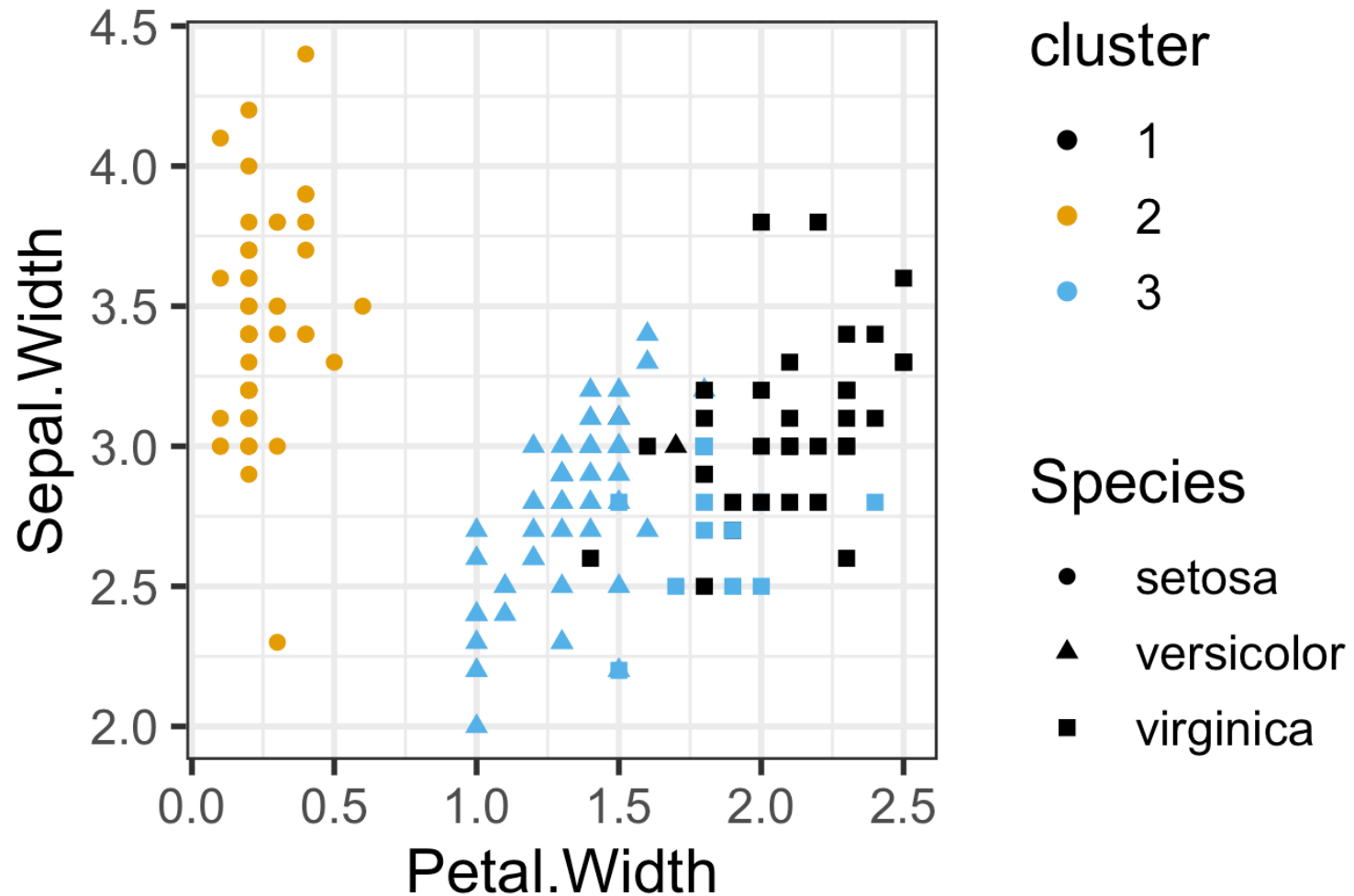
Within cluster sum of squares by cluster:

```
[1] 23.87947 39.82097 15.15100
```

(between_SS / total_SS = 88.4 %)

the clustering (lower is better)

The clusters mostly but not exactly recapitulate the species assignments



How do we determine the right number of means k ?

- Many different methods, see e.g.:
<http://stackoverflow.com/a/15376462/4975218>
- Simplest: plot within-sum-of-squares against k

A bend in within-sum-of-squares indicates the ideal number of clusters

