Gaussian mixture models

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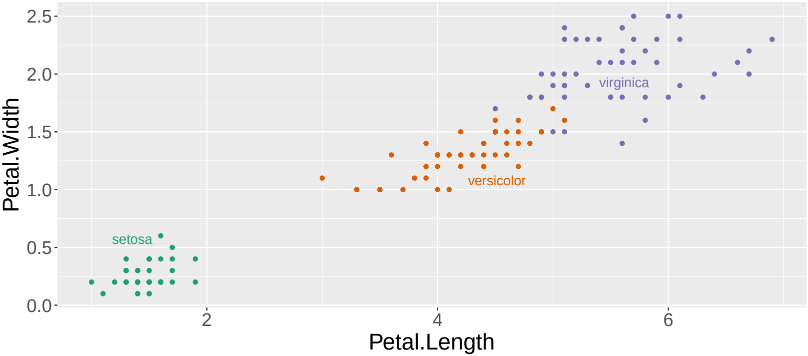
Visualize iris data with labels



Visualize iris data without labels

- Let $X \in \mathbb{R}^{n \times p}$ be the data matrix (input for clustering).
- Example iris $n = 150$ observations, $p = 2$ dimensions.

```
##      Petal.Width Petal.Length
## [1,]         0.2          1.4
## [2,]         0.2          1.4
## [3,]         0.2          1.3
## [4,]         0.2          1.5
```

Gaussian mixture model parameters and EM algorithm

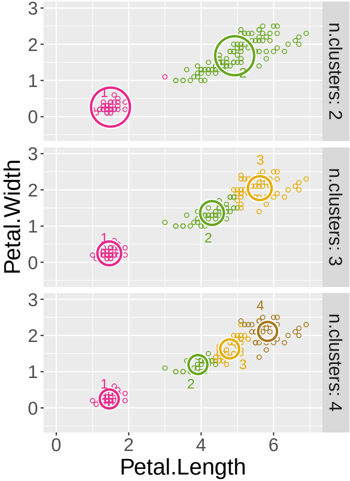
Need to fix number of clusters K, then for every $k \in \{1, \ldots, K\}$ we have cluster-specific parameters $\theta_k = [\mu_k, S_k, \pi_k]$ which are updated during M step,

- mean vector $\mu_k \in \mathbb{R}^p$,
- covariance matrix $S_k \in \mathbb{R}^{p \times p}$, (must be symmetric, positive definite, next slides show optional additional constraints)
- prior weight $\pi_k \in [0, 1]$ (sum over all clusters k must equal one).

During E step we compute the probability matrix $T \in [0, 1]^{n \times K}$, where each row i sums to 1 and each entry T_{ik} is probability that data i is in cluster k.

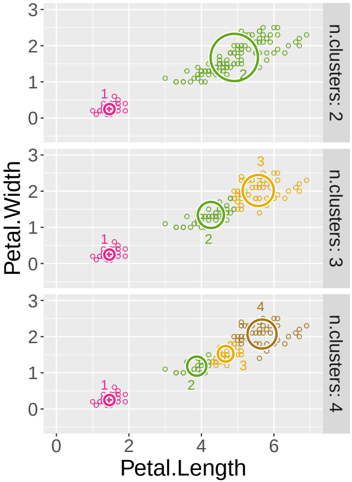
spherical, equal volume

```
##                c1     c1     c2     c2     c3     c3
## width  0.1077 0.0000 0.1077 0.0000 0.1077 0.0000
## length 0.0000 0.1077 0.0000 0.1077 0.0000 0.1077
```



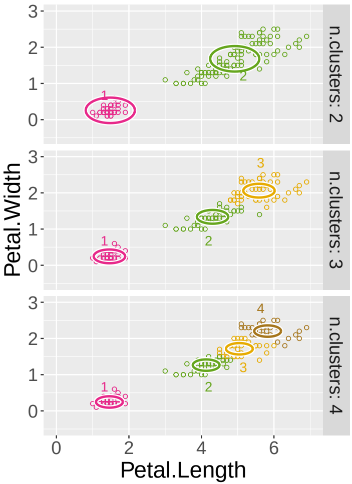
spherical, unequal volume

```
##                 c1     c1     c2     c2     c3     c3
## width  0.0202 0.0000 0.1298 0.0000 0.1837 0.0000
## length 0.0000 0.0202 0.0000 0.1298 0.0000 0.1837
```



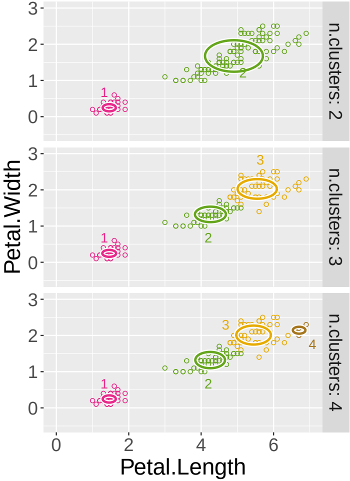
diagonal, equal volume and shape

```
##              c1     c1    c2     c2    c3     c3
## width  0.036 0.0000 0.036 0.0000 0.036 0.0000
## length 0.000 0.1878 0.000 0.1878 0.000 0.1878
```



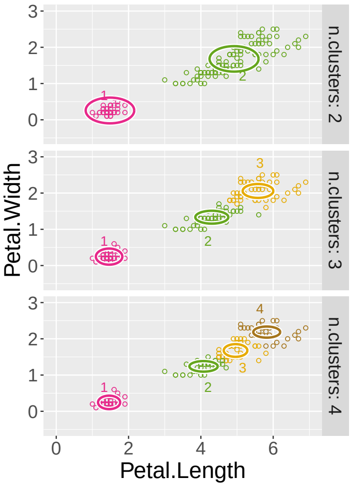
diagonal, varying volume, equal shape

```
##                 c1     c1     c2     c2     c3     c3
## width  0.0091 0.0000 0.0457 0.0000 0.0732 0.0000
## length 0.0000 0.0367 0.0000 0.1837 0.0000 0.2944
```



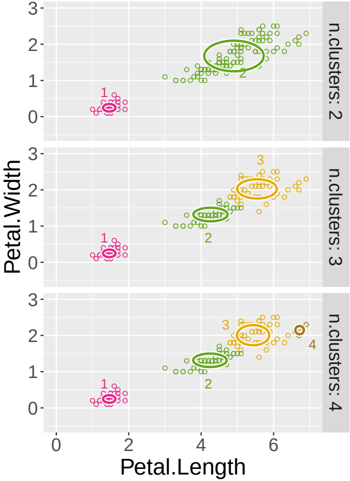
diagonal, equal volume, varying shape

```
##               c1     c1     c2     c2     c3     c3
## width  0.0494 0.0000 0.0317 0.0000 0.0368 0.0000
## length 0.0000 0.1341 0.0000 0.2089 0.0000 0.1802
```



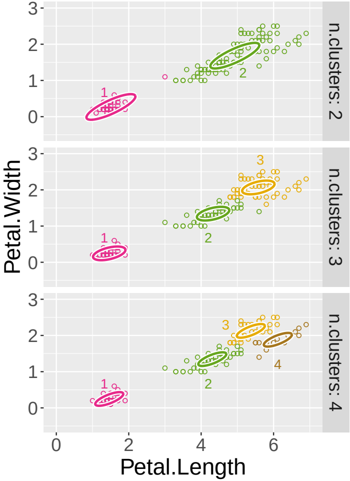
diagonal, varying volume and shape

```
##                c1     c1     c2     c2     c3     c3
## width  0.0109 0.0000 0.0352 0.0000 0.0709 0.0000
## length 0.0000 0.0296 0.0000 0.2243 0.0000 0.3008
```



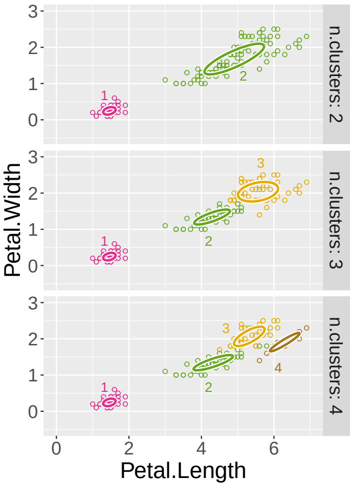
ellipsoidal, equal volume, shape, and orientation

```
##             c1     c1     c2     c2     c3     c3
## width  0.0358 0.0425 0.0358 0.0425 0.0358 0.0425
## length 0.0425 0.2005 0.0425 0.2005 0.0425 0.2005
```

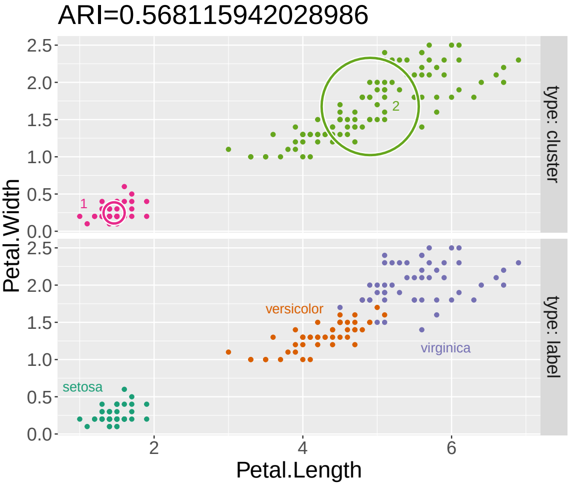


ellipsoidal, varying volume, shape, and orientation

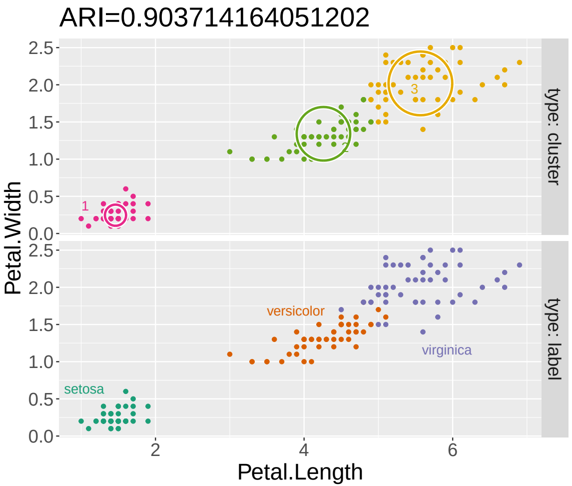
```
##                c1     c1     c2     c2     c3     c3
## width  0.0109 0.0059 0.0428 0.0813 0.0727 0.0482
## length 0.0059 0.0296 0.0813 0.2438 0.0482 0.3065
```



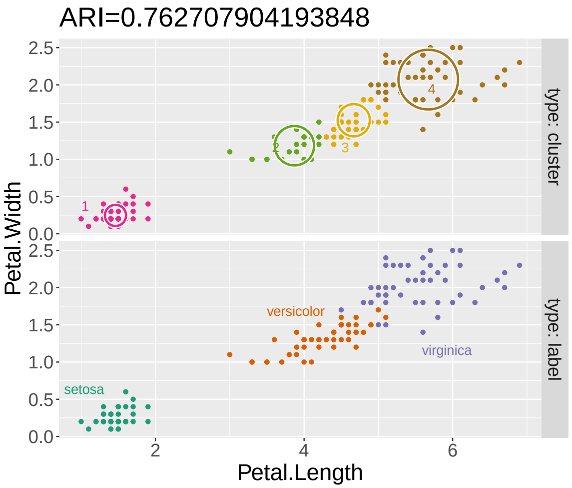
Compare two clusters to labels



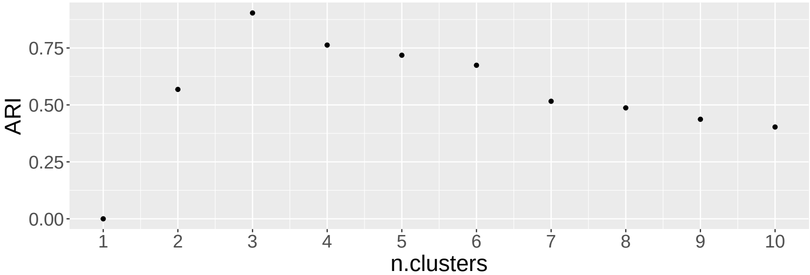
Compare three clusters to labels



Compare four clusters to labels

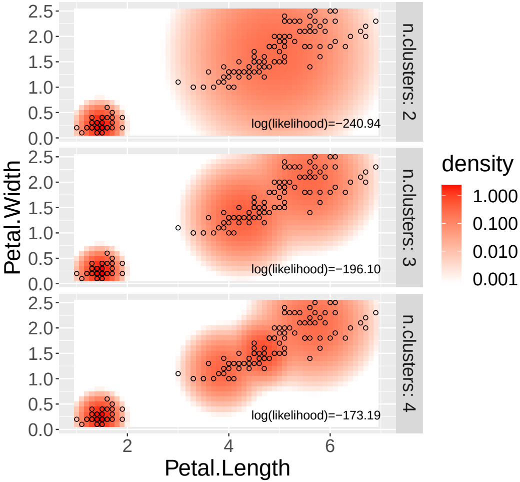


Compute ARI for several clusterings



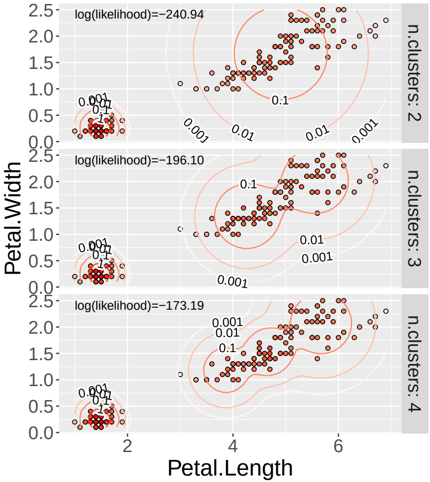
- Which K is best? Clear peak at 3 clusters, which makes sense since there are three species in these data.

Visualization of log likelihood

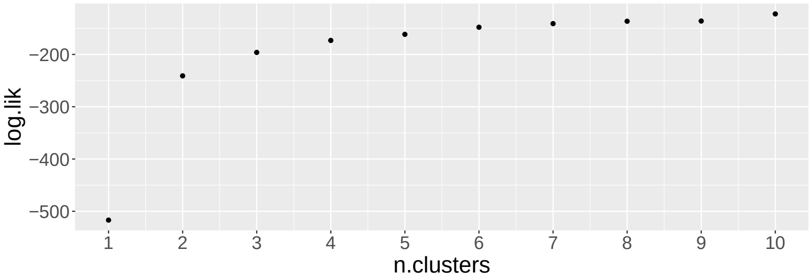


- Darker red means larger density value from learned model.
- The total redness in the data points represents the log likelihood, which is what the EM algorithm attempts to maximize.

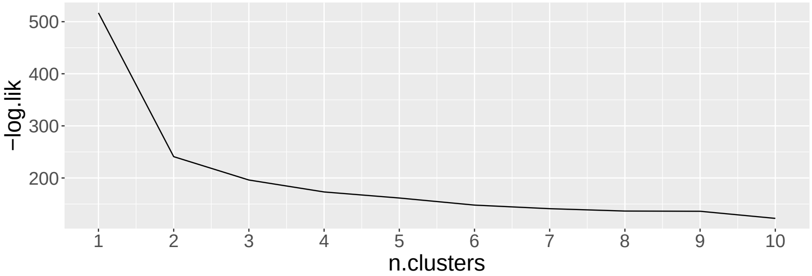
Visualize density using level curves



Compute log likelihood for several clusterings

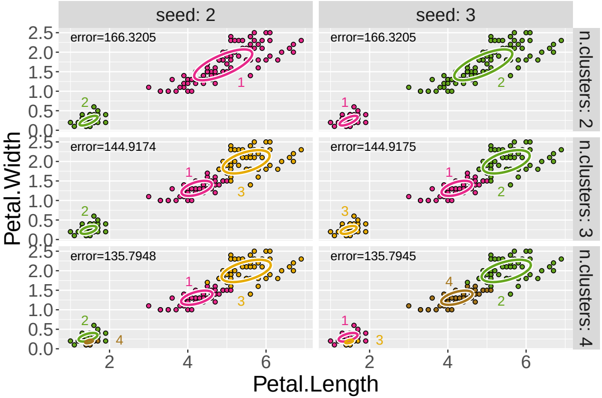


Model selection via error curve analysis (negative log likelihood)



- These error values can be computed using only the input data (labels/outputs are not required).
- In general, for any problem/data set, making this plot and then locating the “kink in the curve” is a good rule of thumb for selecting the number of clusters.

Visualize clusters using two random seeds



- Different seeds used for initial assignment based on K-means.
- EM solution quality depends on random seed (not much variation in these simple data though).

EM algo update rules

Let $f(x, \mu, S)$ be the (multivariate) normal density for a feature vector $x \in \mathbb{R}^p$, a mean vector $\mu \in \mathbb{R}^p$, and a covariance matrix $S \in \mathbb{R}^{p \times p}$.

In the E step we update the probability matrix,

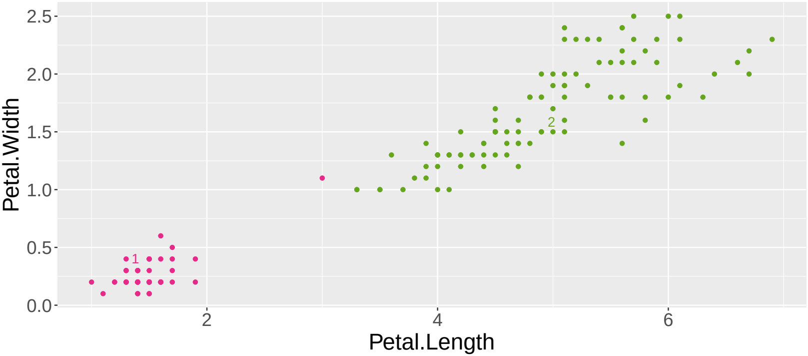
$$T_{ik} \leftarrow \frac{\pi_k f(x_i, \mu_k, S_k)}{\sum_{k=1}^{K} \pi_k f(x_i, \mu_k, S_k)}$$

.

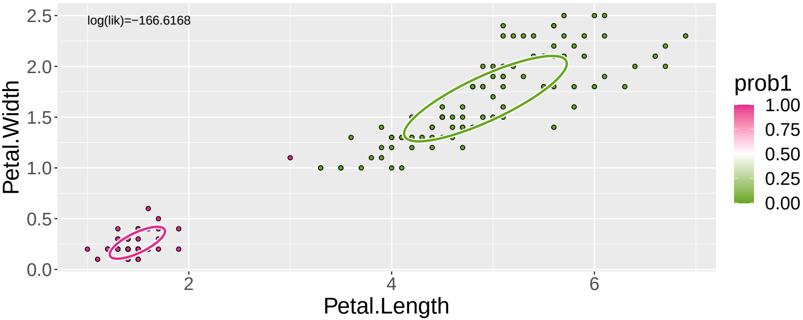
In the M step we update the cluster parameters,

- $\pi_k \leftarrow \frac{1}{n} \sum_{i=1}^{n} T_{i,k}$,
- $\mu_k \leftarrow \frac{\sum_{i=1}^{k} T_{i,k} x_i}{\sum_{i=1}^{k} T_{i,k}}$,
- $S_k \leftarrow \frac{\sum_{i=1}^{k} T_{i,k} (x_i - \mu_k)(x_i - \mu_k)^\intercal}{\sum_{i=1}^{k} T_{i,k}}$.

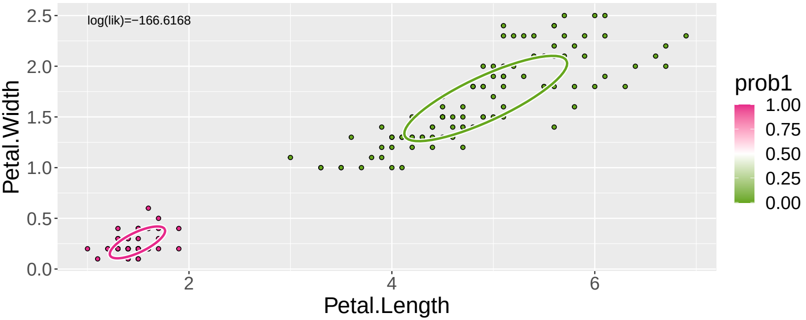
EM algo starting with K-means assignments



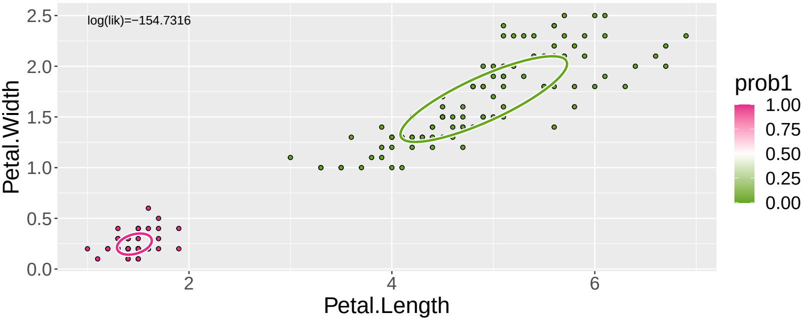
Compute weights, means, covariance matrices



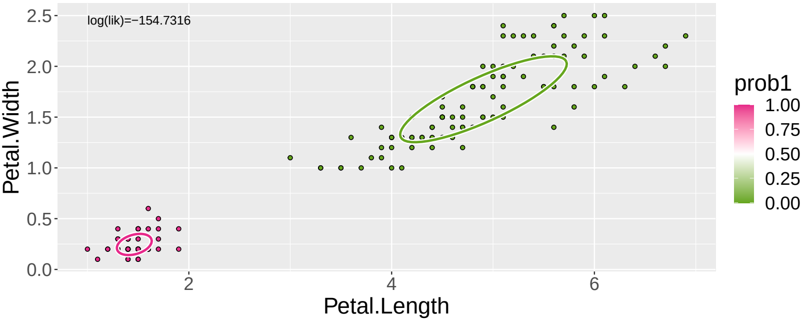
Cluster probabilities updated



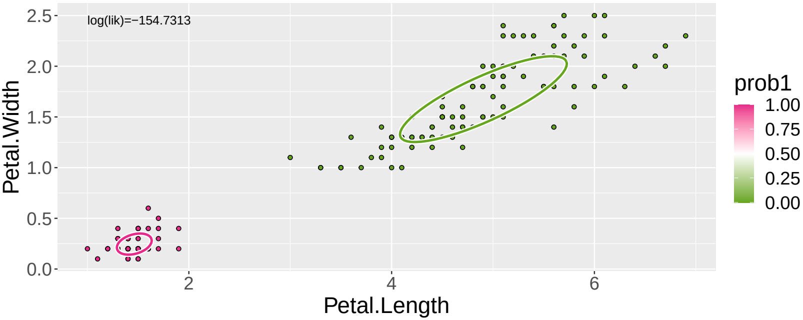
Compute new cluster parameters



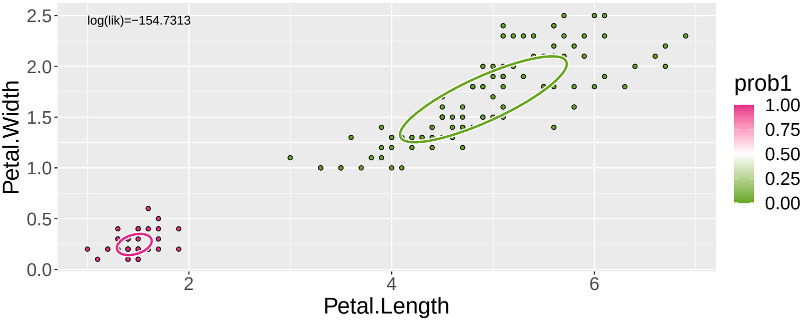
Compute new cluster/data probabilities



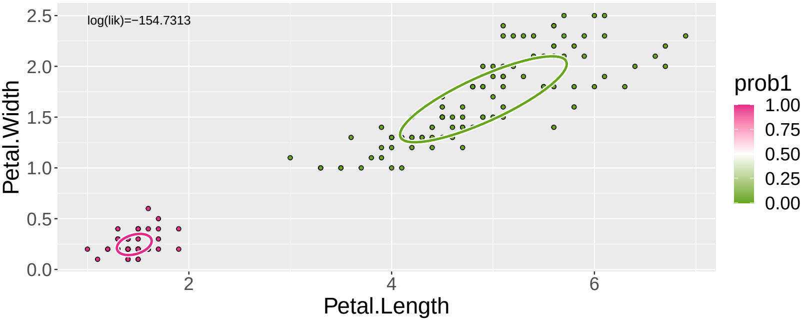
Compute cluster parameters iteration 3



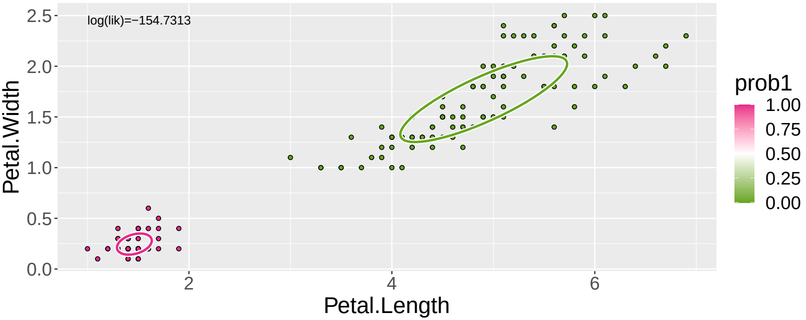
Compute probabilities iteration 3



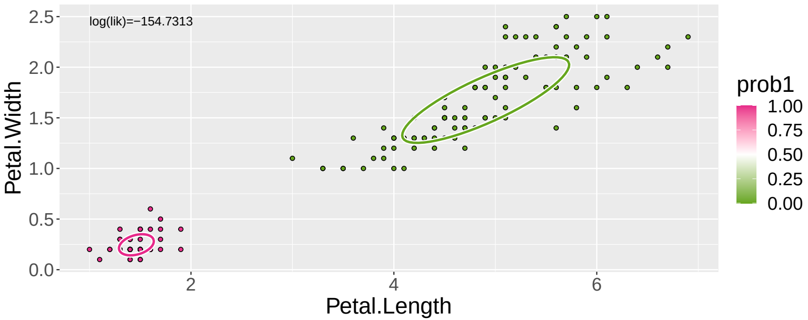
Compute cluster parameters iteration 4



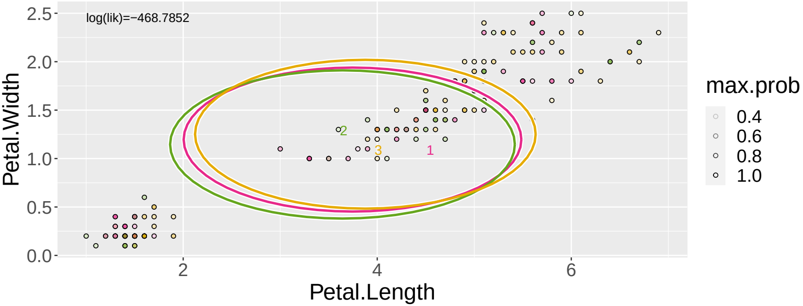
Compute probabilities iteration 4



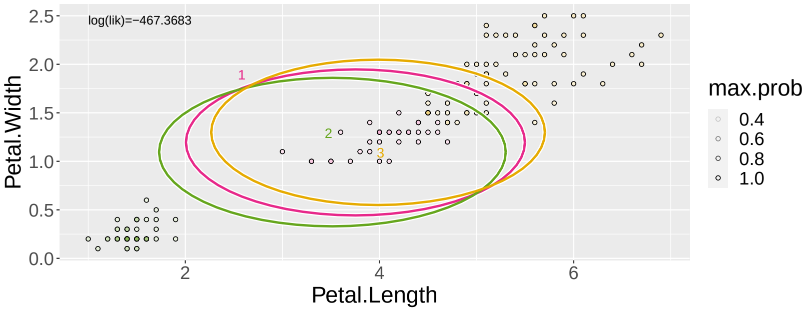
Compute cluster parameters iteration 5 (no change = stop)



Three clusters, diagonal constraint, random initialization

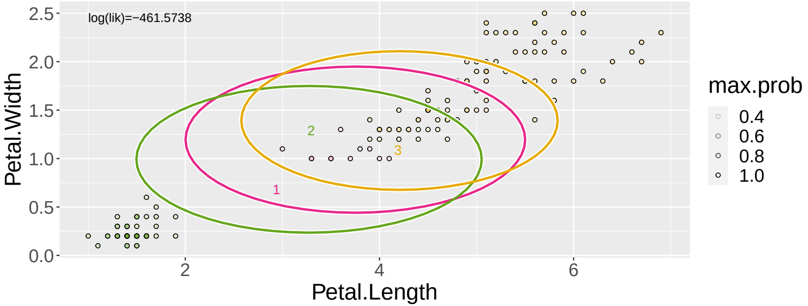


iteration 2



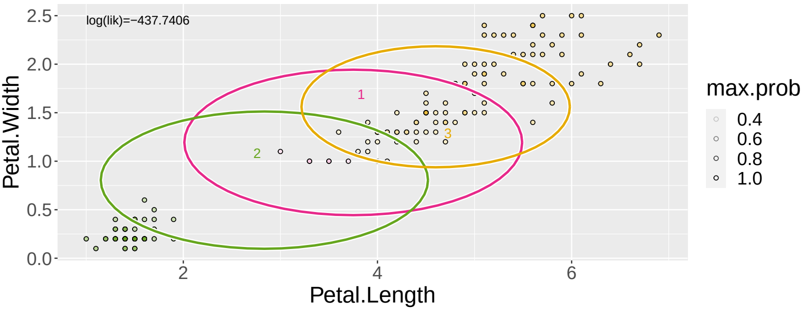
log(lik)=−467.3683
1
2
3
Petal.Width
Petal.Length
2.5
2.0
1.5
1.0
0.5
0.0
2
4
6
max.prob
0.4
0.6
0.8
1.0

iteration 3



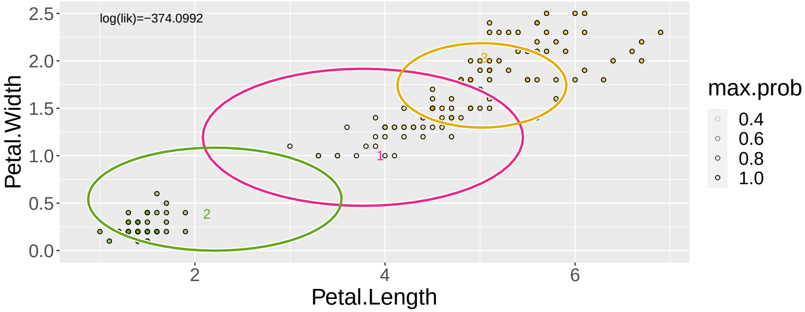
log(lik)=−461.5738
2.5
2.0
1.5
1.0
0.5
0.0
Petal.Width
2
4
6
Petal.Length
1
2
3
max.prob
0.4
0.6
0.8
1.0

iteration 4



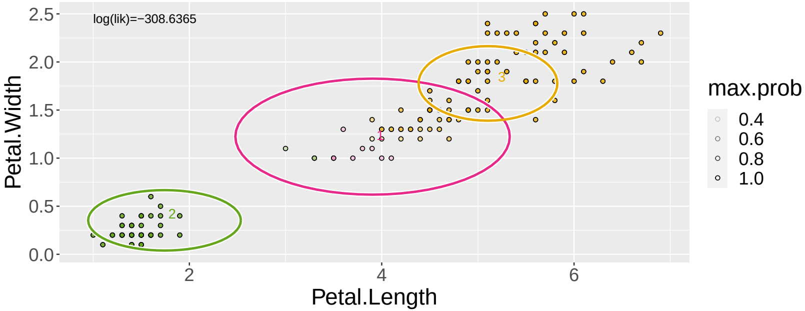
log(lik)=−437.7406
1
2
3
Petal.Width
Petal.Length
2.5
2.0
1.5
1.0
0.5
0.0
2
4
6
max.prob
0.4
0.6
0.8
1.0

iteration 5



log(lik)=−374.0992
Petal.Width
Petal.Length
2.5
2.0
1.5
1.0
0.5
0.0
2
4
6
1
2
3
max.prob
0.4
0.6
0.8
1.0

iteration 6



log(lik)=−308.6365
2.5
2.0
1.5
1.0
0.5
0.0
Petal.Width
2
4
6
Petal.Length
1
2
3
max.prob
0.4
0.6
0.8
1.0

iteration 7

log(lik)=−211.7579
2.5
2.0
1.5
1.0
0.5
0.0
Petal.Width
2
4
6
Petal.Length
1
2
3
max.prob
0.4
0.6
0.8
1.0

iteration 8

log(lik)=−181.2220
2.5
2.0
1.5
1.0
0.5
0.0
Petal.Width
2
4
6
Petal.Length
1
2
3
max.prob
0.4
0.6
0.8
1.0

iteration 9


log(lik)=−171.9739
Petal.Width
Petal.Length
2.5
2.0
1.5
1.0
0.5
0.0
2
4
6
1
2
3
max.prob
0.4
0.6
0.8
1.0

iteration 10

iteration 11

iteration 12

iteration 13

iteration 14

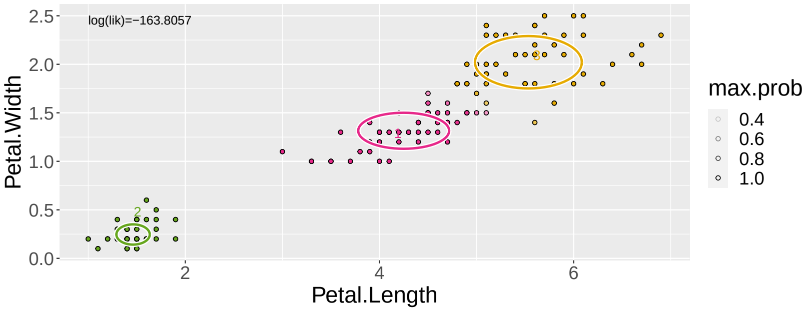
iteration 15

iteration 16

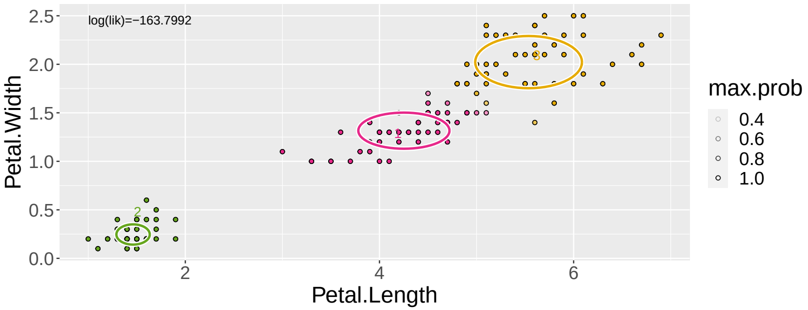
iteration 17

iteration 18

iteration 19



iteration 20



iteration 21