# Gaussian mixture models

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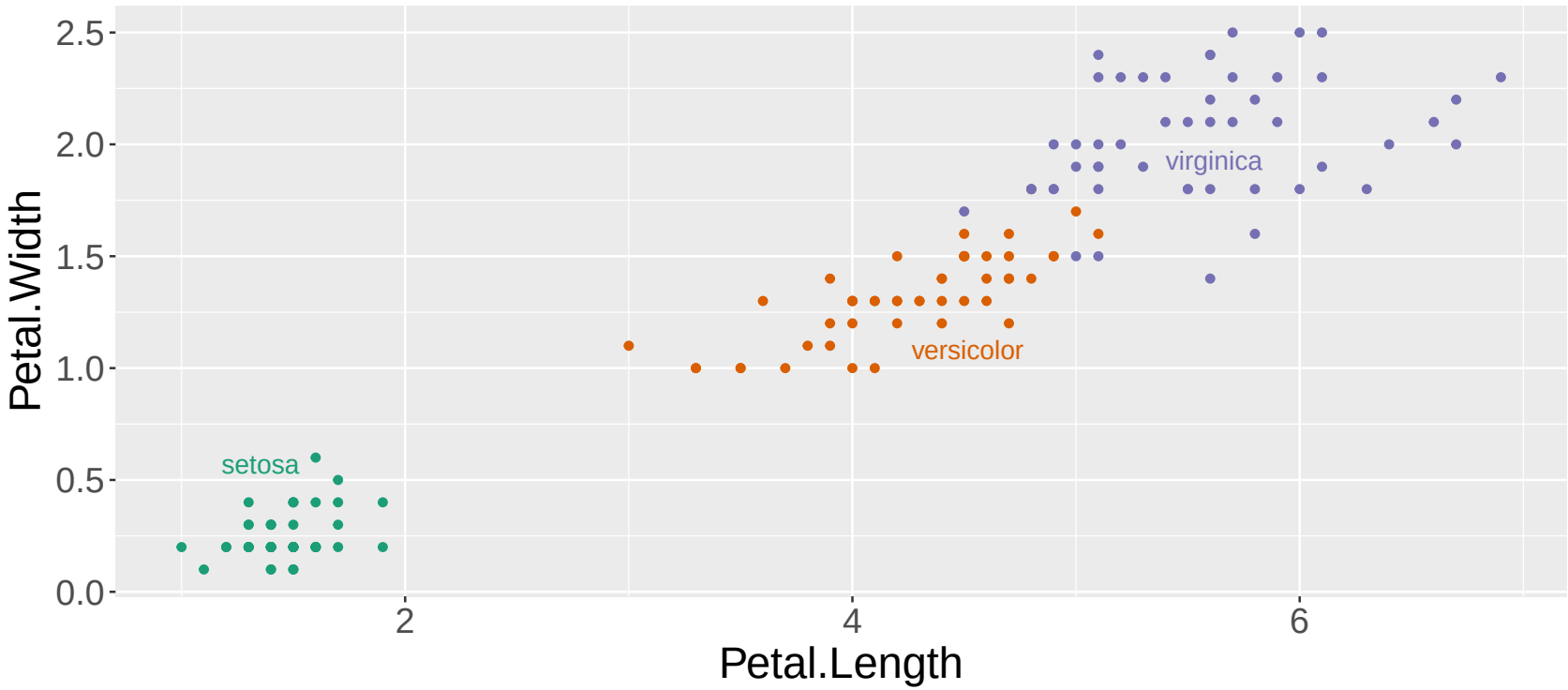
# Visualize iris data with labels



# Visualize iris data without labels

- Let $X = [x_1 \cdots x_n]^\intercal \in \mathbb{R}^{n \times p}$ be the data matrix (input for clustering), where $x_i \in \mathbb{R}^p$ is the input vector for observation $i$.
- 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

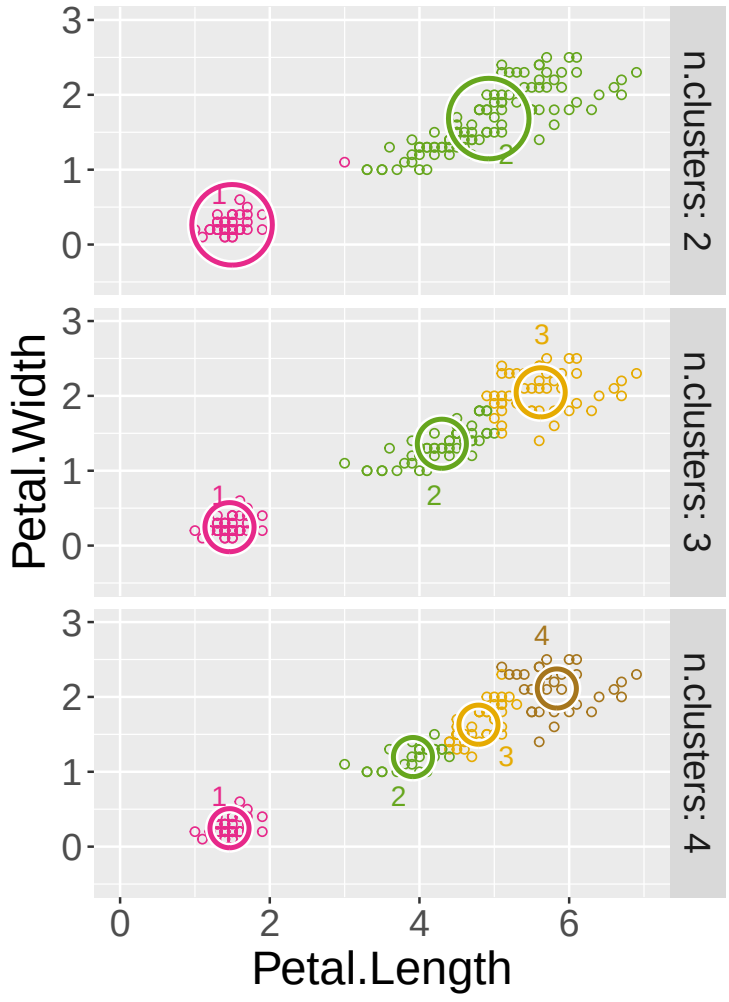
Need to fix number of clusters $K$, then for every $k \in \{1, \ldots, K\}$ we have cluster-specific parameters $\theta_k = [\mu_k, S_k, \pi_k]$ which are updated during M step,

- 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 $k$.

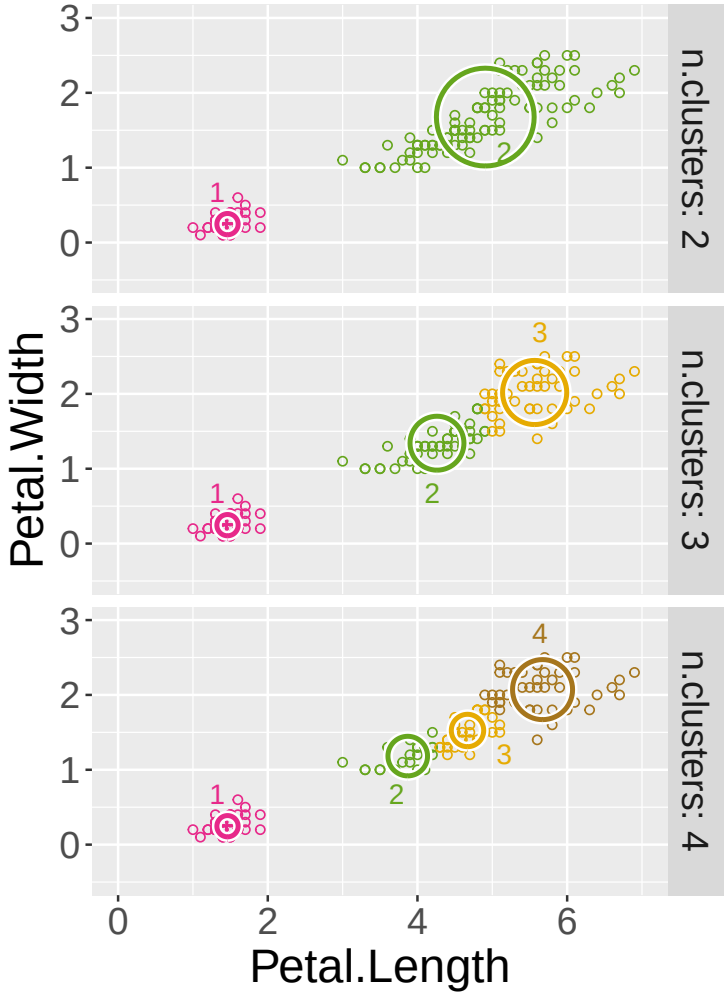
# spherical, equal volume

```
##                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
```



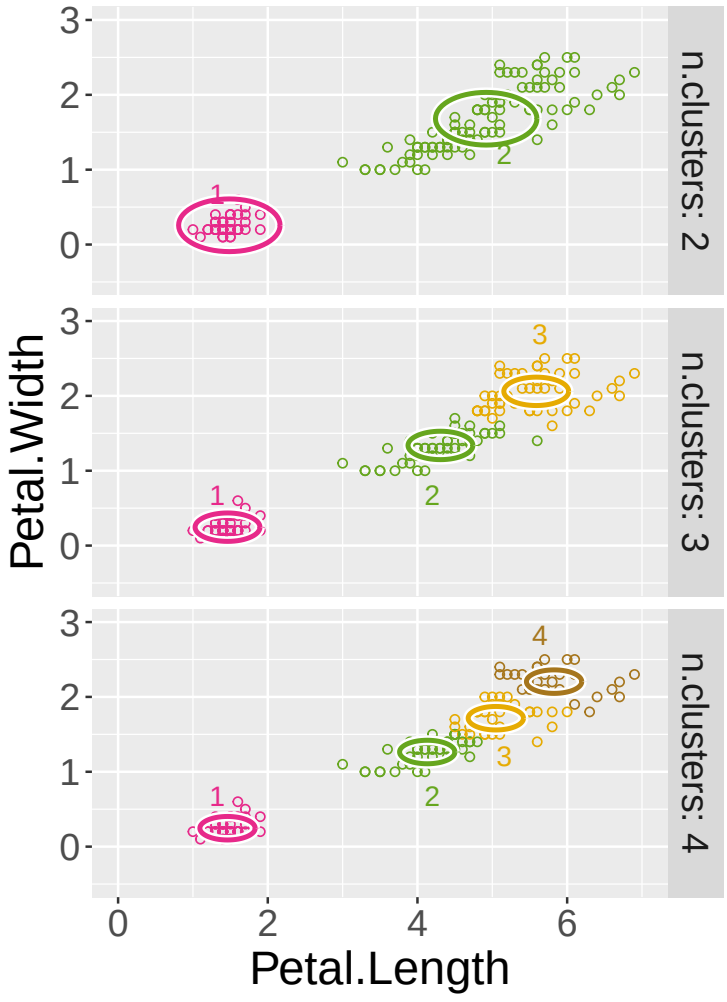
# spherical, unequal volume

```
##                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
```



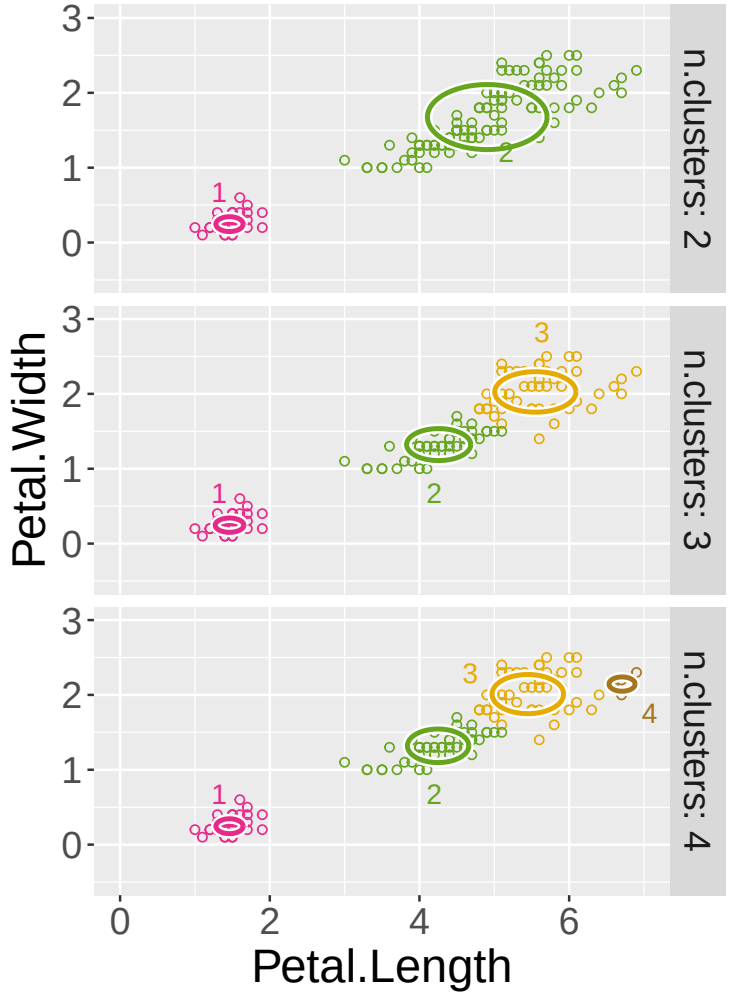
# diagonal, equal volume and shape

```
##              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
```



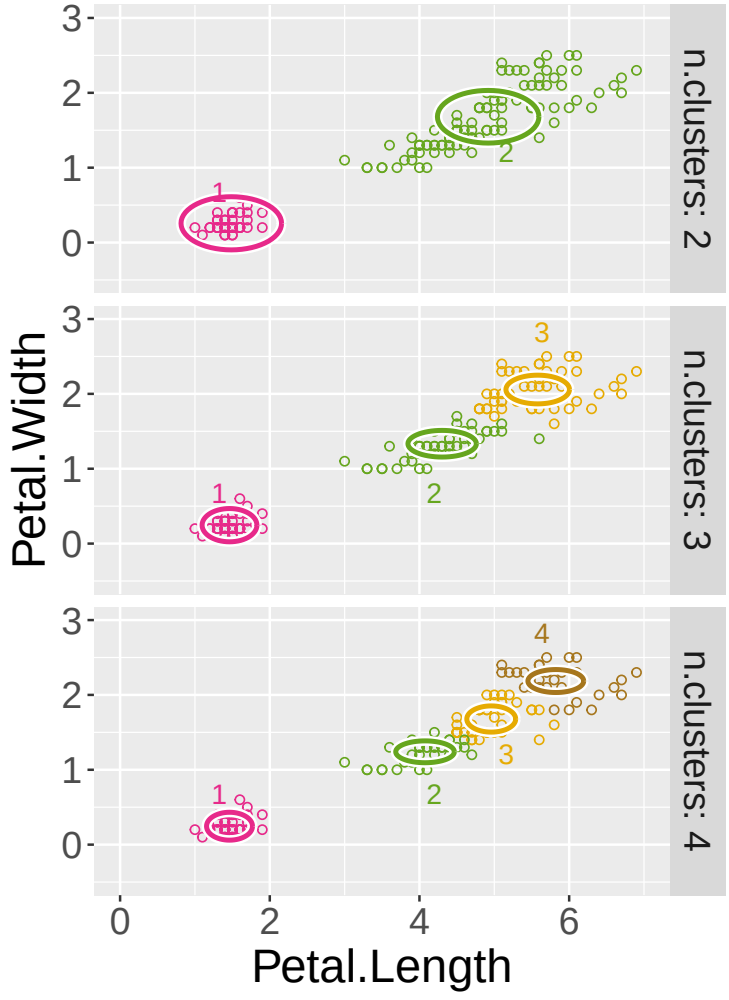
# diagonal, varying volume, equal shape

```
##                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
```



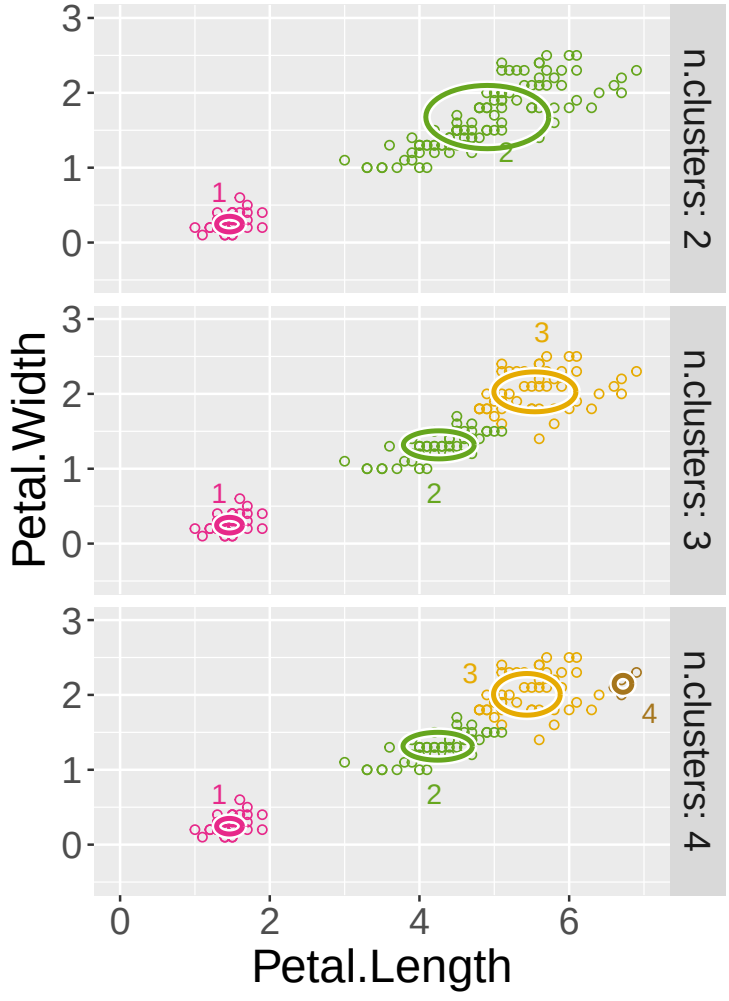
# diagonal, equal volume, varying shape

```
##                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
```



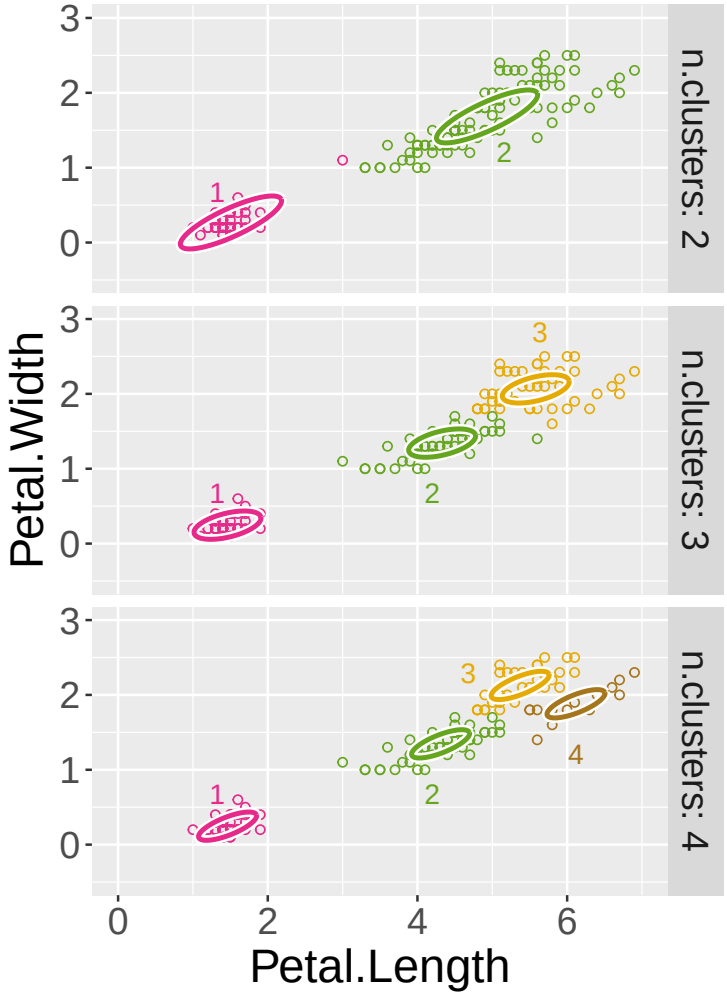
# diagonal, varying volume and shape

```
##                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
```



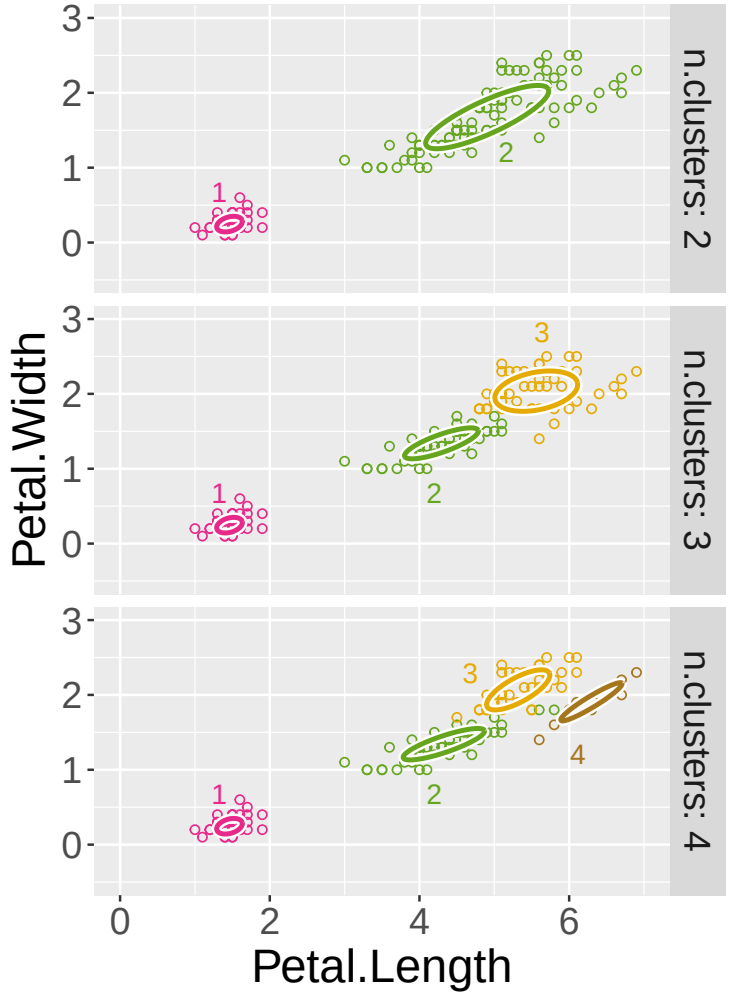
# ellipsoidal, equal volume, shape, and orientation

```
##                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
```

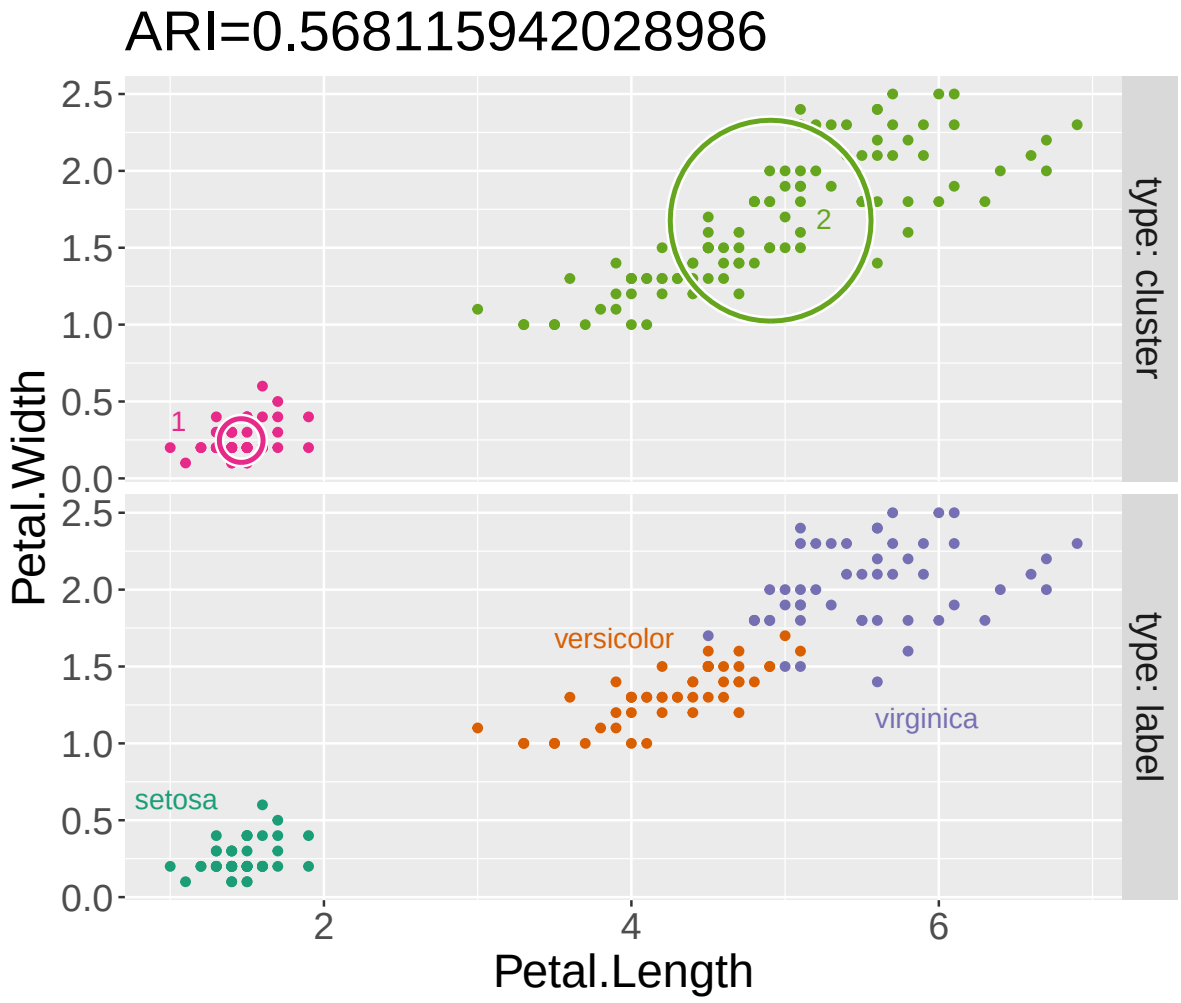


# ellipsoidal, varying volume, shape, and orientation

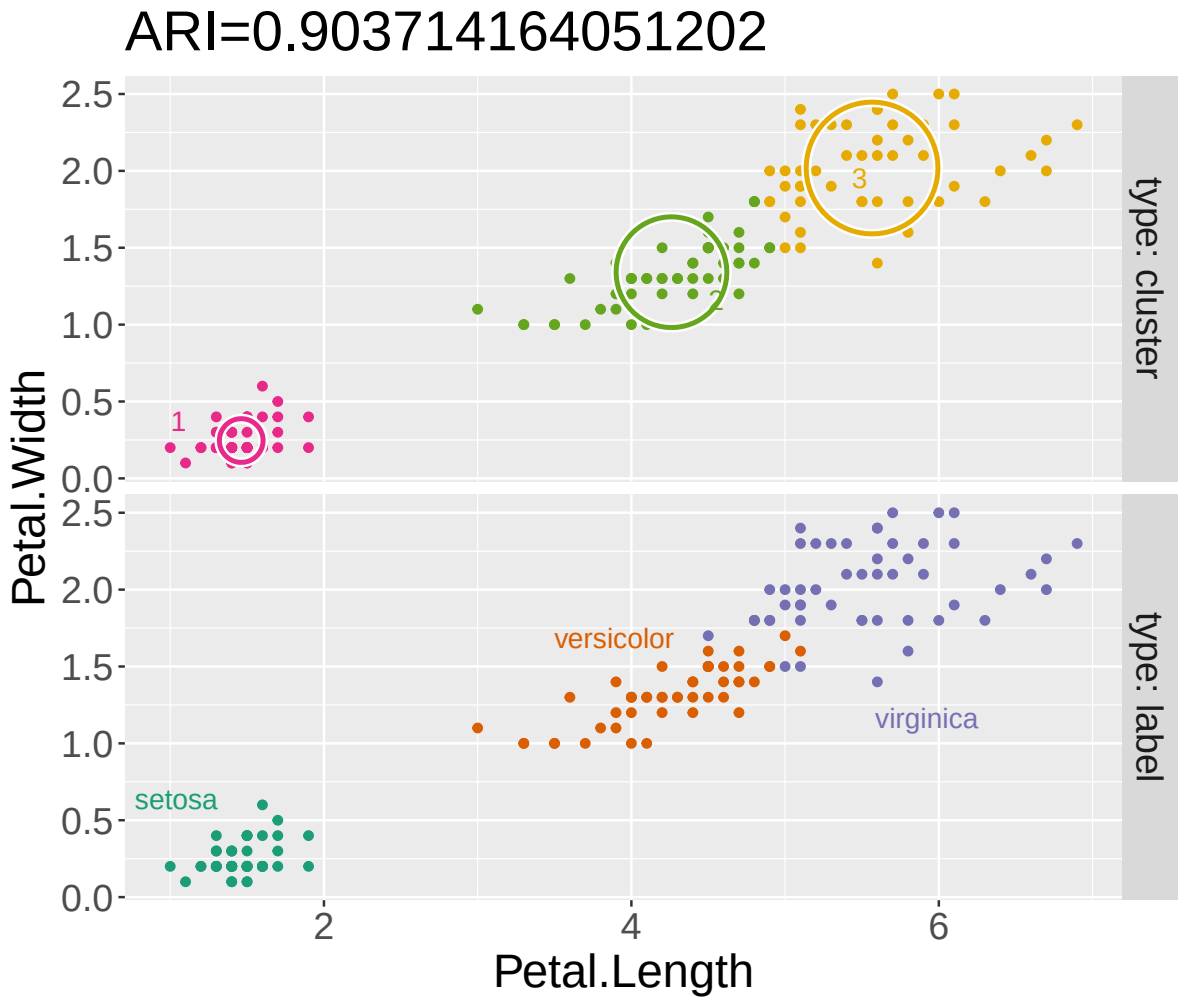
```
##                c1      c1      c2      c2      c3      c3
## width  0.0109 0.0059 0.0428 0.0813 0.0727 0.0482
## length 0.0059 0.0296 0.0813 0.2438 0.0482 0.3065
```



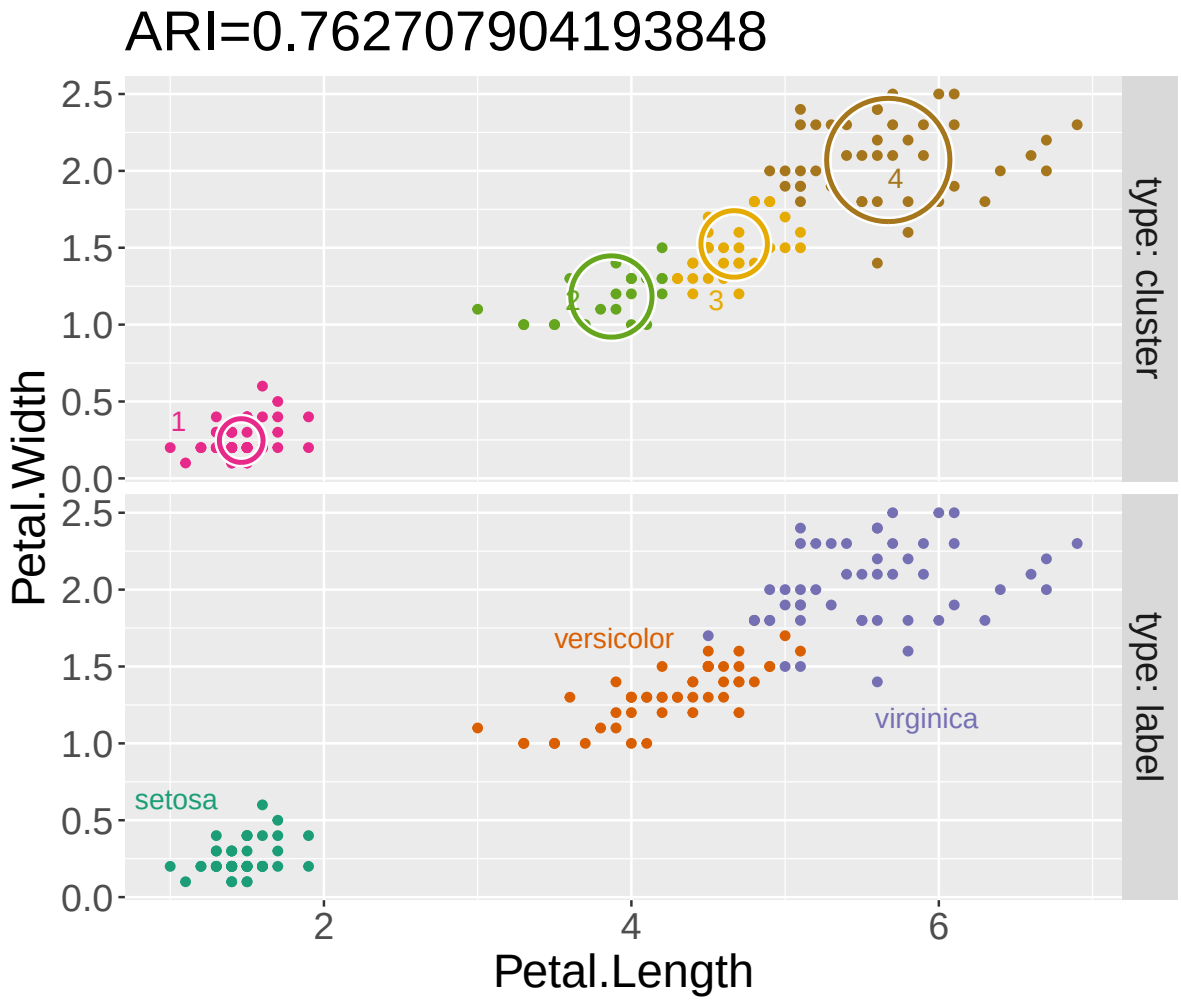
# Compare two clusters to labels



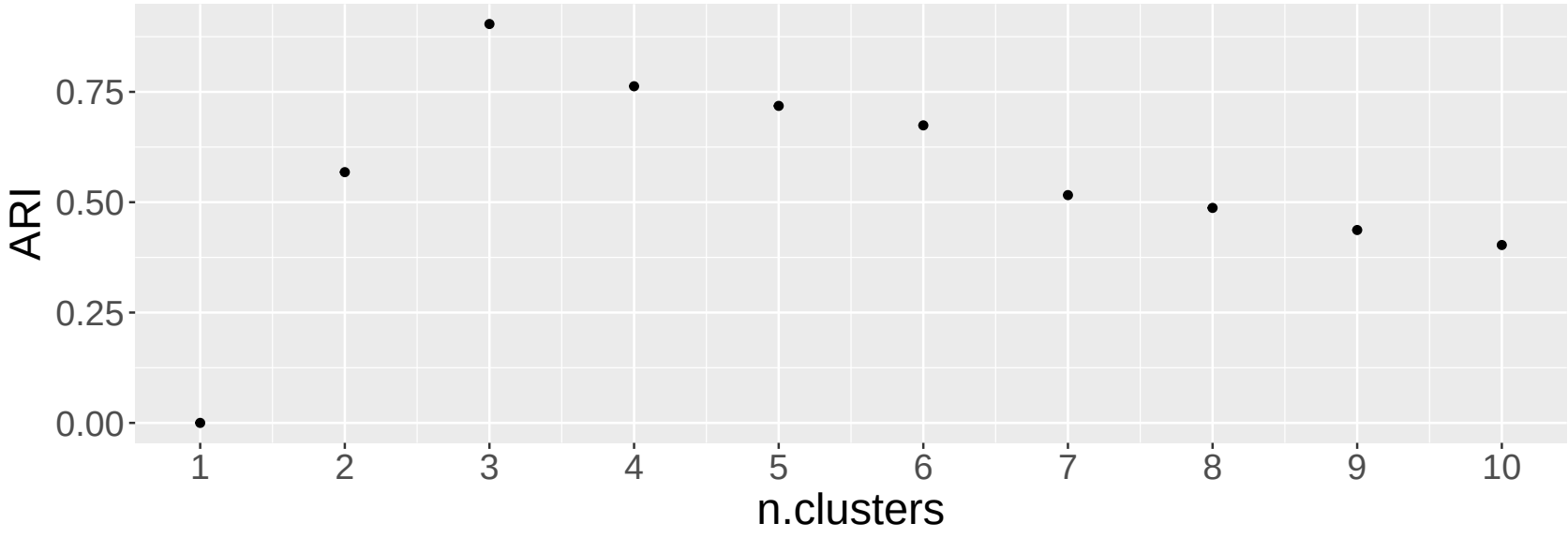
# Compare three clusters to labels



# Compare four clusters to labels

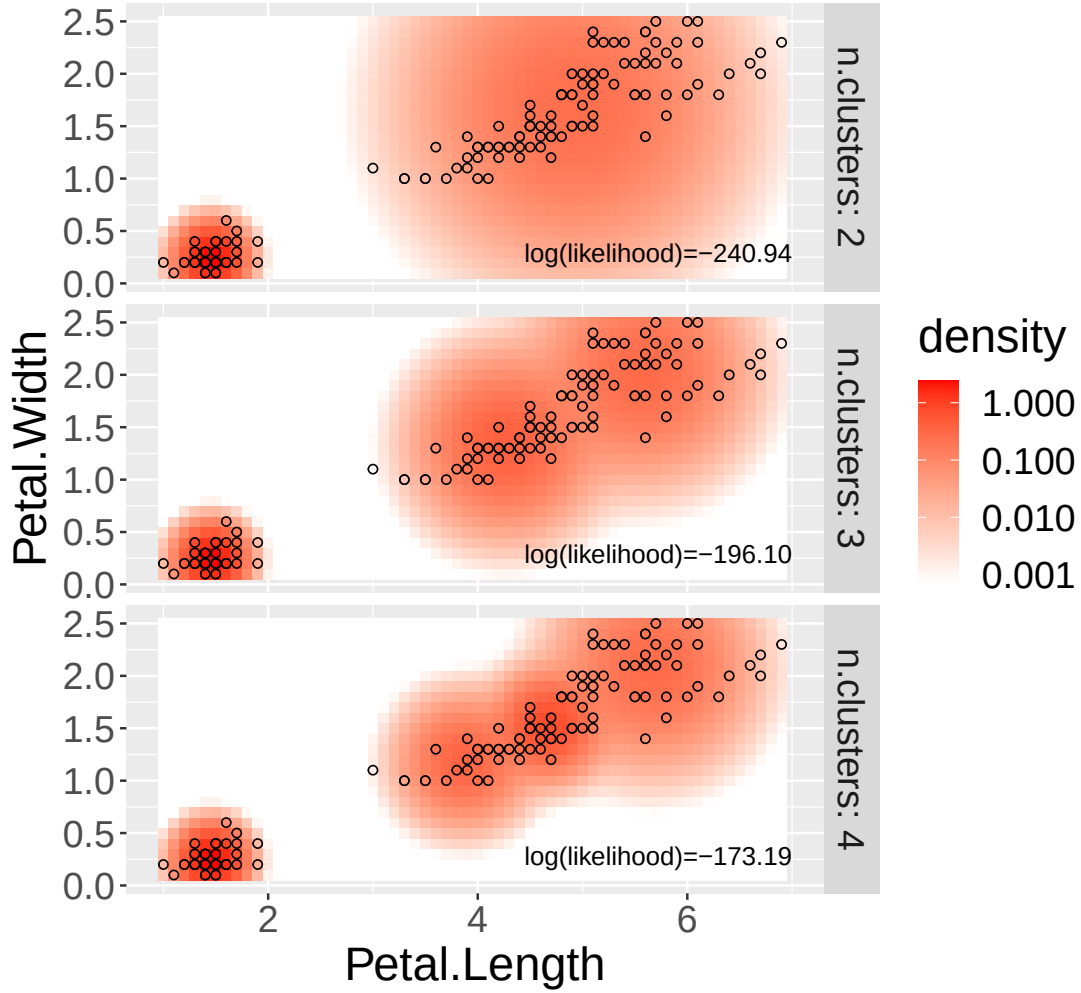


# Compute ARI for several clusterings



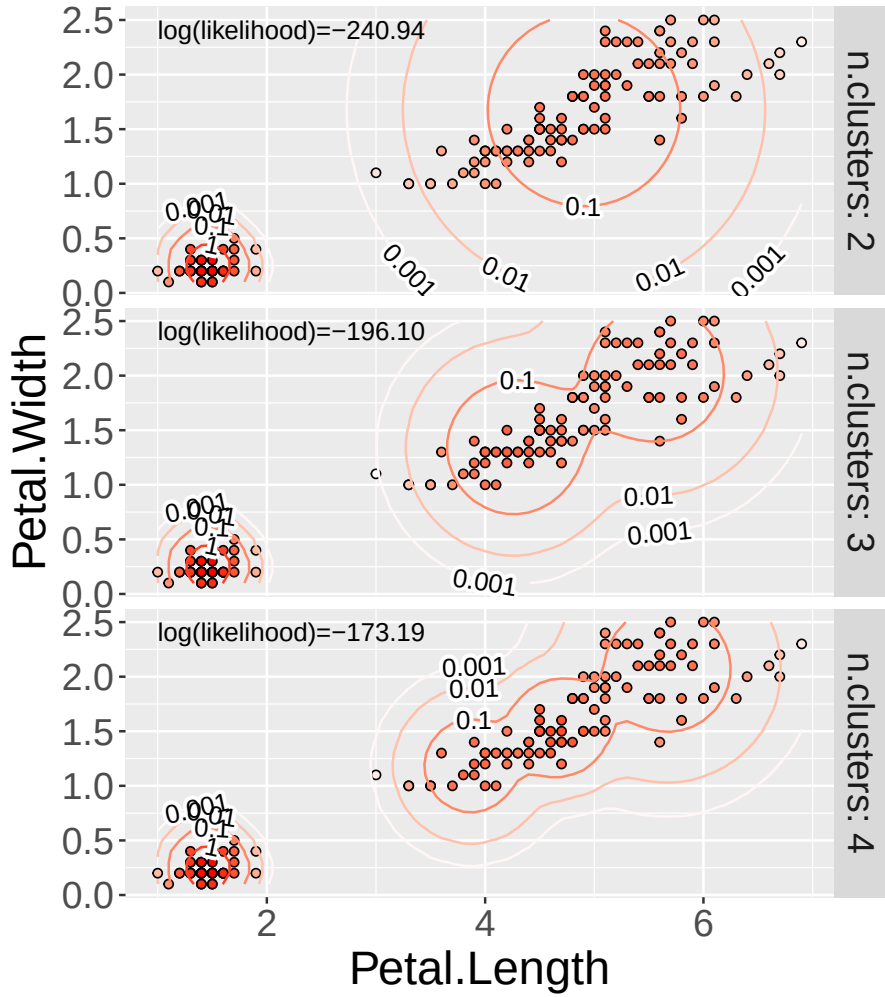

- Which K is best? Clear peak at 3 clusters, which makes sense since there are three species in these data.

# Visualization of log likelihood

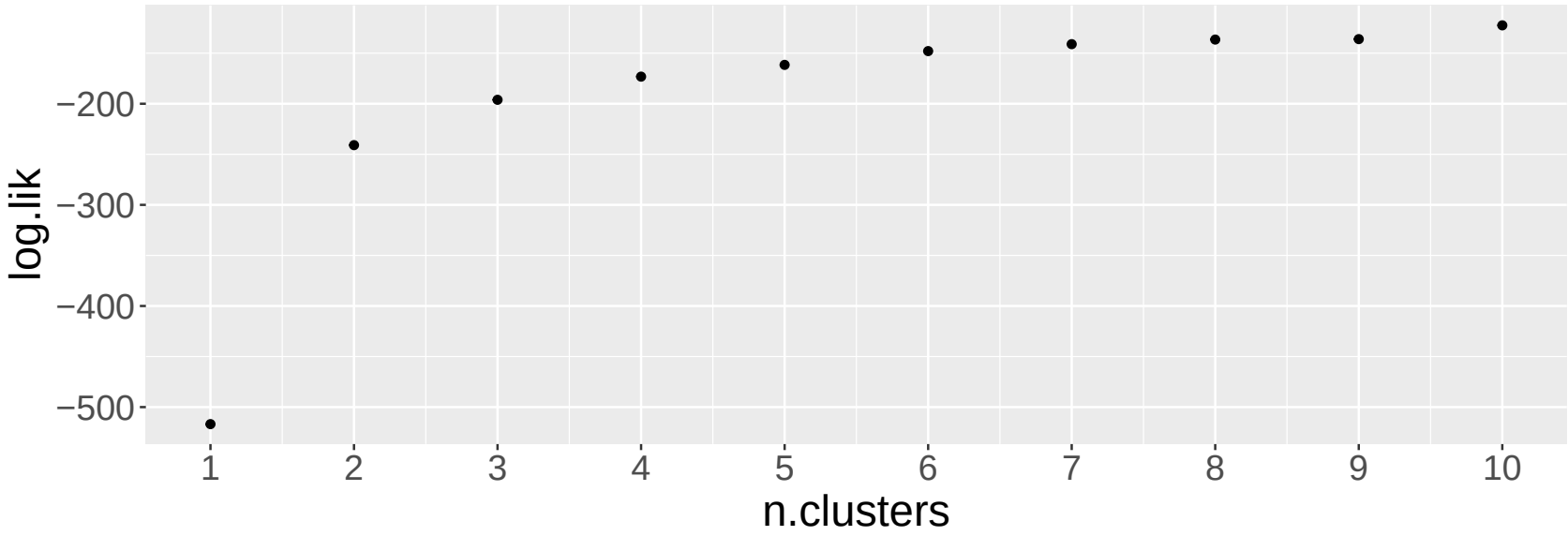



- Darker red means larger density value from learned model.
- The total redness in the data points represents the log likelihood, which is what the EM algorithm attempts to maximize.

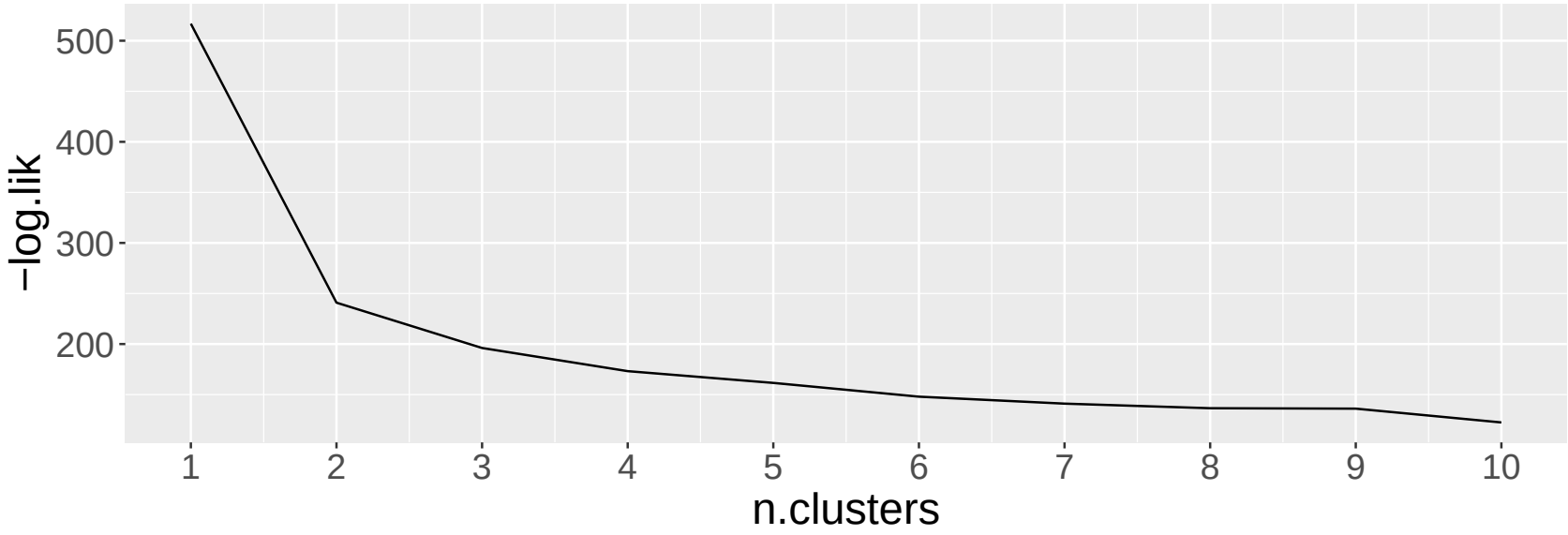
# Visualize density using level curves



# Compute log likelihood for several clusterings

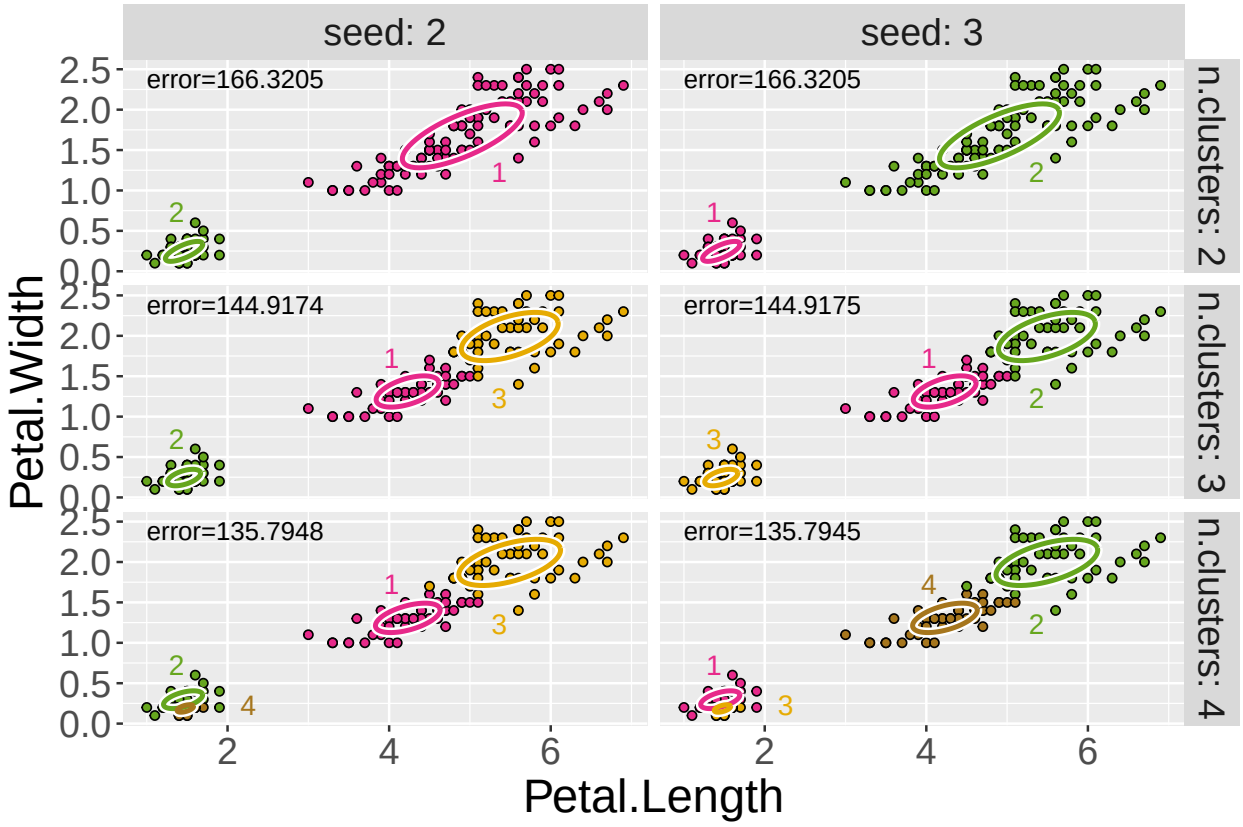


# Model selection via error curve analysis (negative log likelihood)




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

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,

- $\pi_k \leftarrow \frac{1}{n} \sum_{i=1}^{n} T_{i,k}$,
- $\mu_k \leftarrow \frac{\sum_{i=1}^{n} T_{i,k} x_i}{\sum_{i=1}^{n} T_{i,k}}$,
- $S_k \leftarrow \frac{\sum_{i=1}^{n} T_{i,k} (x_i - \mu_k)(x_i - \mu_k)^\intercal}{\sum_{i=1}^{n} T_{i,k}}$ (no constraints).

# Where do these update rules come from?

The goal of the algorithm is to find model parameters that maximize the log likelihood, $\log L(x, \theta, T)$.

$$\max_{\theta} \log L(x, \theta, T)$$

$$\max_{T} \log L(x, \theta, T)$$

- Use gradient condition to derive $T, \theta$ which maximize the likelihood given the data and other parameters.
- Covariance constraints affect the $\theta$ update rule. For example diagonal covariance update,
- $S_k \leftarrow \frac{\sum_{i=1}^{n} \text{Diag}[T_{i,k}(x_i - \mu_k)(x_i - \mu_k)^\intercal]}{\sum_{i=1}^{n} T_{i,k}}$ (diagonal constraint).
- $j$-th entry/feature of $S_k$ is $\sum_{i=1}^{n} T_{i,k} D_{i,j}^2$ where $D \in \mathbb{R}^{n \times p}$ is the difference matrix $X - \mu_k$. (avoids matrix multiplication, linear rather than quadratic time in feature dimension $p$)

# Numerical issues (underflow)

To avoid numerical issues in EM algorithm we need to

- Store log density, update via log-sum-exp trick, to avoid non-finite probability values in E step.

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

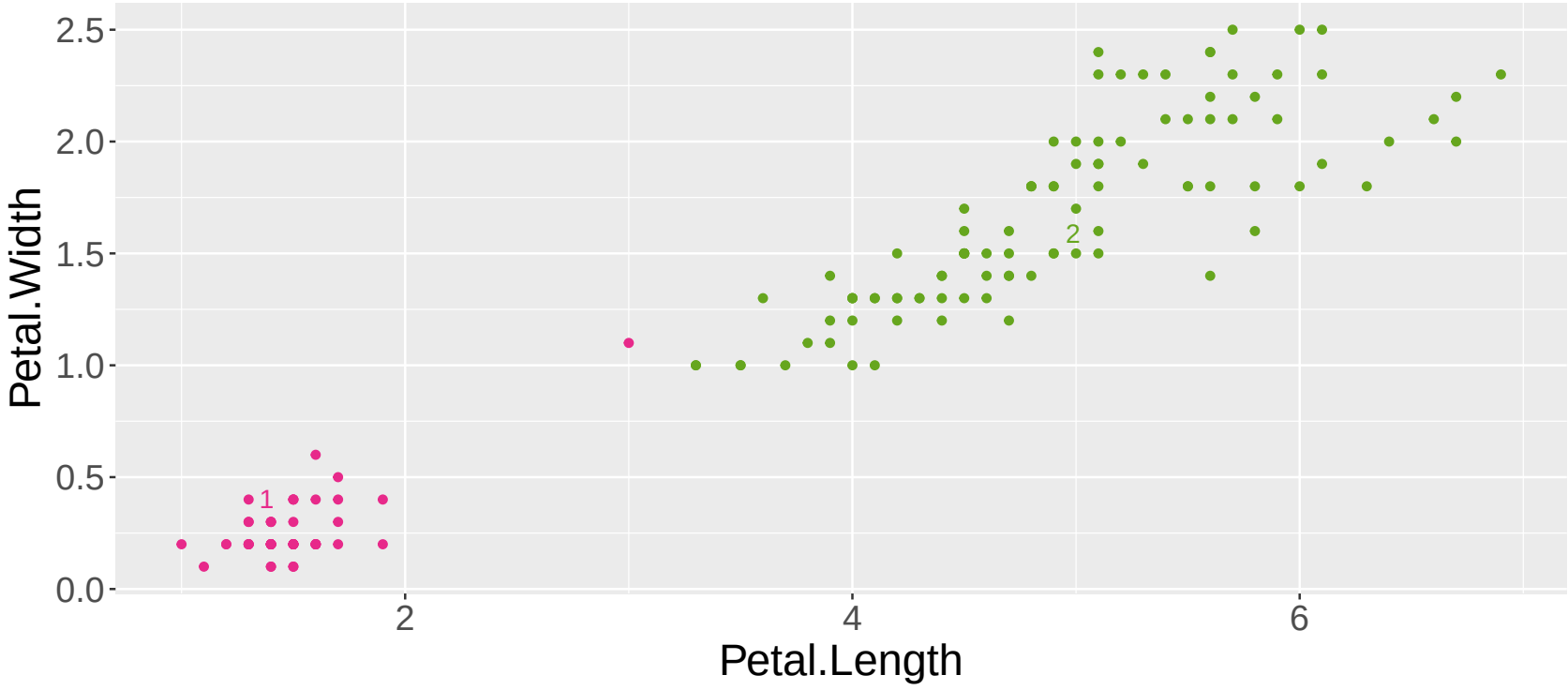
$$\log T_{ik} \leftarrow \log \pi_k + \log f(x_i, \mu_{k'}, S_{k'}) - Z$$

$$Z = M + \log[e^M \sum_{k'=1}^{K} \pi_{k'} e^{\log f(x_i, \mu_{k'}, S_{k'}) - M}]$$

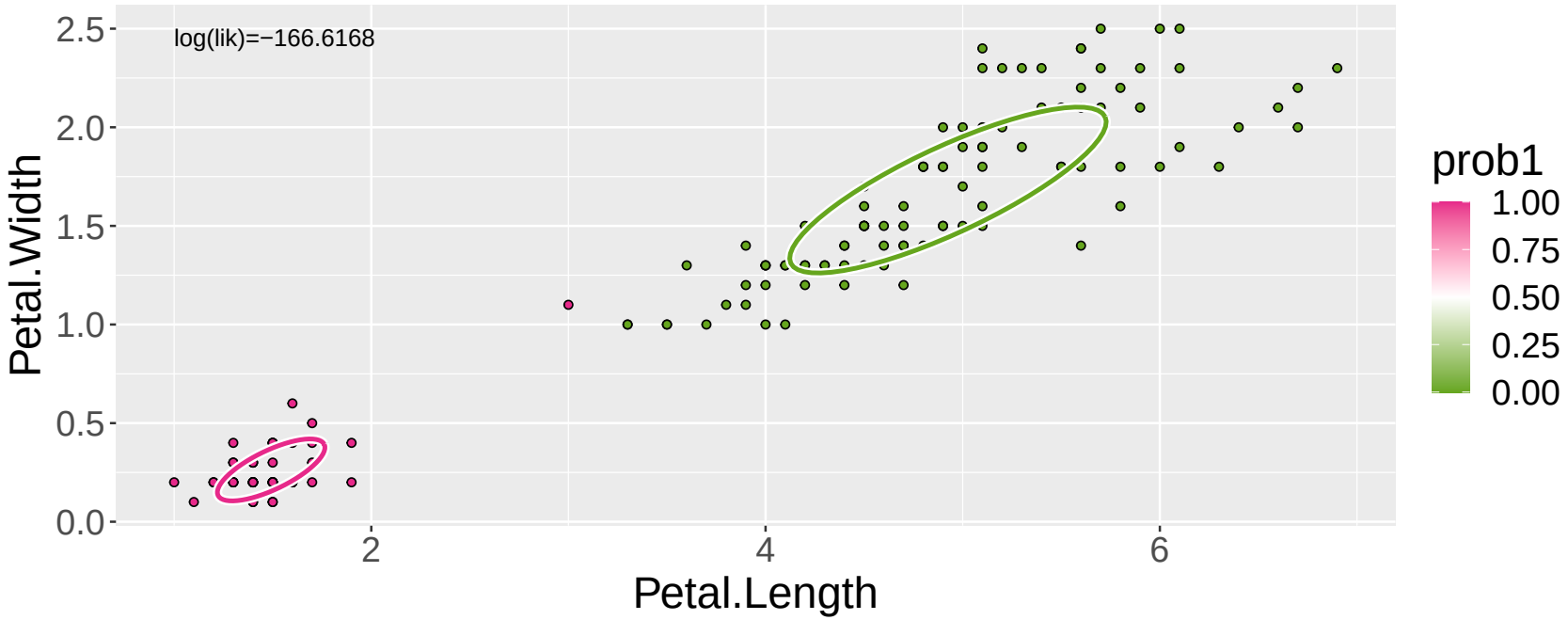
$$M = \max_{k' \in \{1,\ldots,K\}} \log f(x_i, \mu_{k'}, S_{k'})$$

- Add a small number, $\lambda = 10^{-6}$ to the diagonal of the covariance matrix to avoid zero variance in M step, $S_k \leftarrow \frac{\sum_{i=1}^{n} T_{i,k}(x_i - \mu_k)(x_i - \mu_k)^\intercal}{\sum_{i=1}^{n} T_{i,k}} + \lambda I_p$.

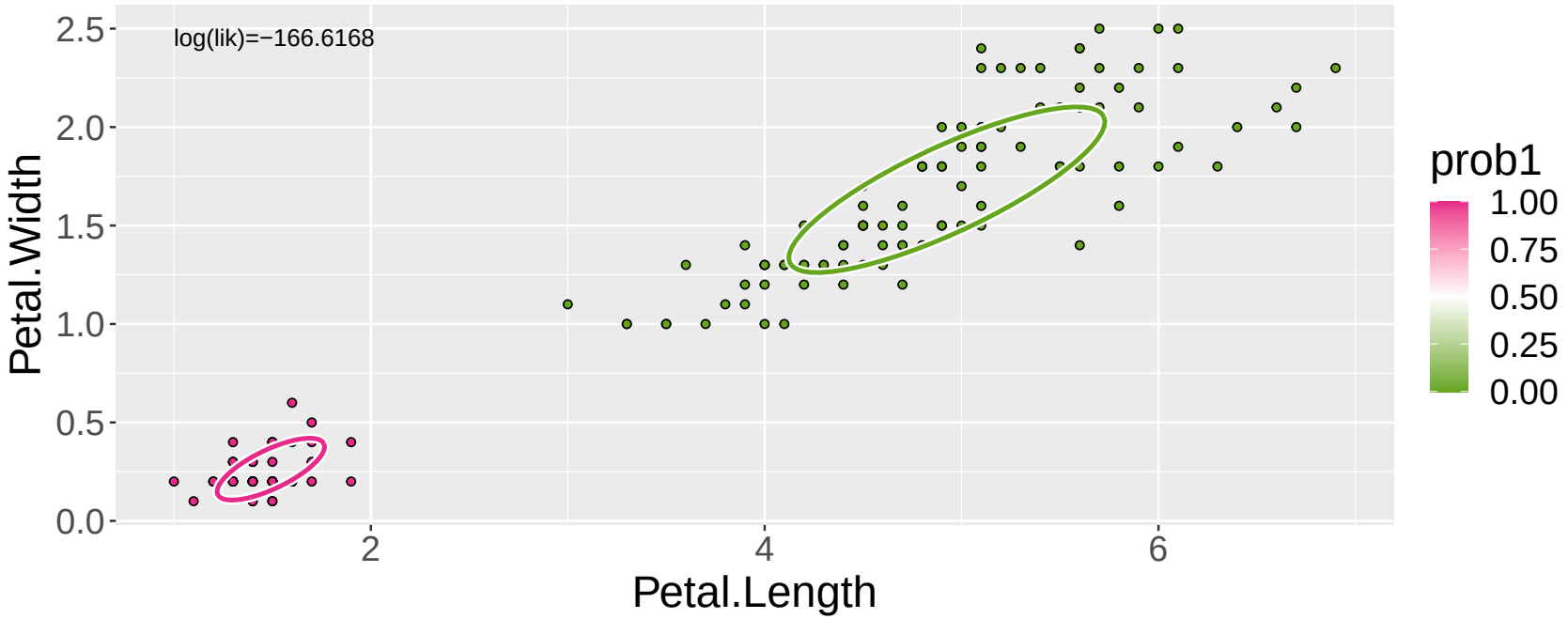
# EM algo starting with K-means assignments



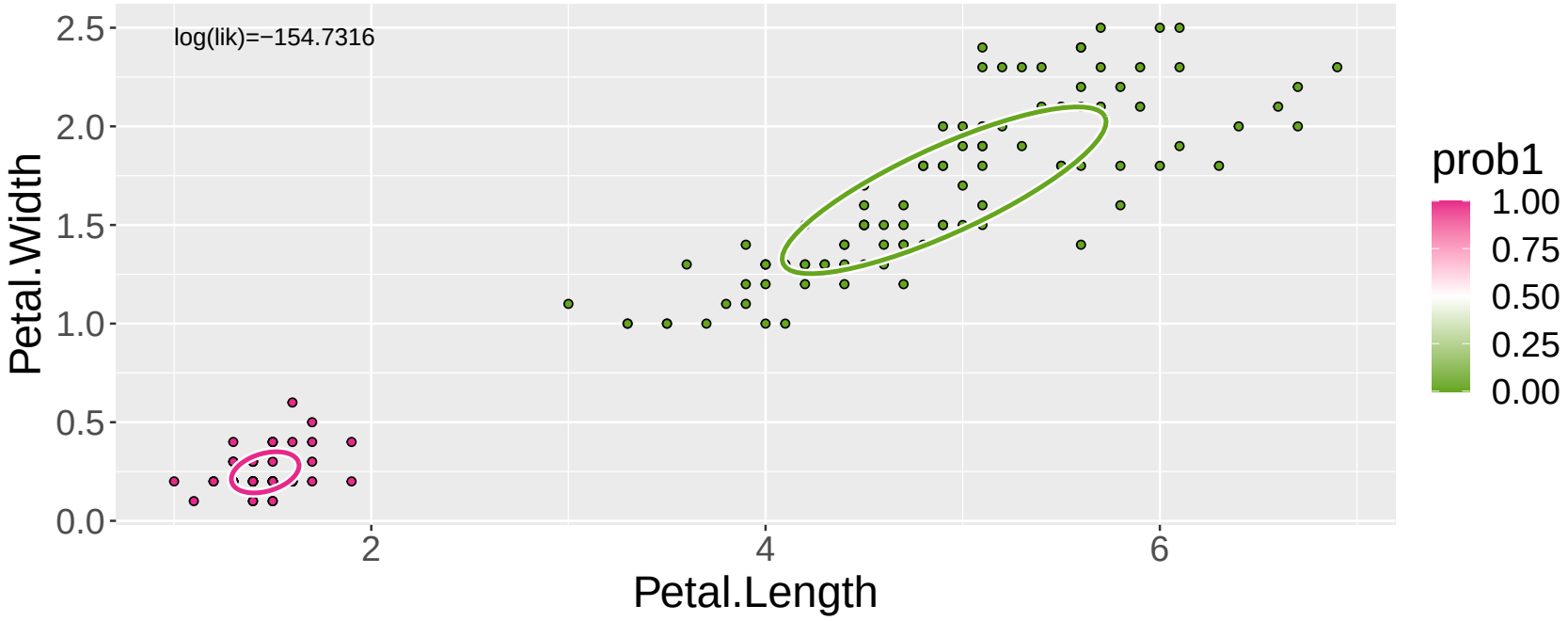
# Compute weights, means, covariance matrices



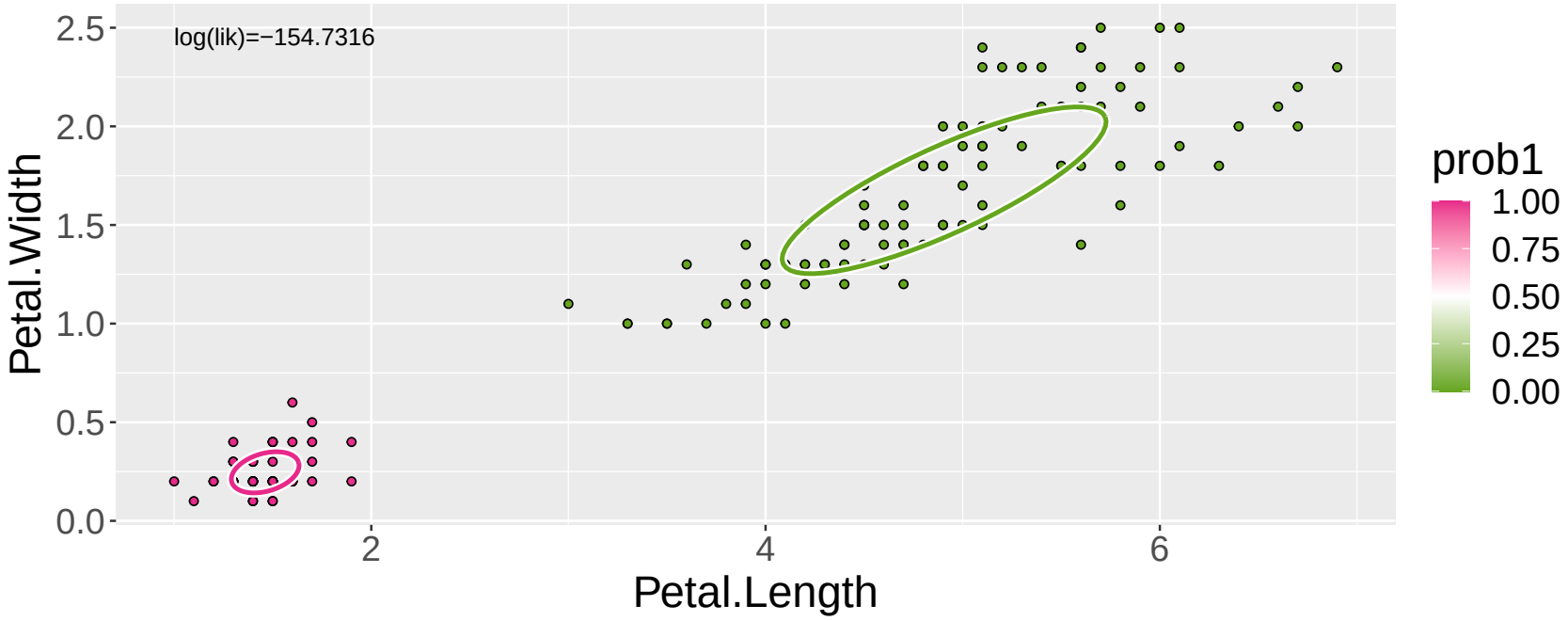
# Cluster probabilities updated



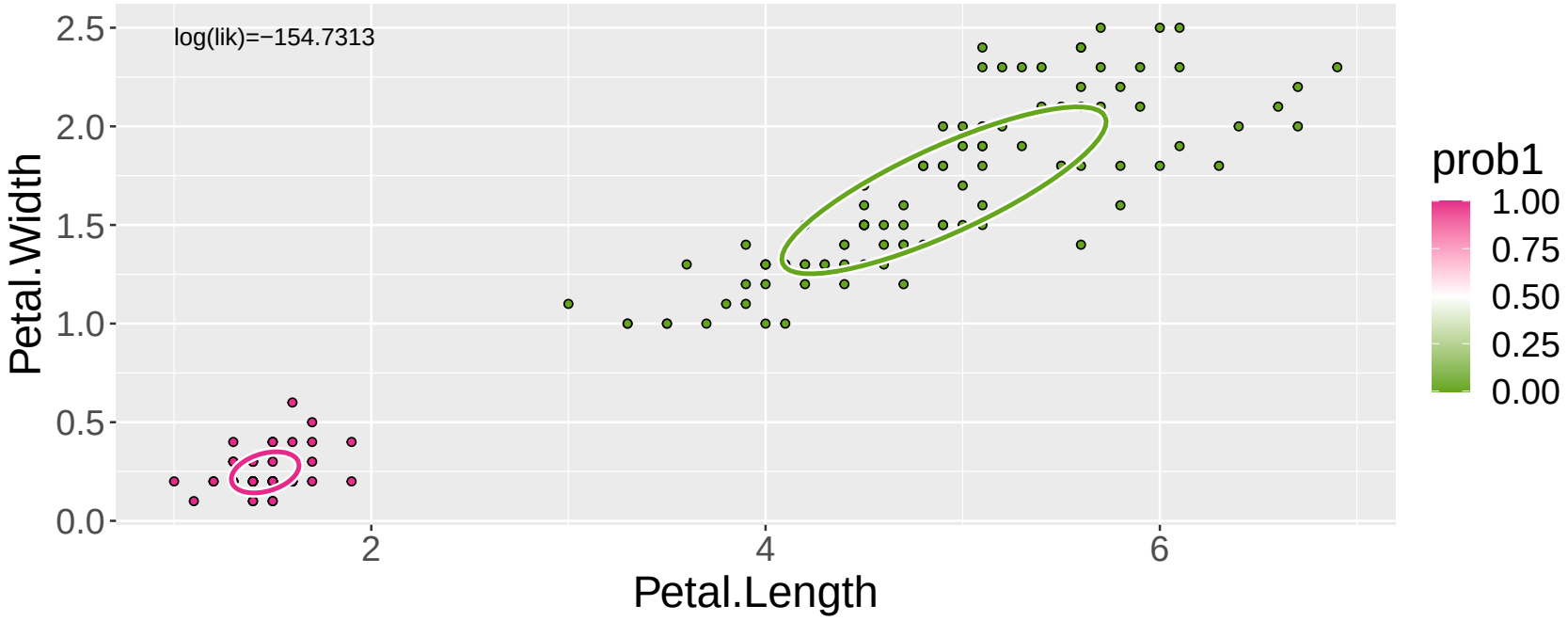
# Compute new cluster parameters



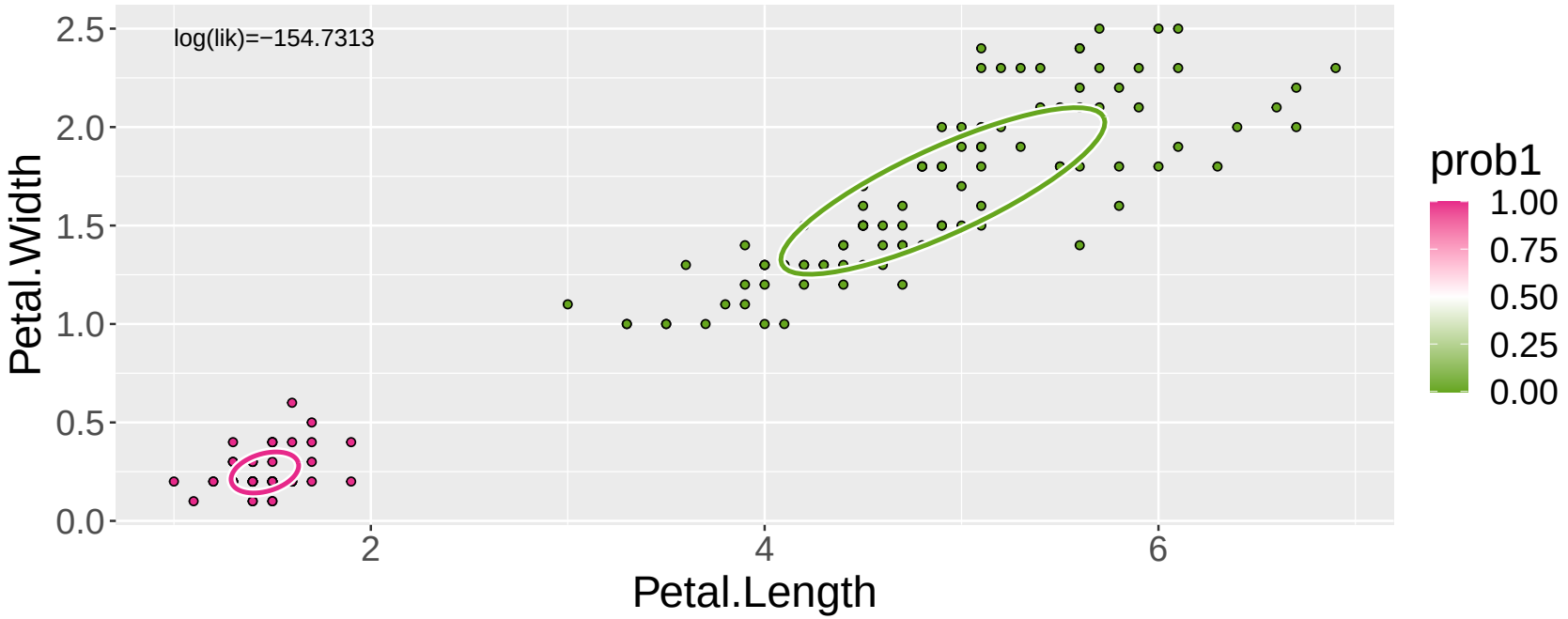
# Compute new cluster/data probabilities



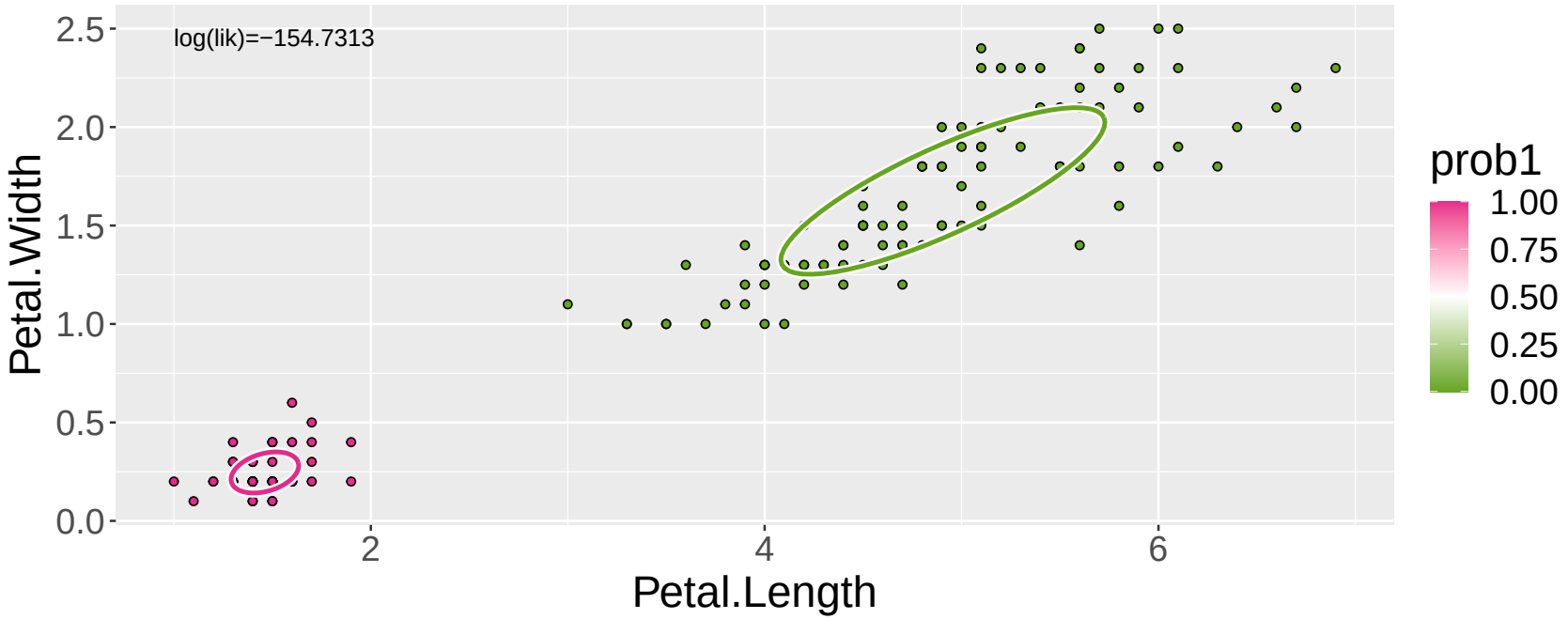
# Compute cluster parameters iteration 3



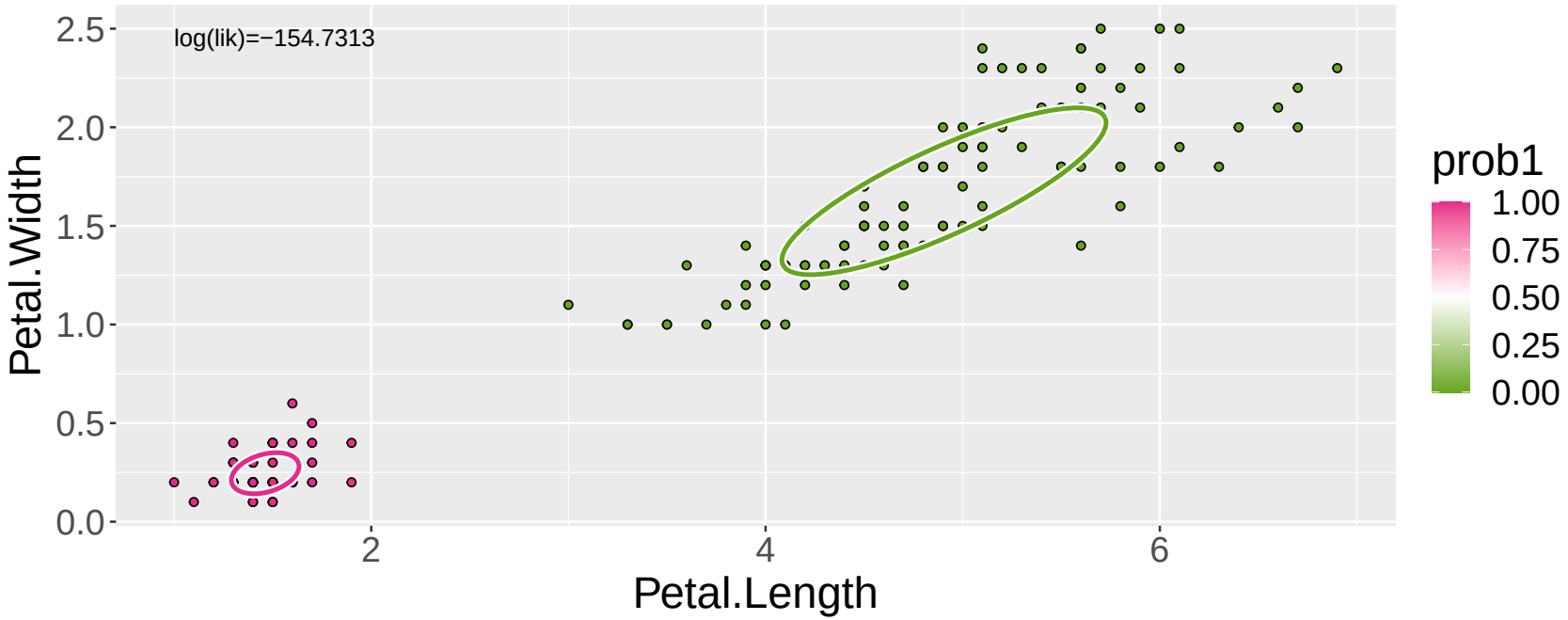
# Compute probabilities iteration 3



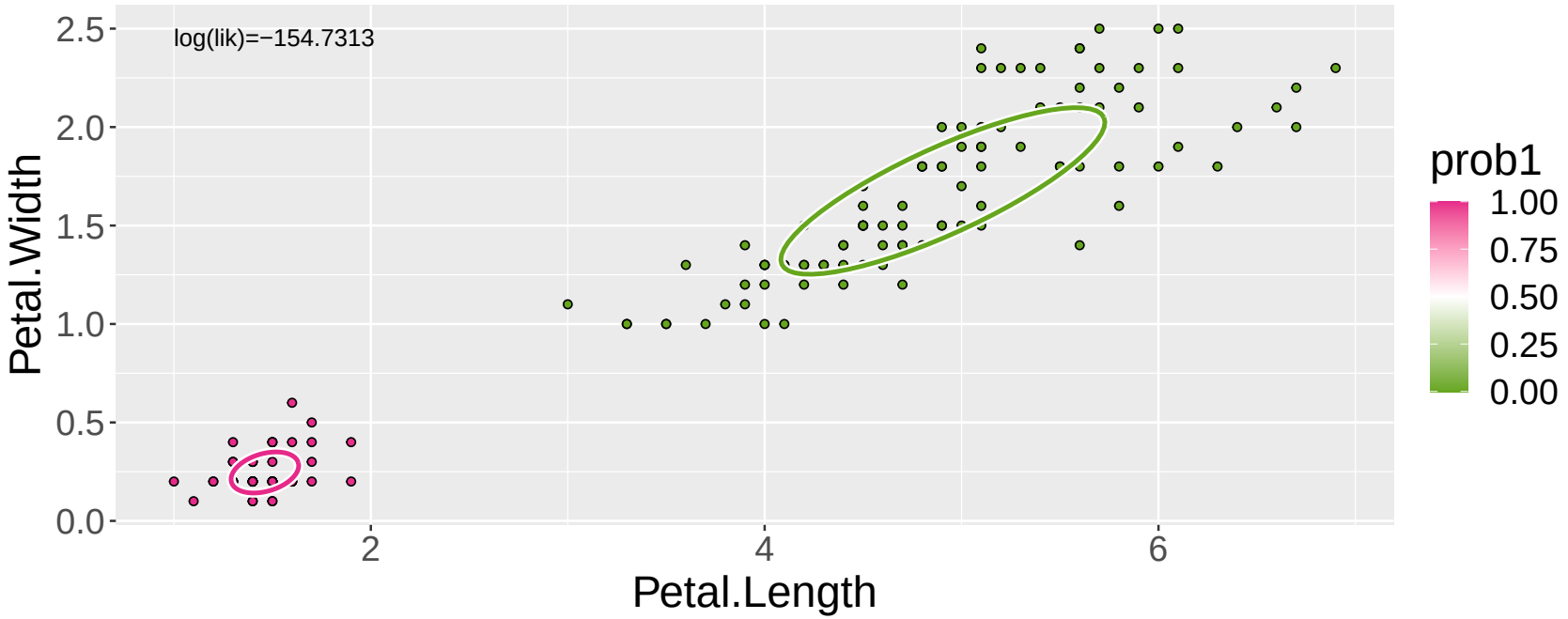
# Compute cluster parameters iteration 4



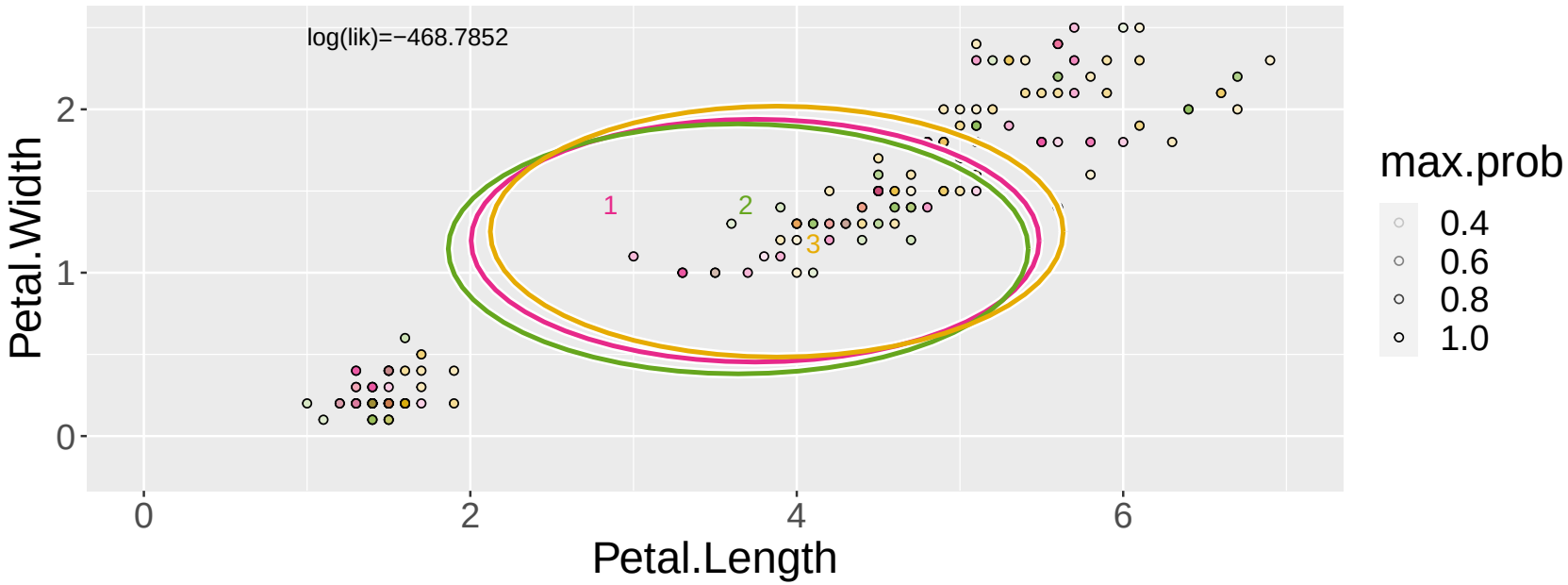
# Compute probabilities iteration 4



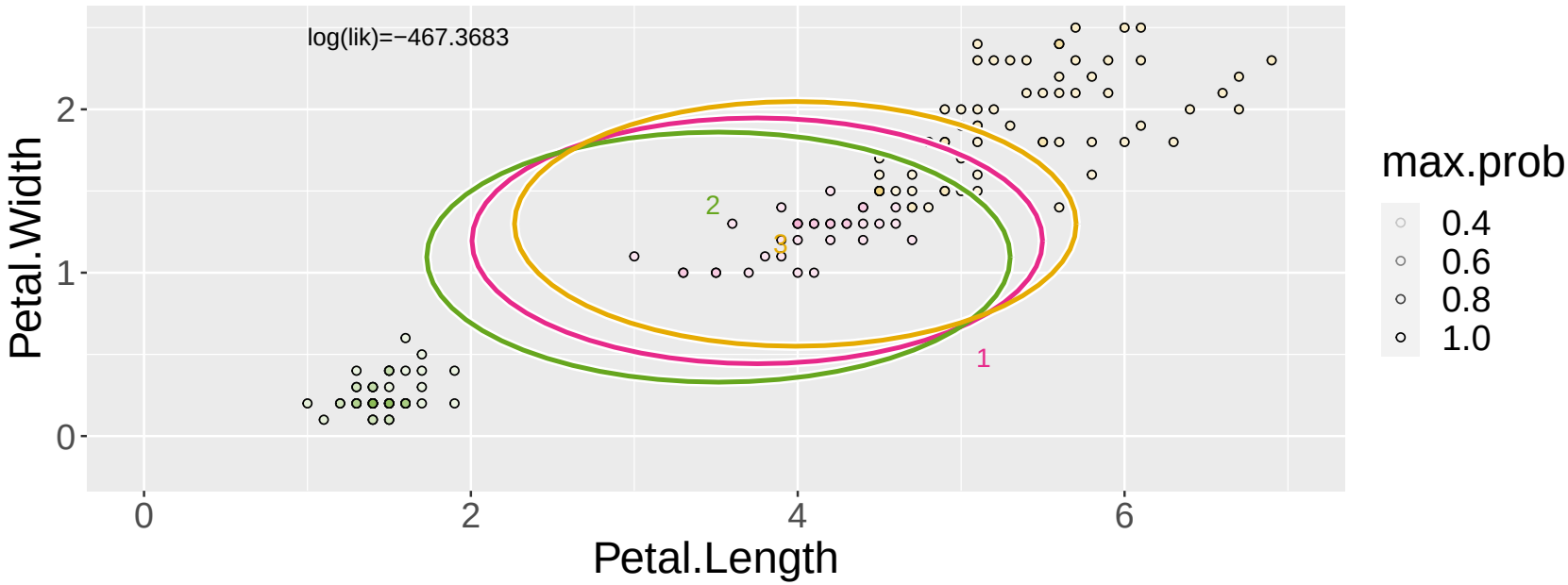
# Compute cluster parameters iteration 5 (no change = stop)



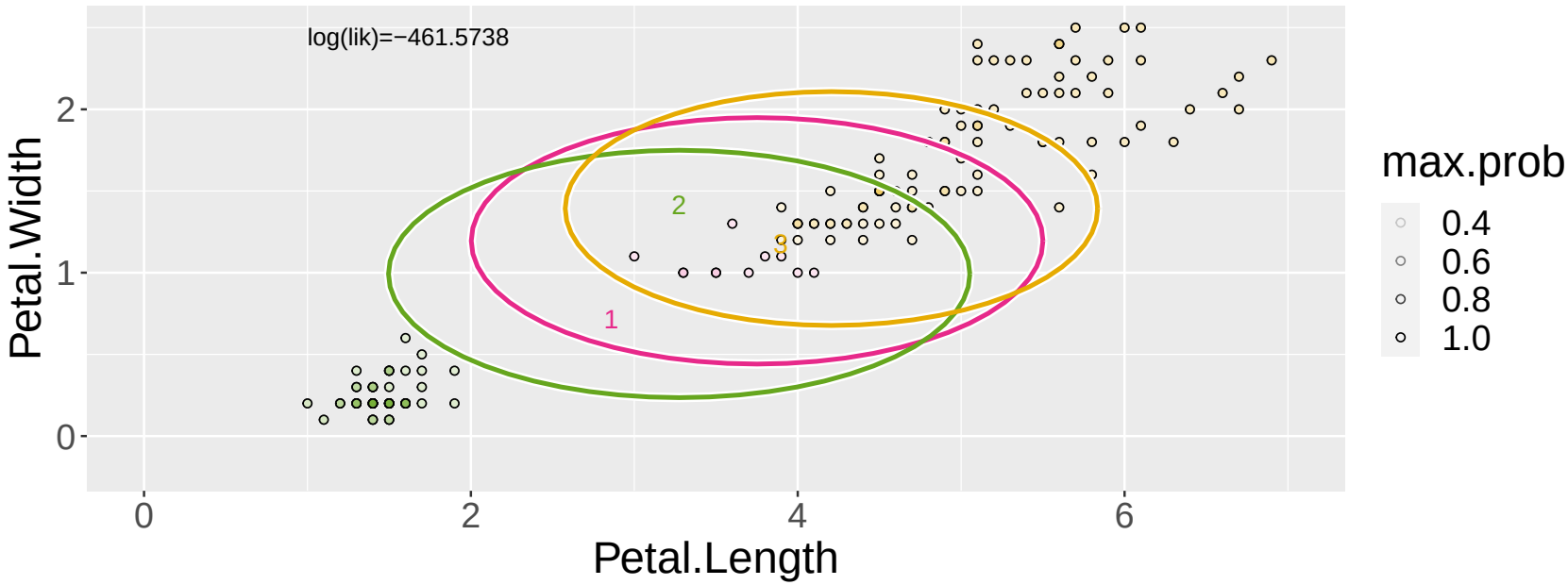
# Three clusters, diagonal constraint, random initialization



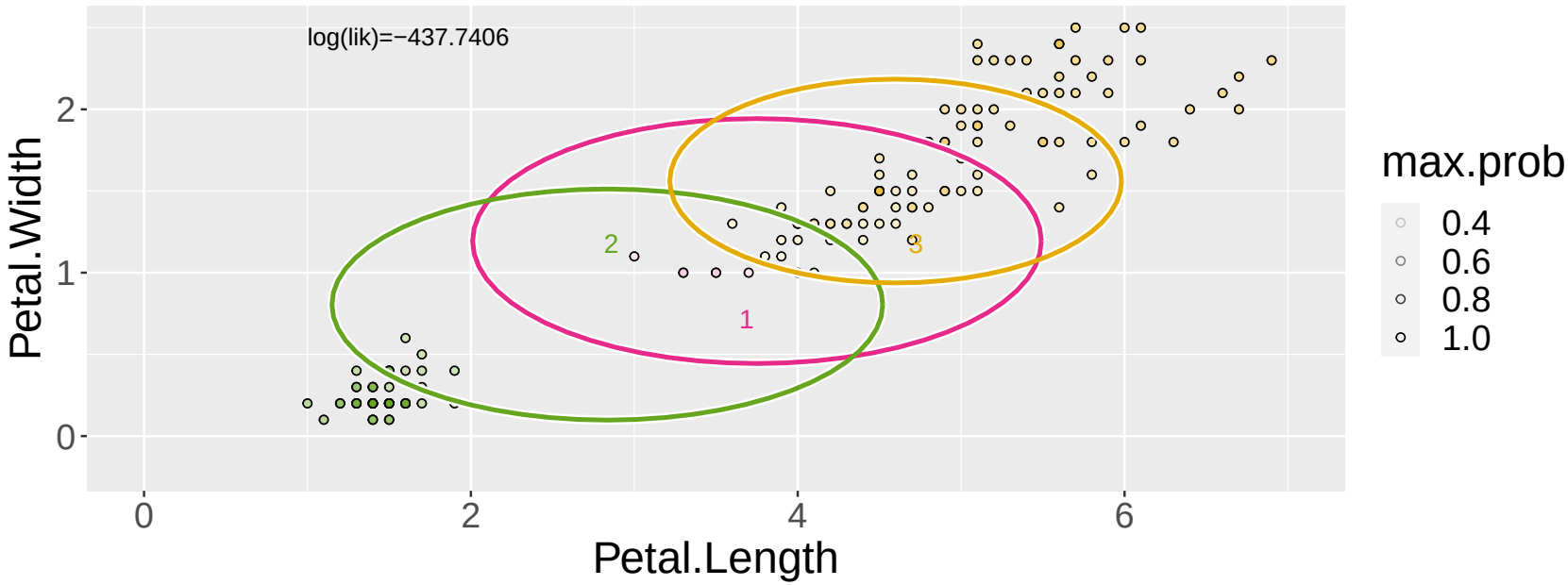
# iteration 2


log(lik)=−467.3683
Petal.Width
Petal.Length
0
1
2
0
2
4
6
2
3
1
max.prob
0.4
0.6
0.8
1.0

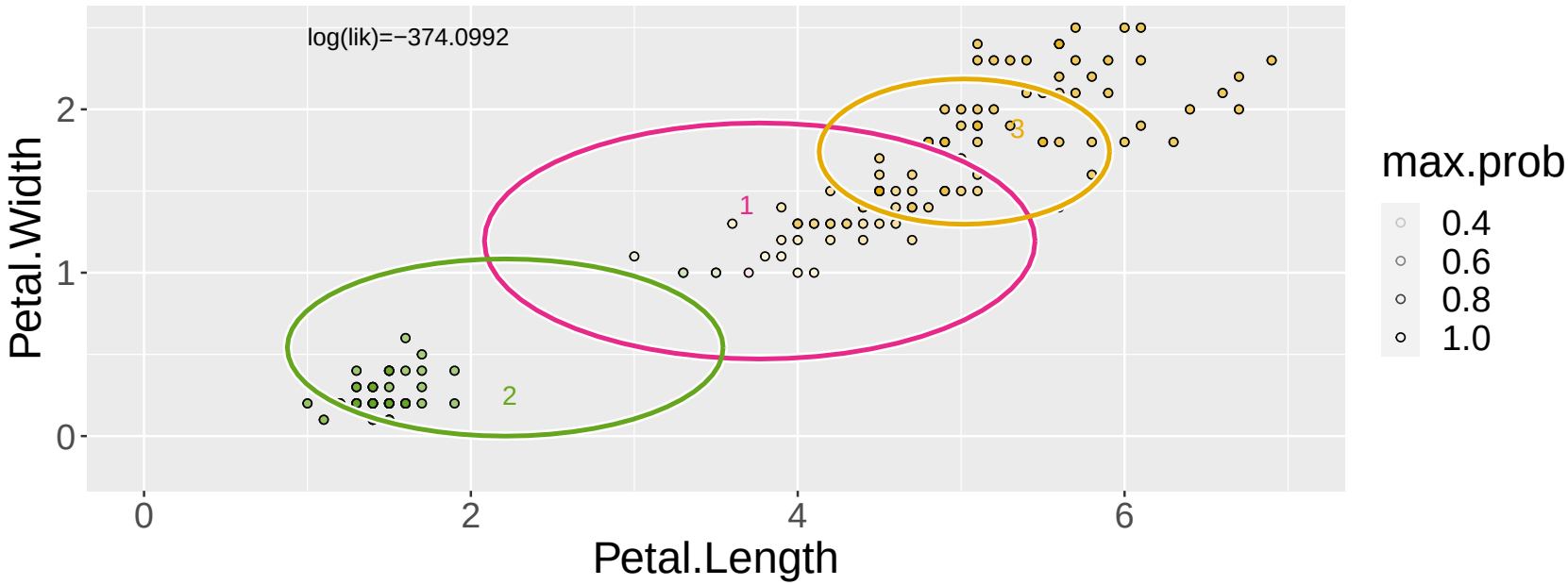
# iteration 3


log(lik)=−461.5738
Petal.Width
Petal.Length
0
1
2
0
2
4
6
1
2
3
max.prob
0.4
0.6
0.8
1.0

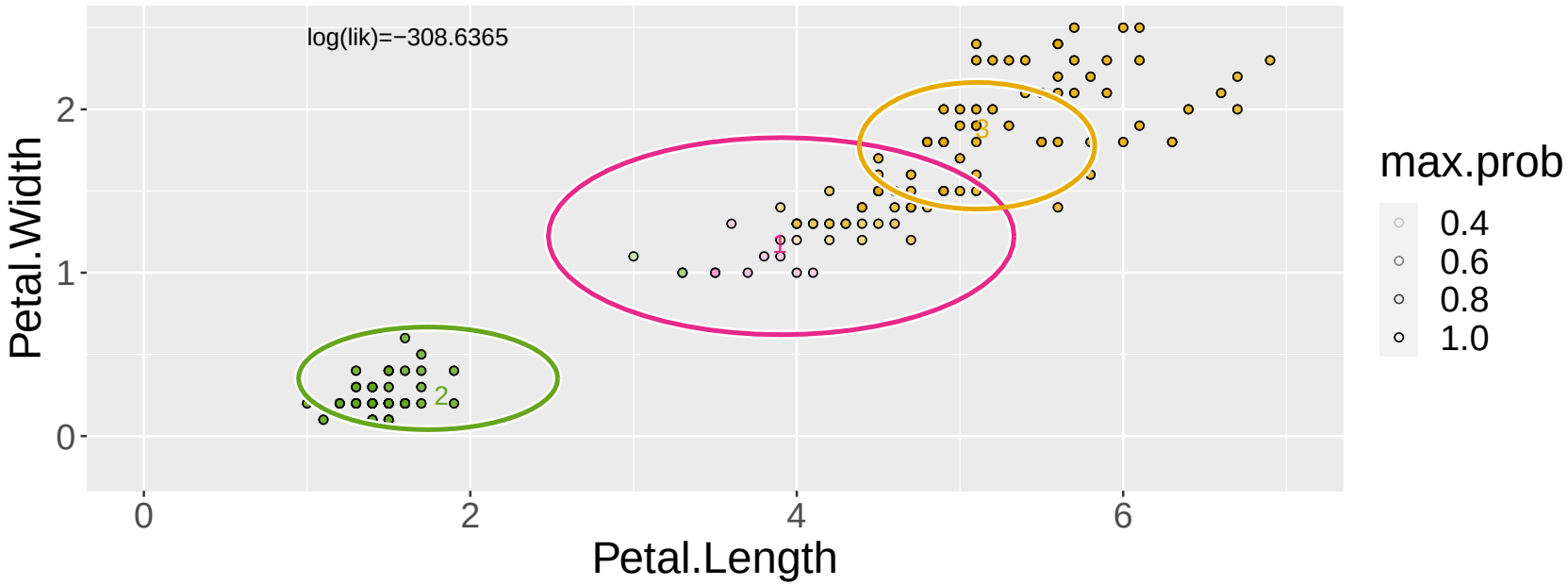
# iteration 4


log(lik)=−437.7406
Petal.Width
Petal.Length
0
1
2
0
2
4
6
1
2
3
max.prob
0.4
0.6
0.8
1.0

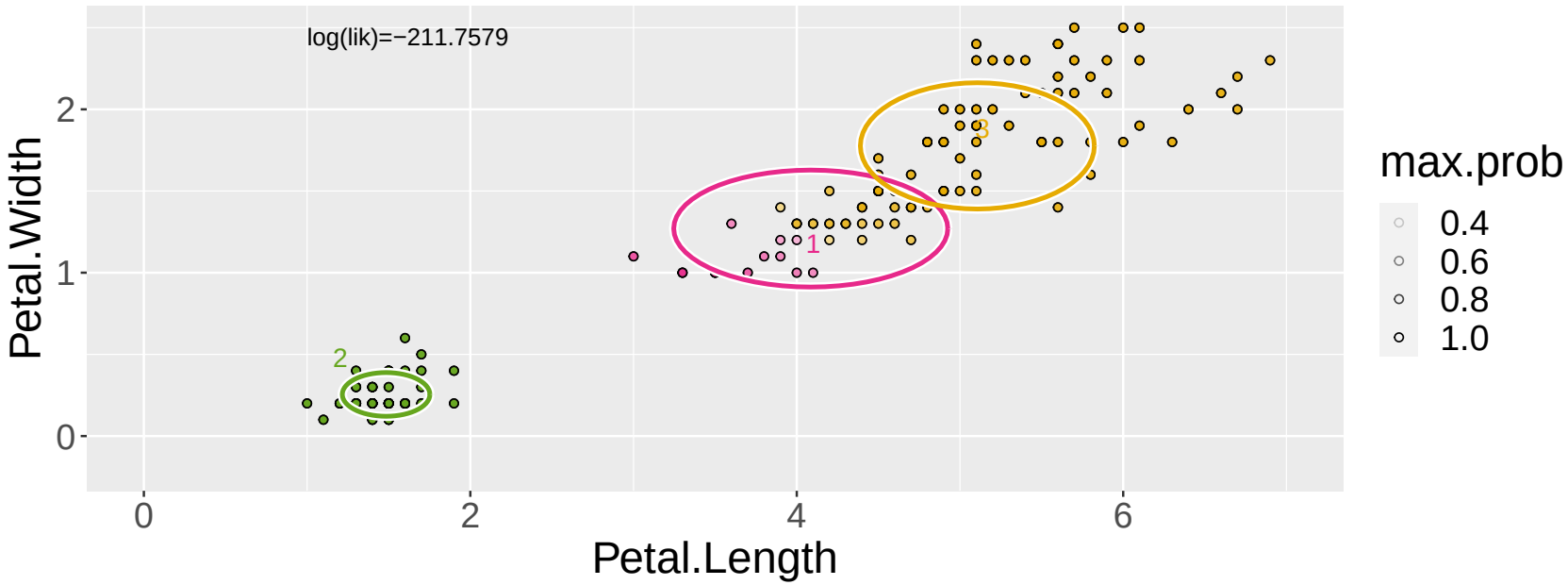
# iteration 5


log(lik)=−374.0992
Petal.Width
Petal.Length
0
1
2
0
2
4
6
1
2
3
max.prob
0.4
0.6
0.8
1.0

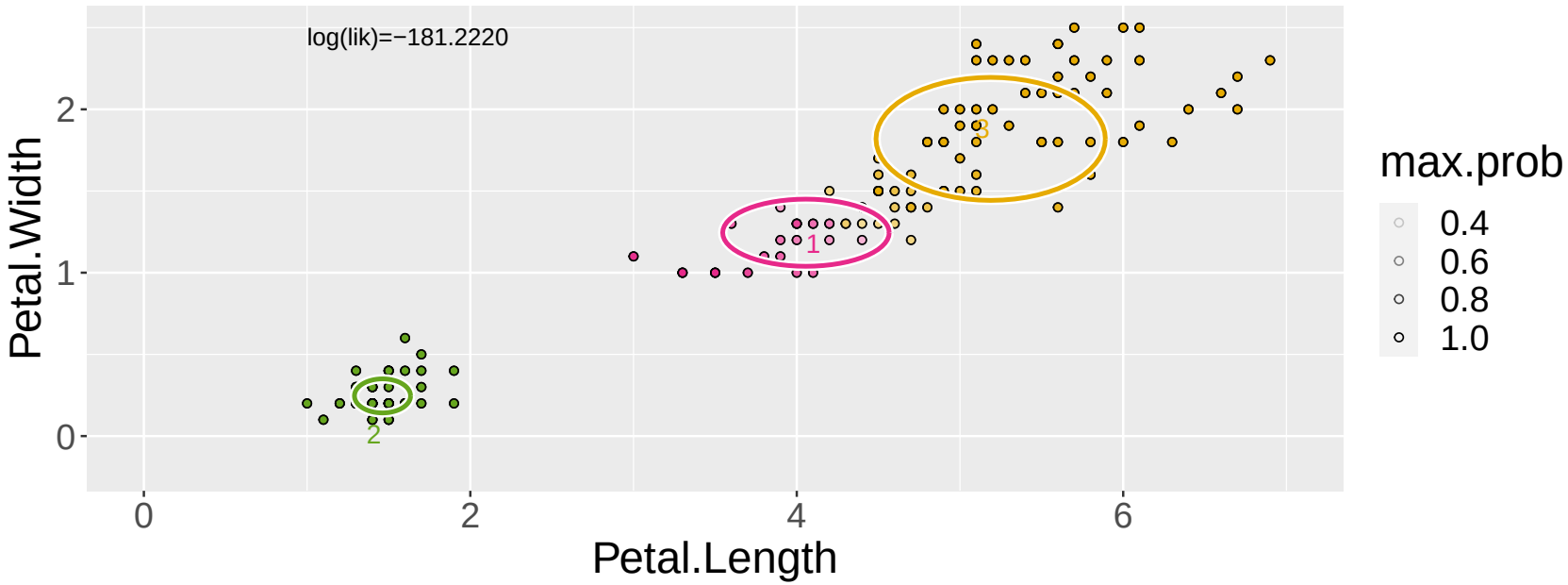
# iteration 6


log(lik)=−308.6365
Petal.Width
Petal.Length
0
1
2
0
2
4
6
1
2
3
max.prob
0.4
0.6
0.8
1.0

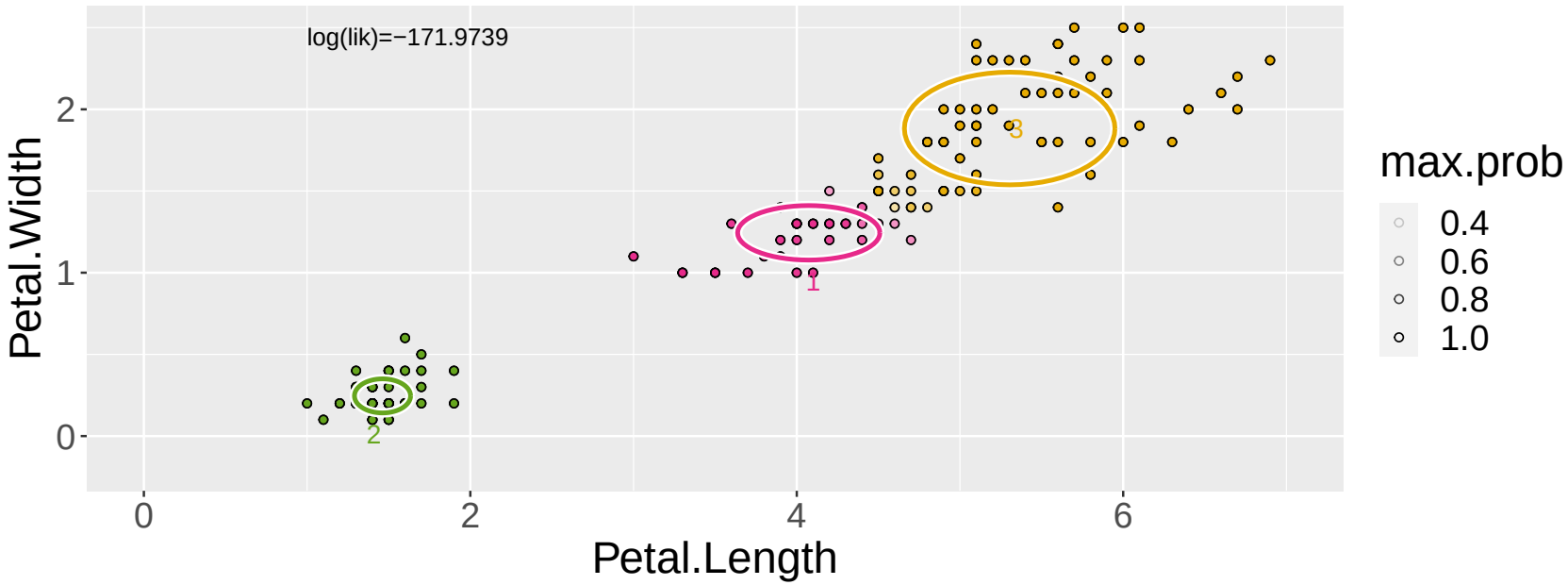
# iteration 7


log(lik)=−211.7579
Petal.Width
Petal.Length
0
1
2
0
2
4
6
1
2
3
max.prob
0.4
0.6
0.8
1.0

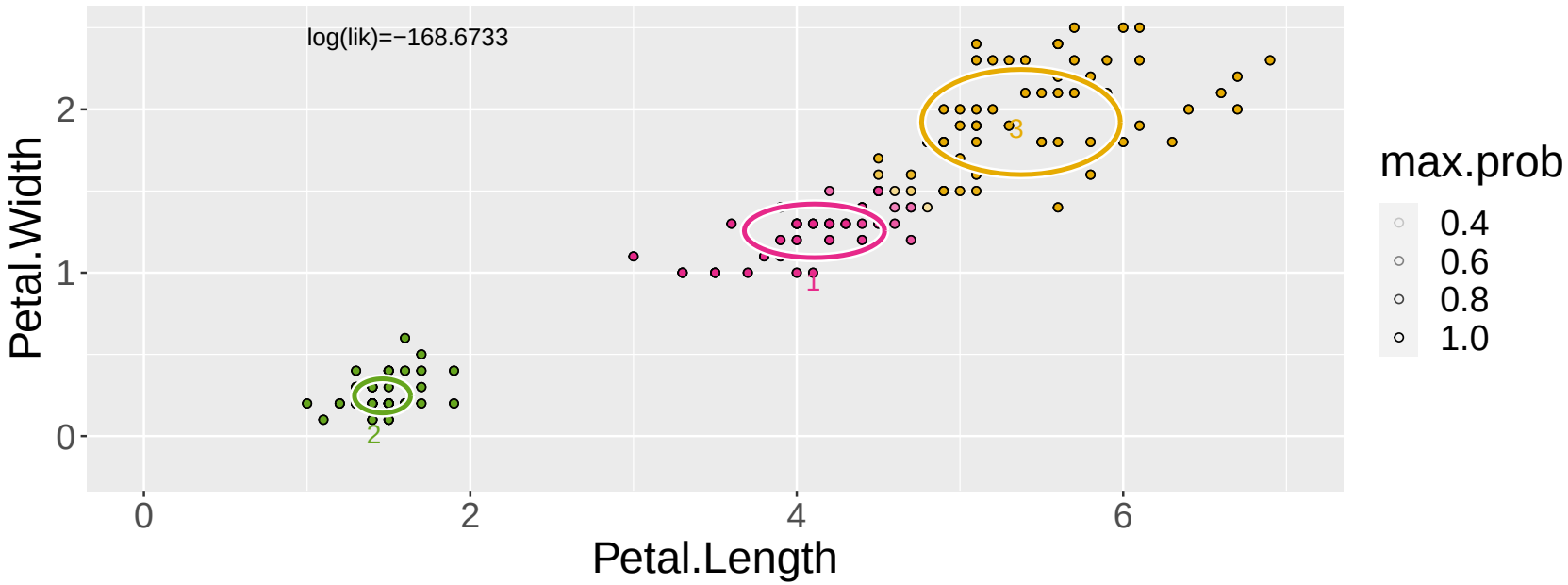
# iteration 8


log(lik)=−181.2220
Petal.Width
Petal.Length
0
1
2
3
0
2
4
6
max.prob
0.4
0.6
0.8
1.0

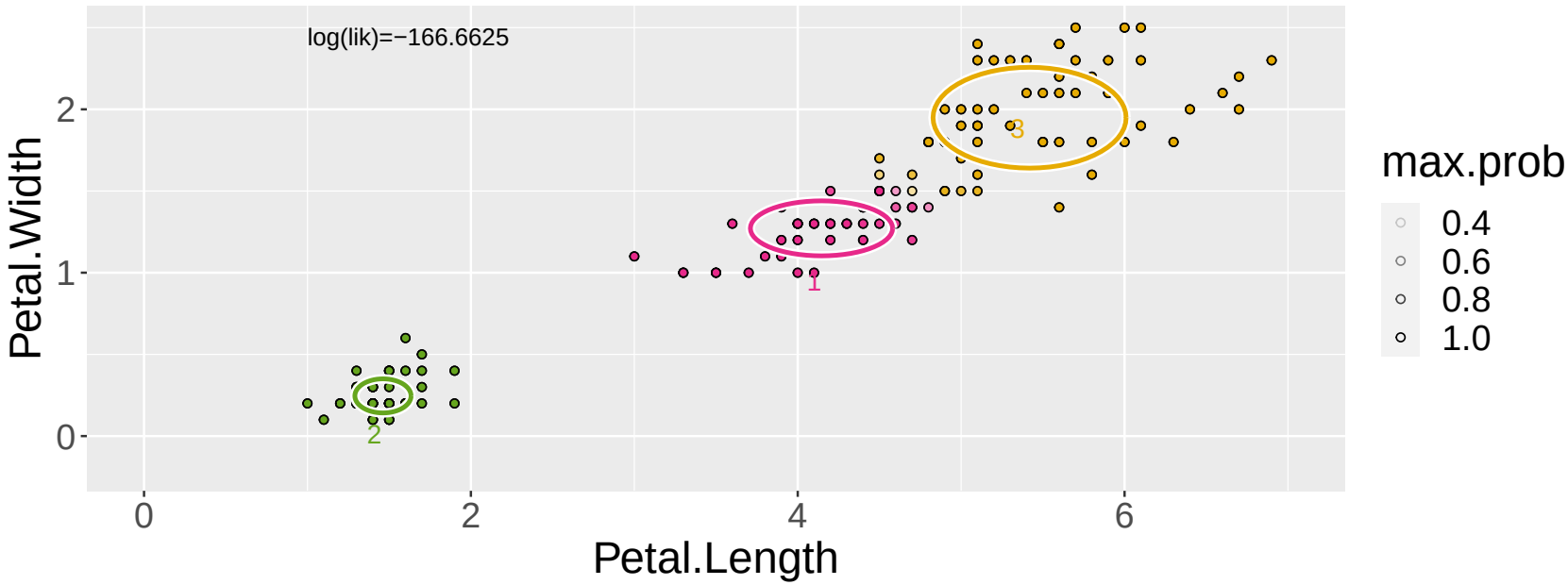
# iteration 9


log(lik)=−171.9739
Petal.Width
Petal.Length
0
1
2
3
0
2
4
6
max.prob
0.4
0.6
0.8
1.0

# iteration 10

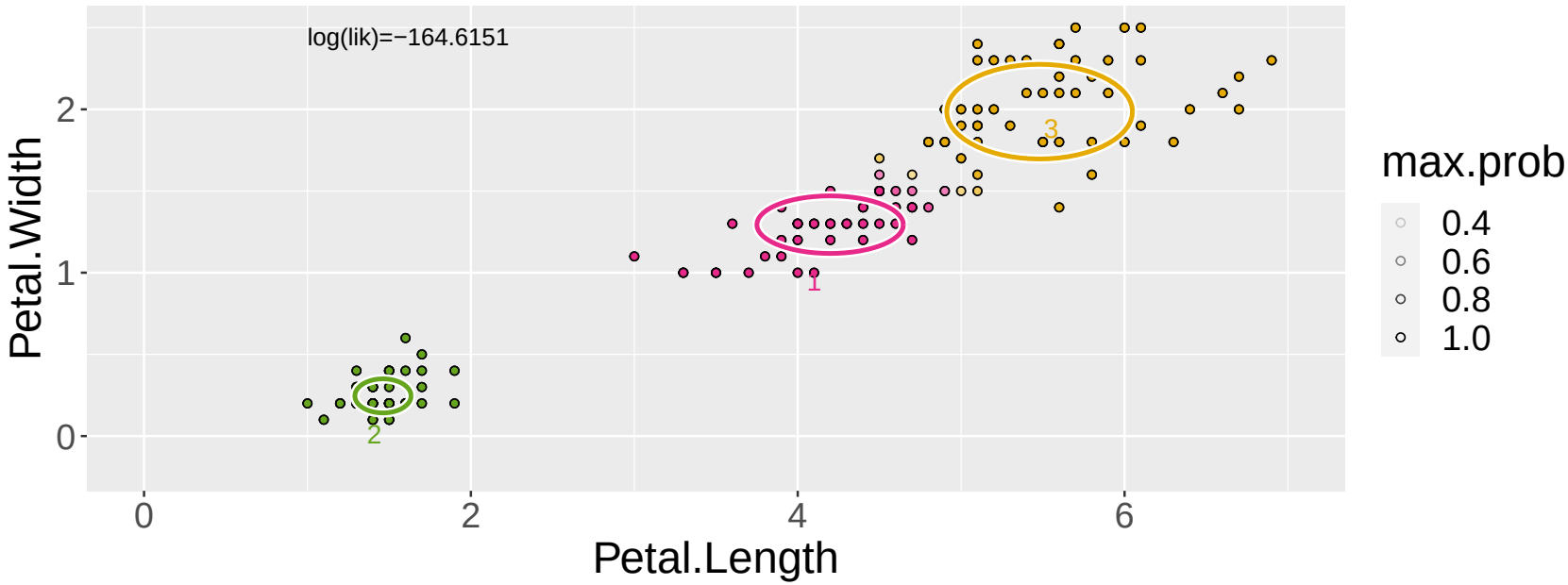


# iteration 11



# iteration 12

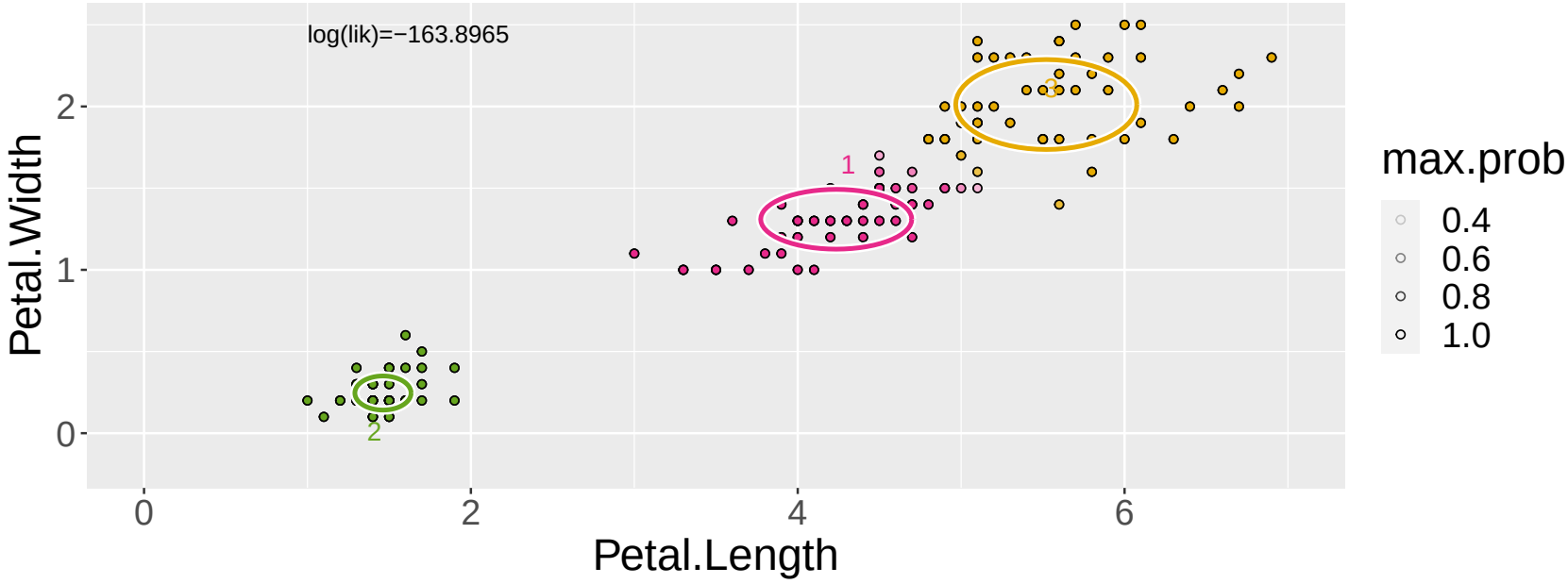
# iteration 13



# iteration 14

# iteration 15

# iteration 16



# iteration 17

# iteration 18

# iteration 19

# iteration 20

# Possible Exam Questions

- How many real number parameters in an unconstrained gaussian mixture model for data with $p = 5$ features?
- What hyper-parameter is common to K-means and Gaussian mixtures? (A hyper-parameter is a model choice that must be fixed before running the learning/EM algorithm)
- What hyper-parameter is unique to Gaussian mixtures?
- What cluster parameter is common to K-means and Gaussian mixtures?
- What cluster parameters are present in Gaussian mixtures but not in K-means?

# Possible exam questions 2

- We say K-means uses hard assignment and Gaussian mixtures uses soft assignment – what values are used in the probability/assignment matrix in each case?
- The K-means and Gaussian mixtures have similar learning algorithms. What are the main steps in common and what is the difference?
- In K-means we compute the squared error, and in Gaussian mixtures we compute the negative log likelihood – these values INCREASE or DECREASE as the number of clusters increase? These values INCREASE or DECREASE as the number of iterations of the learning algorithm increases?