Machine Learning I

MICRO-455

Classification with GMM and KNN

The Teaching Team

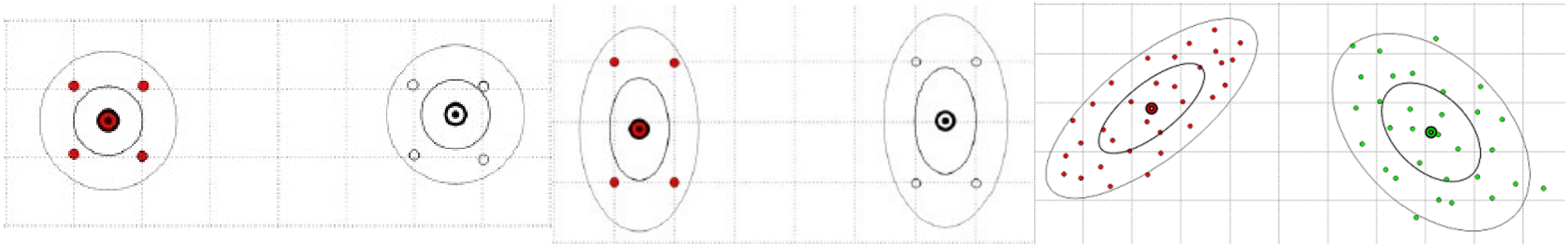
EPFL

Fall 2025

LASA

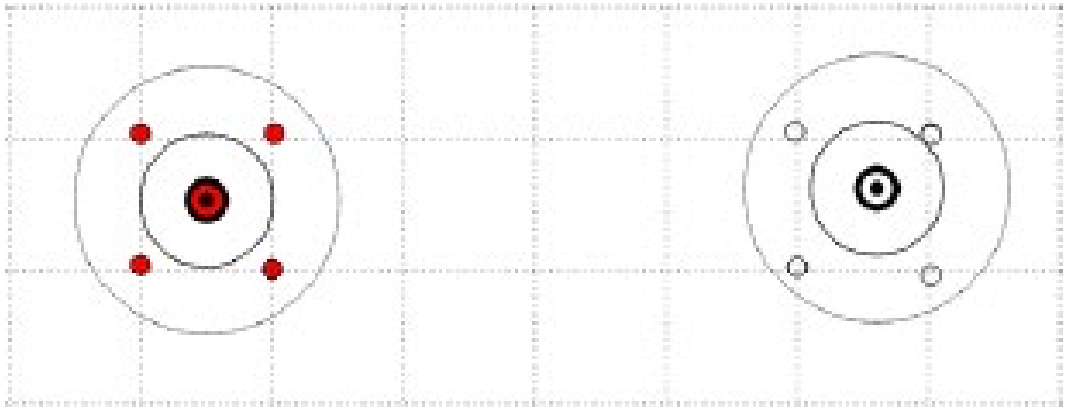
Q1.A

- Drawing the classification boundary.
  - Two classes, each fitted with a single Gauss function.
  - Two classes have the *same* number of datapoints.
  - The Gauss functions are *not* normalized.



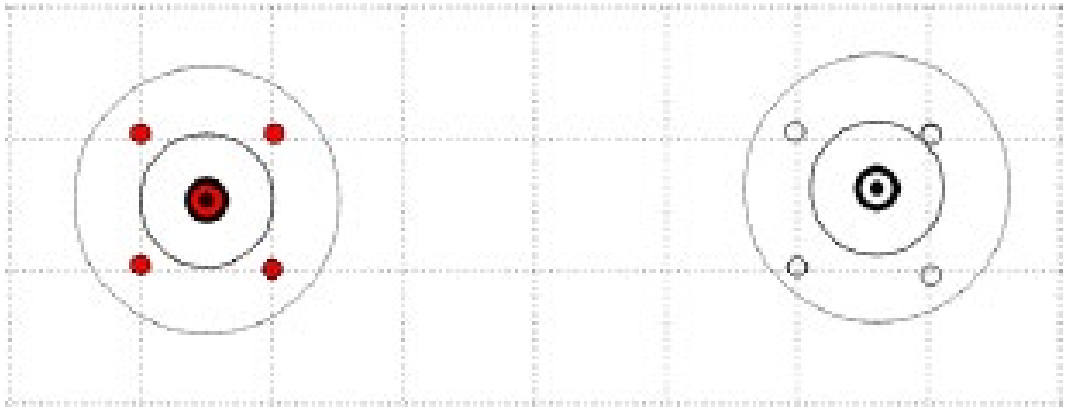
Q1.A > a

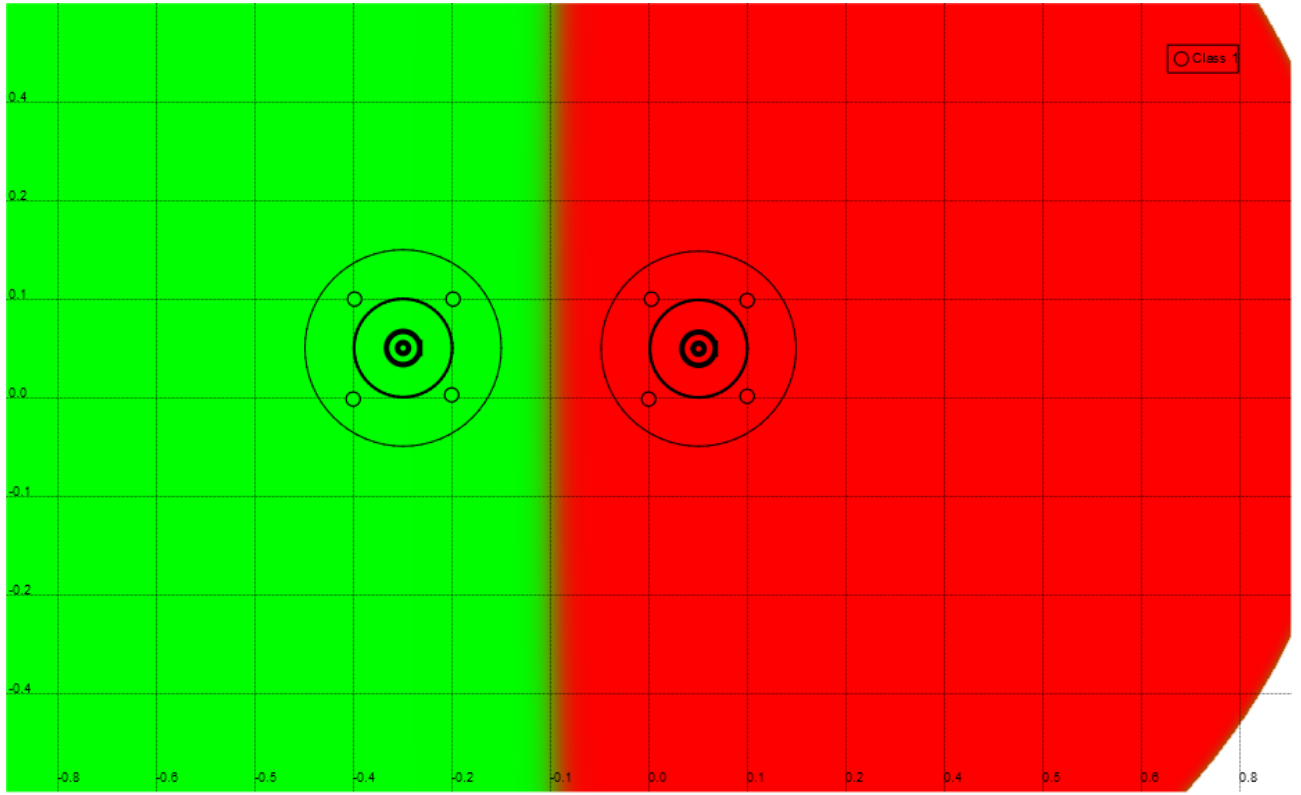
- Identical spherical covariance matrices.



Q1.A > a

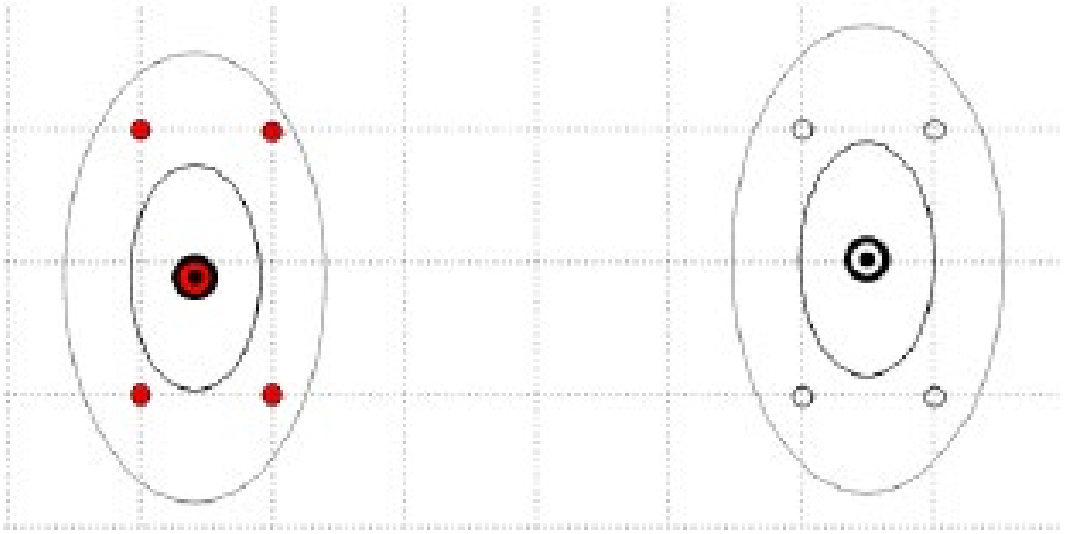
- Identical spherical covariance matrices.
- Linear boundary is equidistant from the two centroids.





Q1.A > b

- Identical diagonal covariance matrices.



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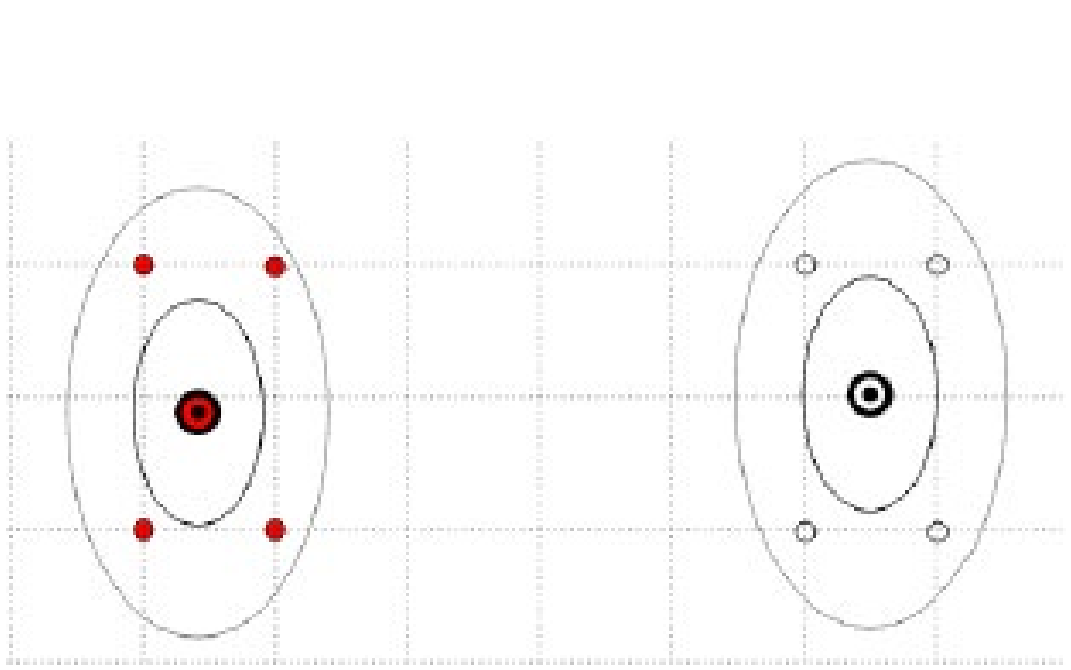
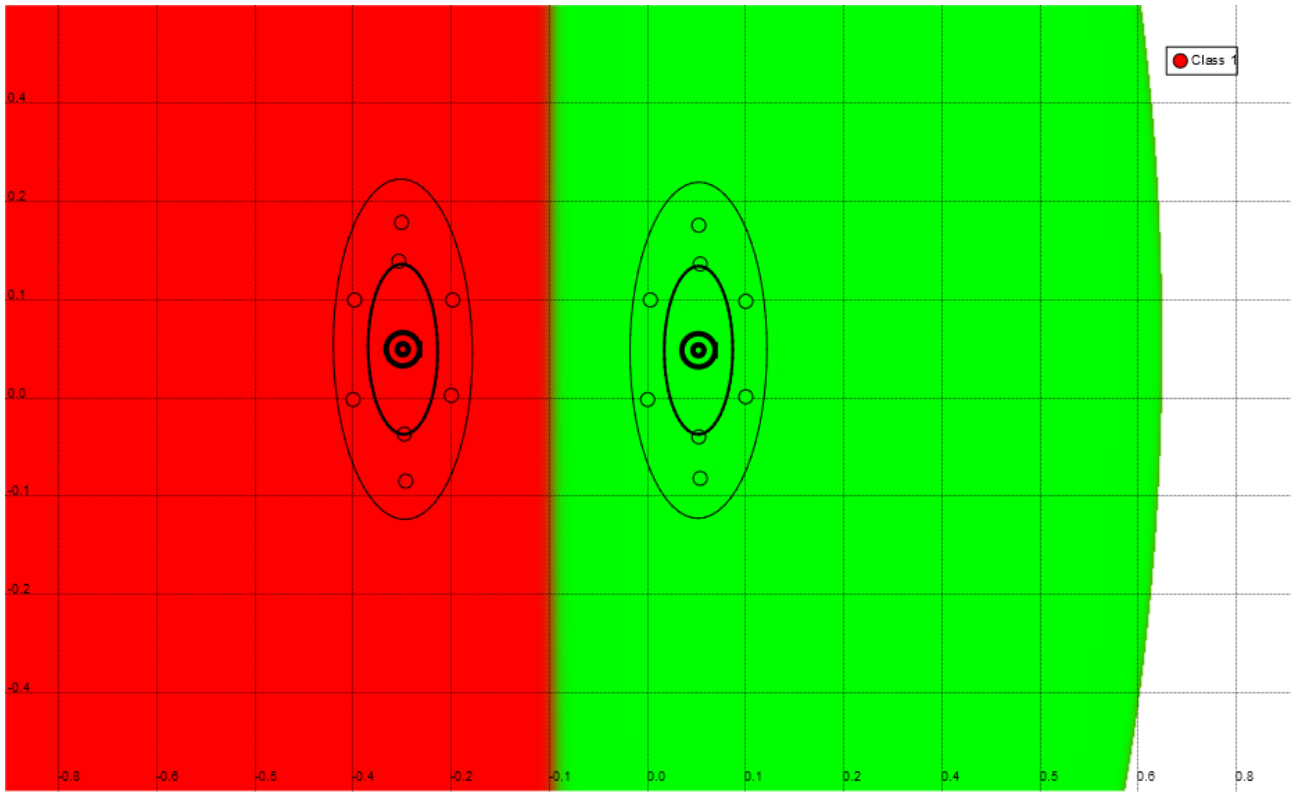
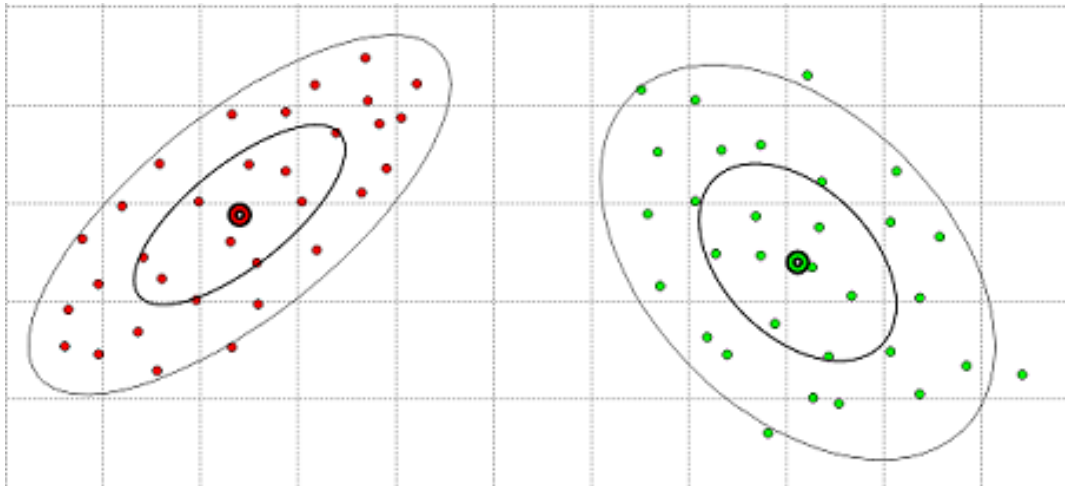




Q1.A > c

- Full covariance matrices.



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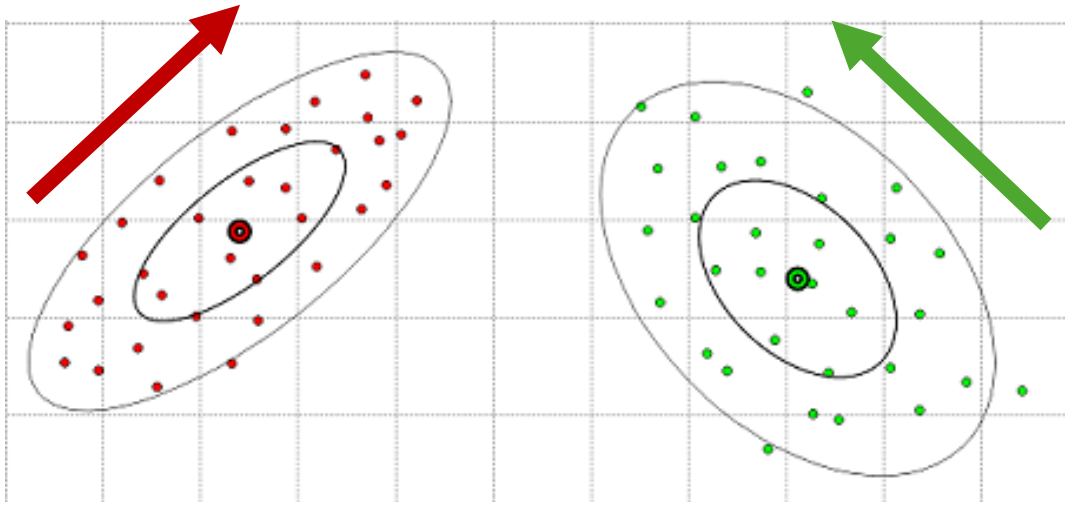
- Full covariance matrices.
- Notice the direction of spread (variance) for each Gaussian.



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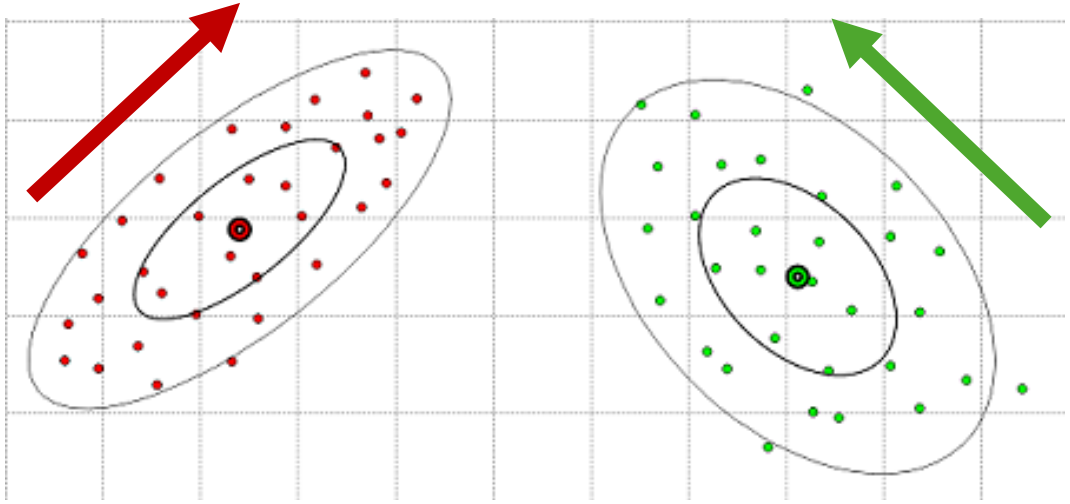

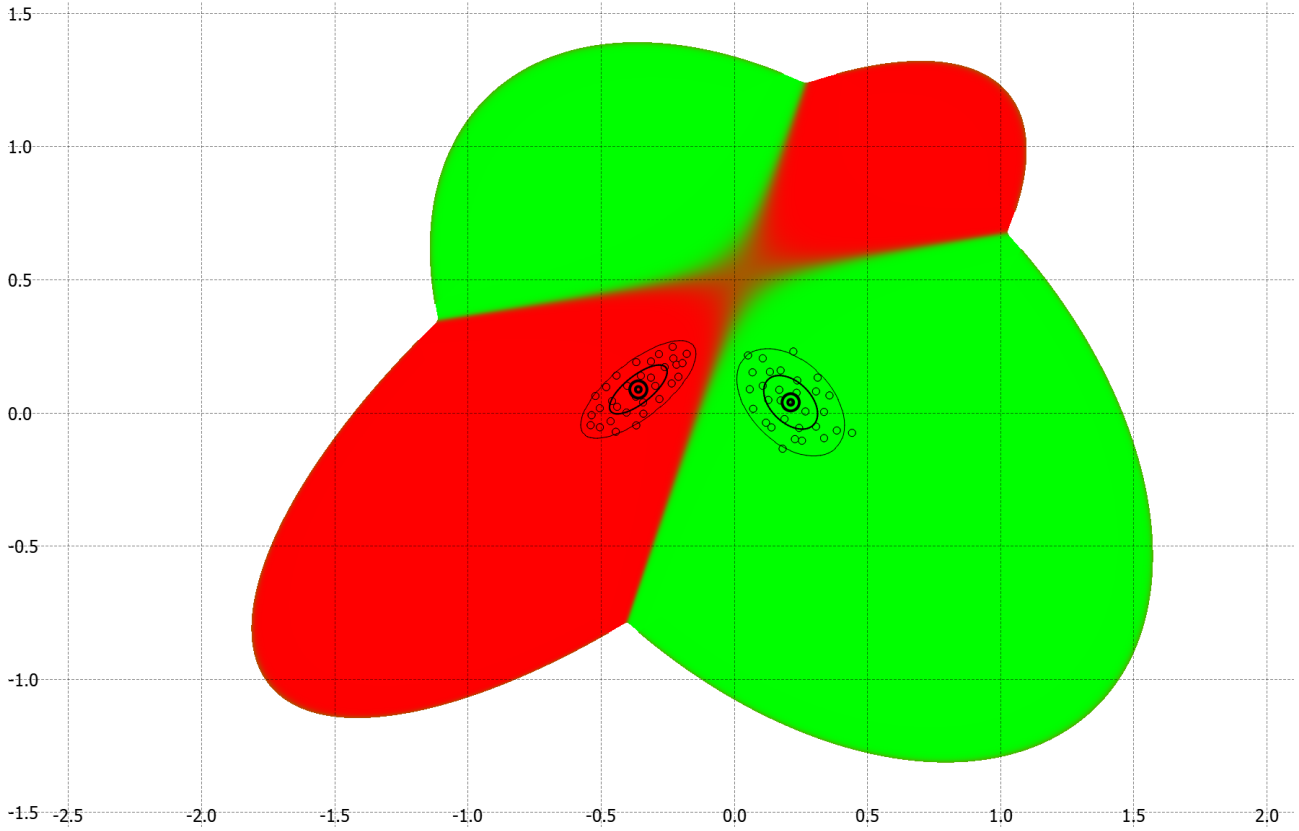

Q1.B

- Studying the effect of the number of datapoints per class on the classification boundary.
  - Two classes, each fitted with a single Gauss function.
  - Two classes have identical covariance matrices.

$$-\frac{1}{2}(x-\mu^1)^\top\Sigma^{-1}(x-\mu^1)+\ln p(y=1) = -\frac{1}{2}(x-\mu^2)^\top\Sigma^{-1}(x-\mu^2)+\ln p(y=2)$$

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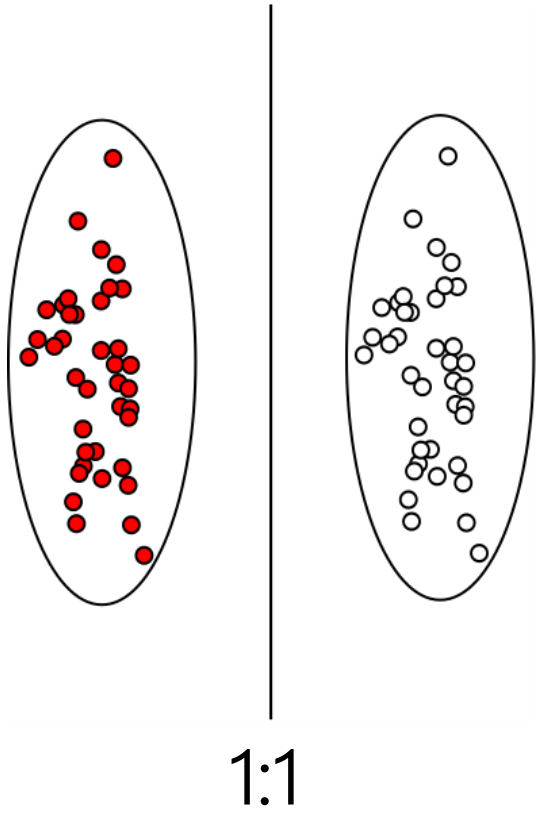

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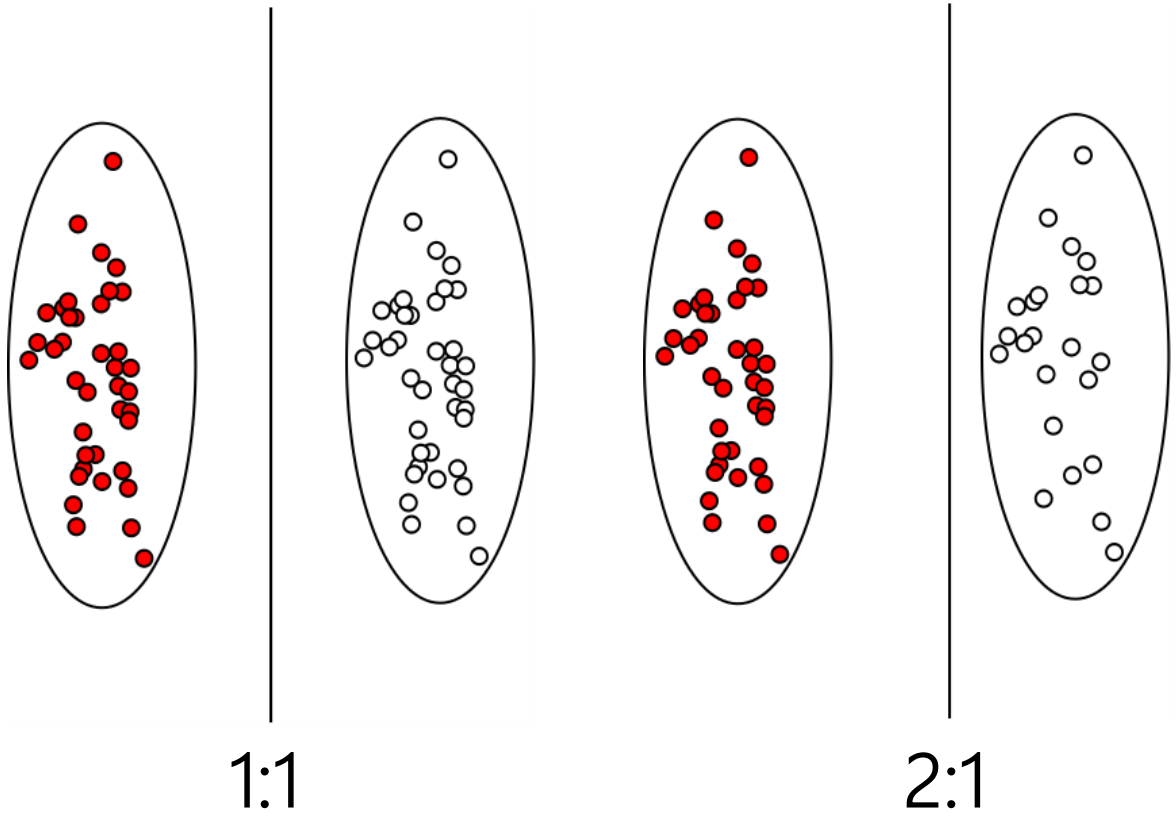

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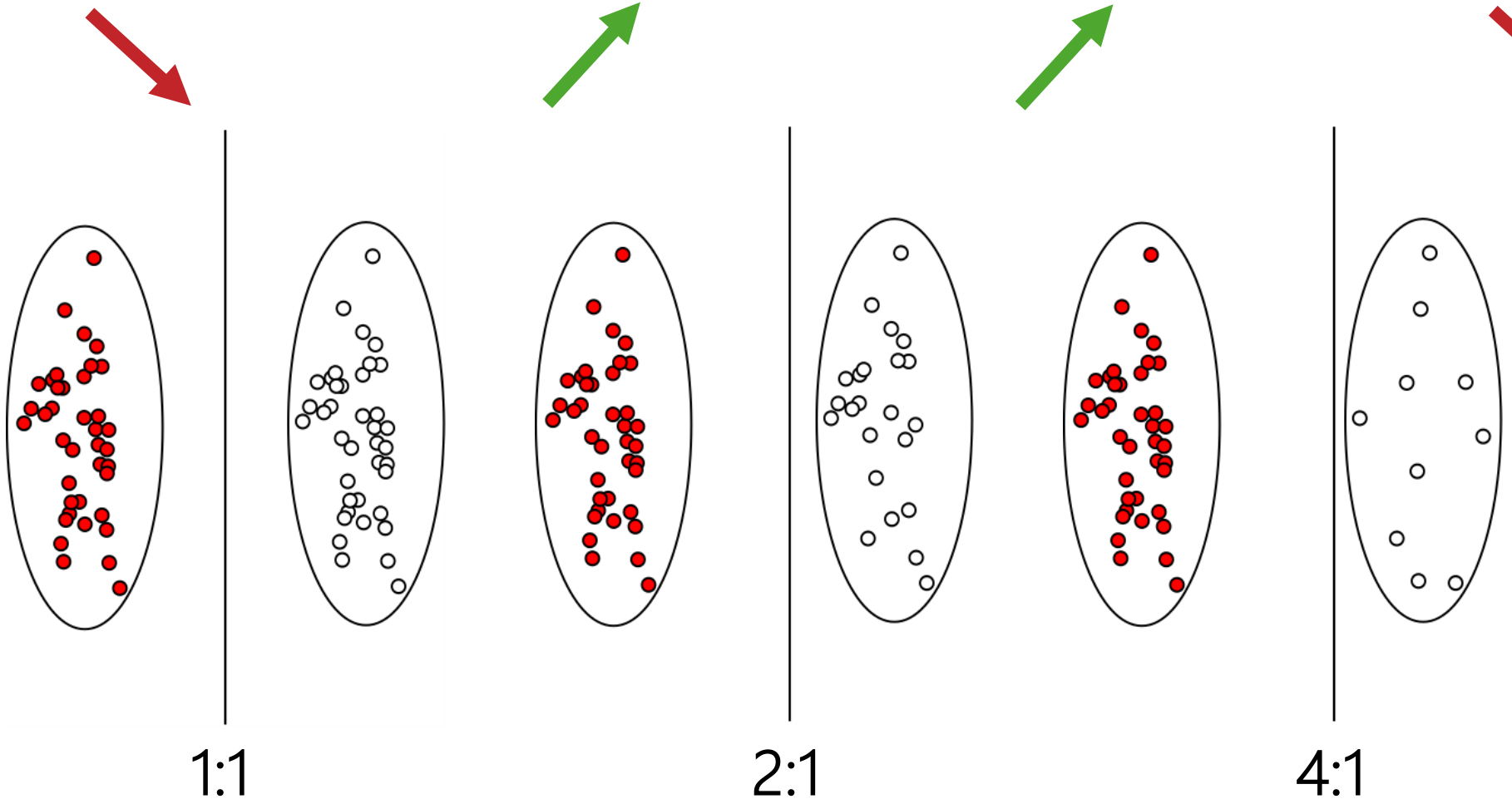
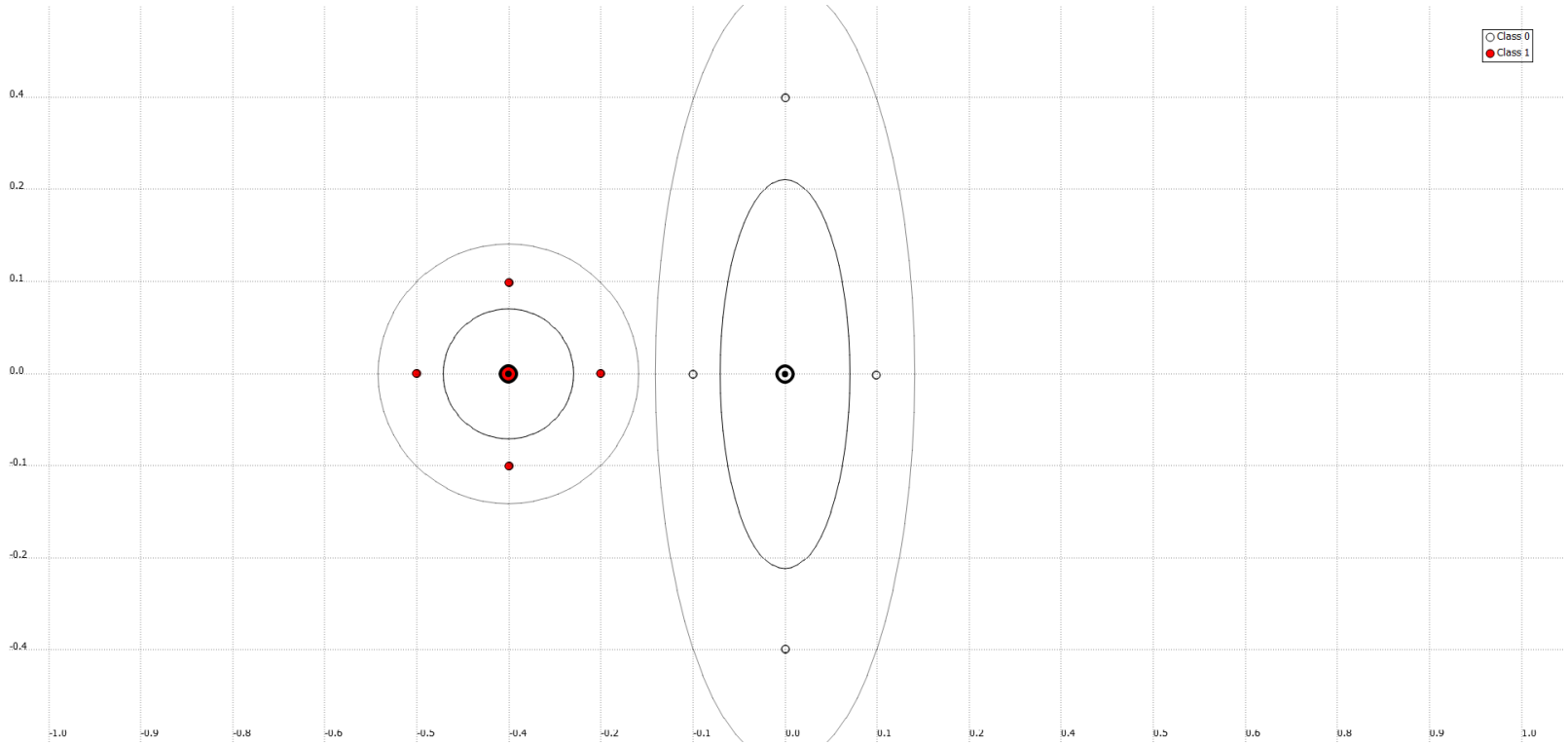


Q1.C

- Drawing the classification boundary when the Gauss functions are *normalized* and the covariance matrices are different.
  - Both Gaussian distributions have the same variance along the X-axis.



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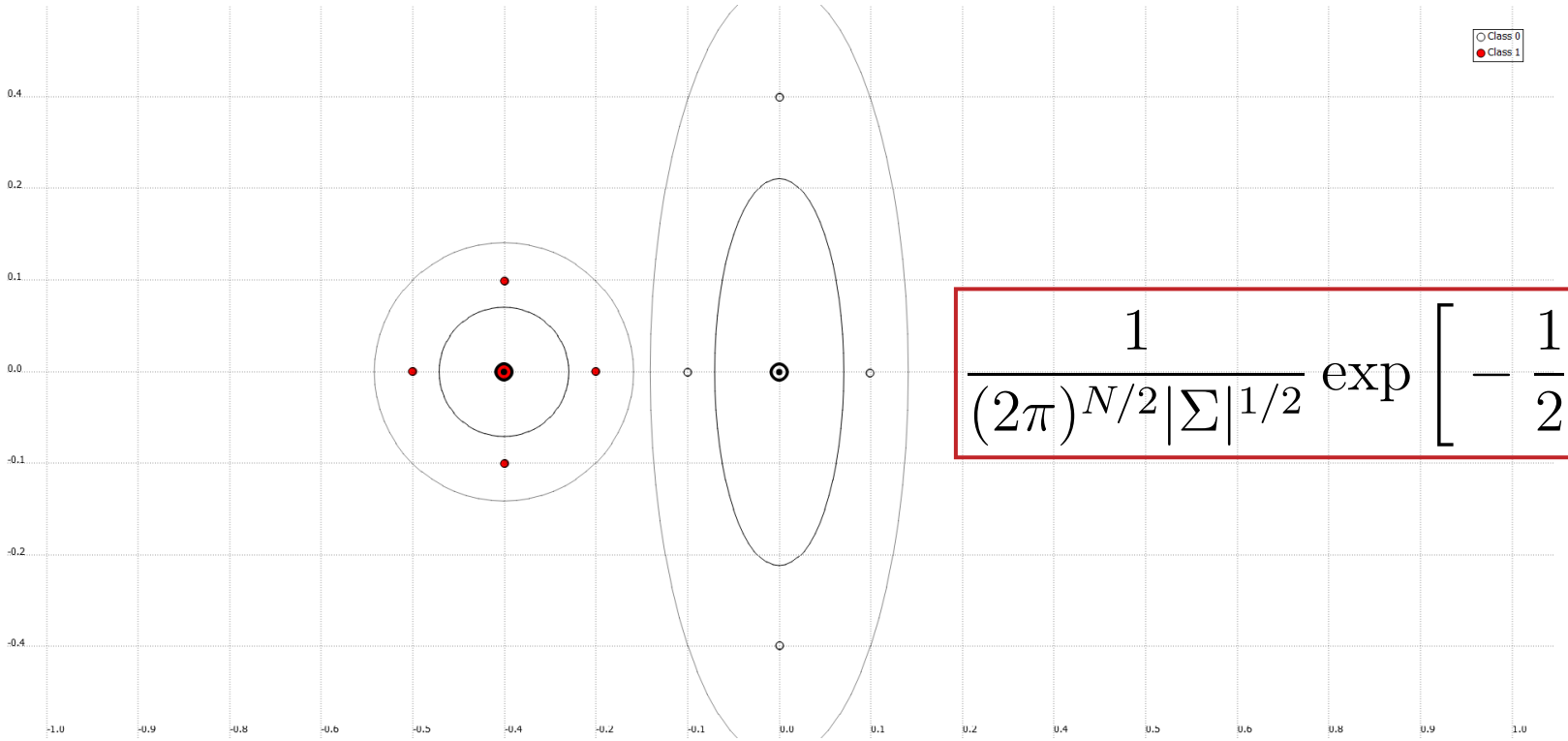

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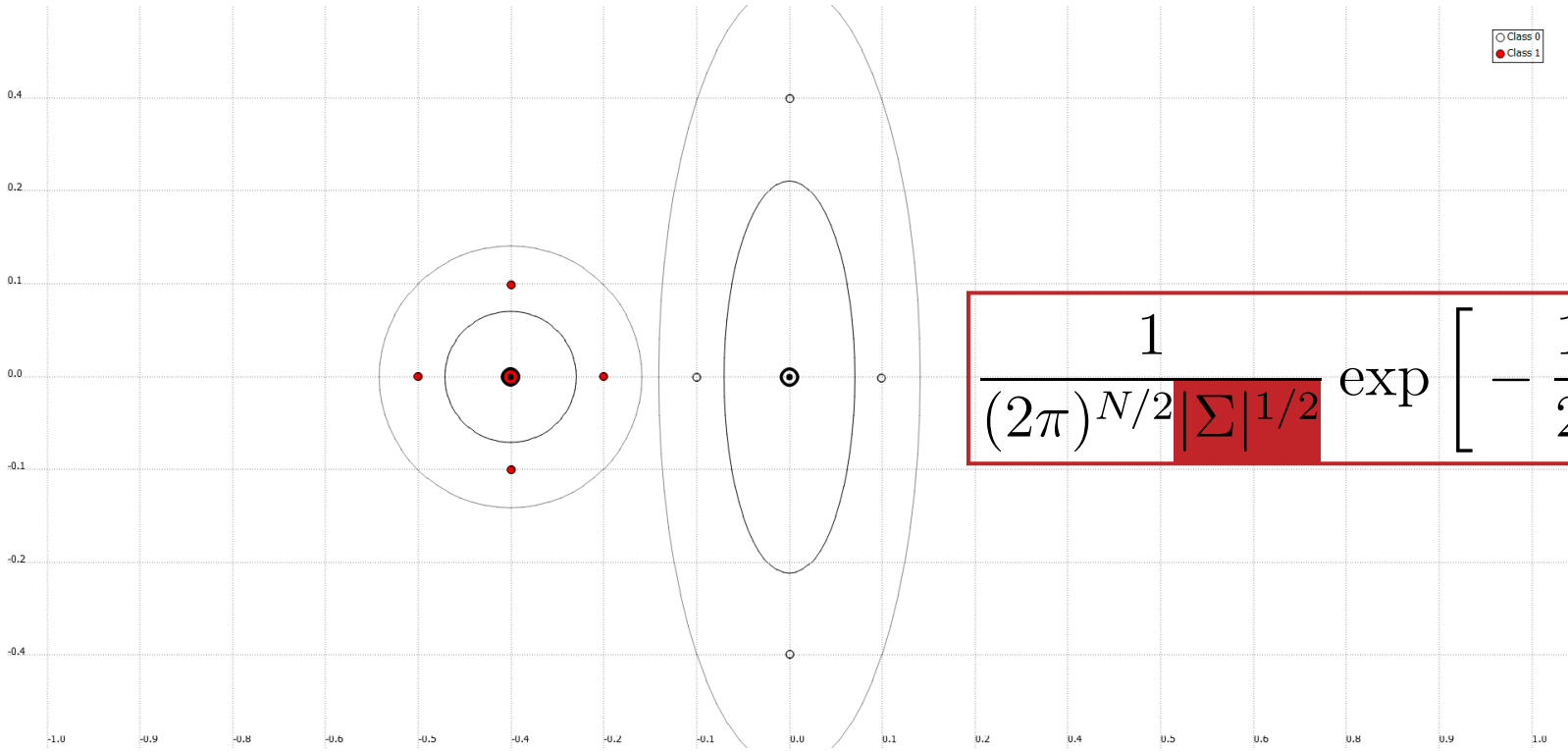

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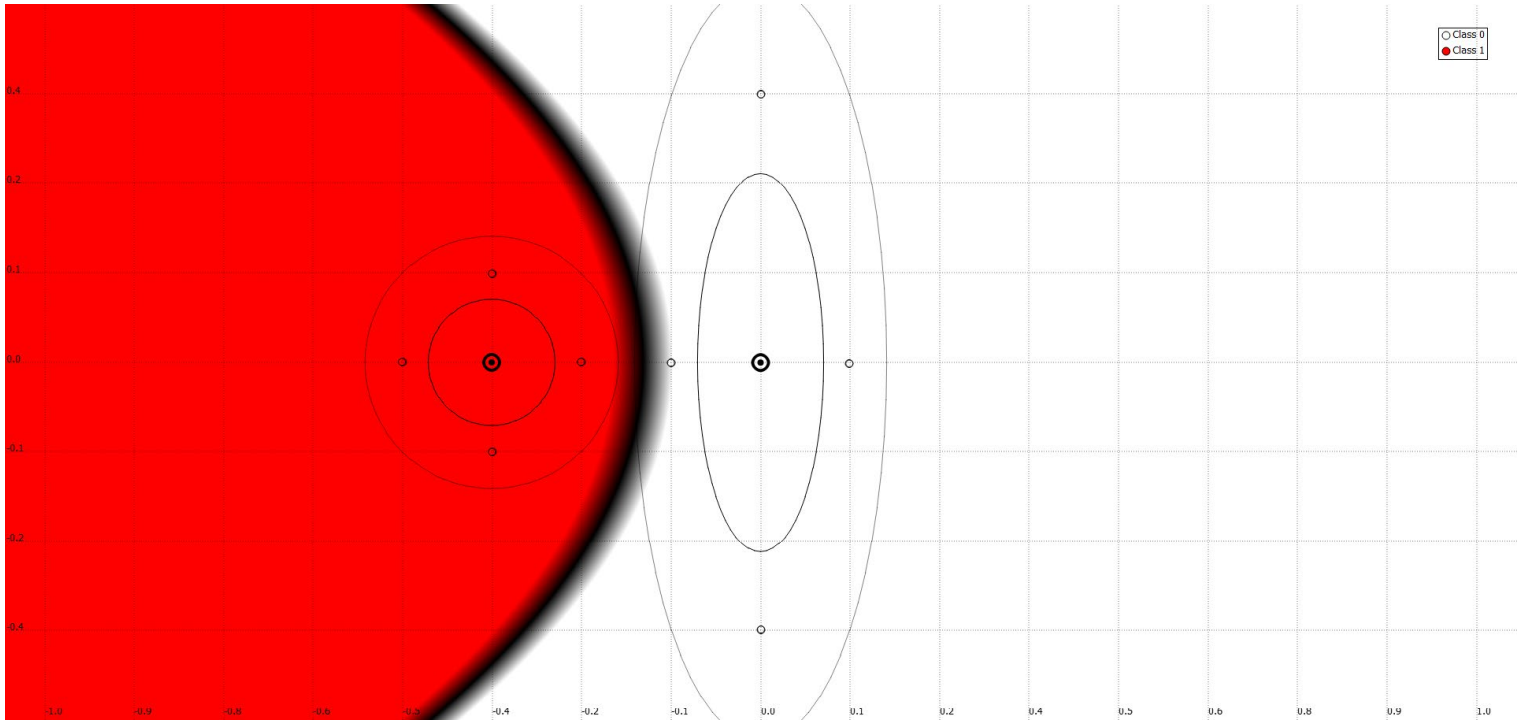
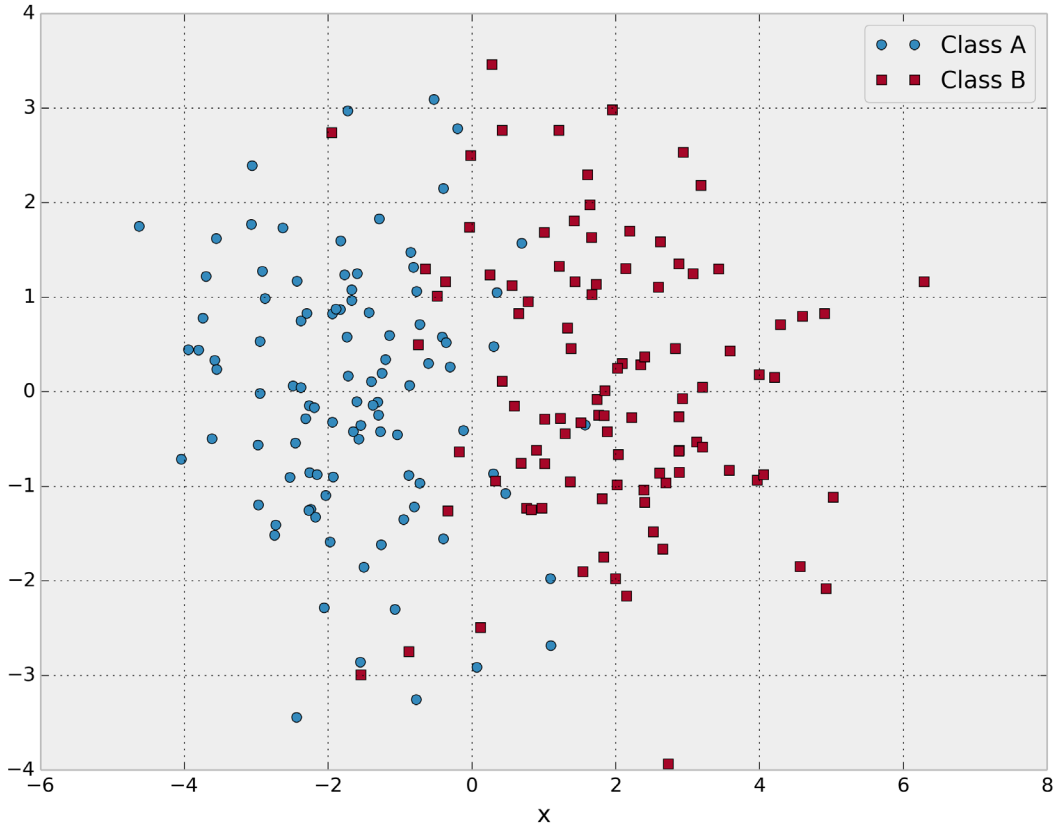
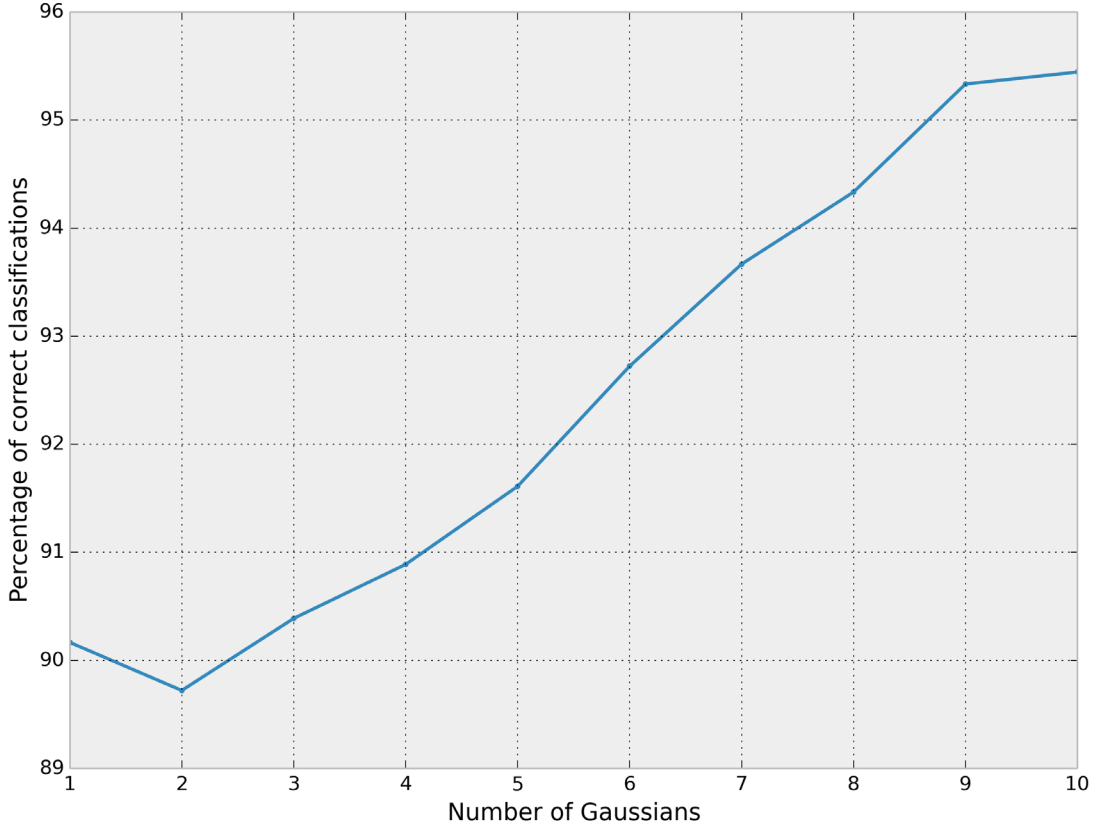


Q2.A

- Choosing the number of Gauss functions in GMM based on the performance of the classifier.





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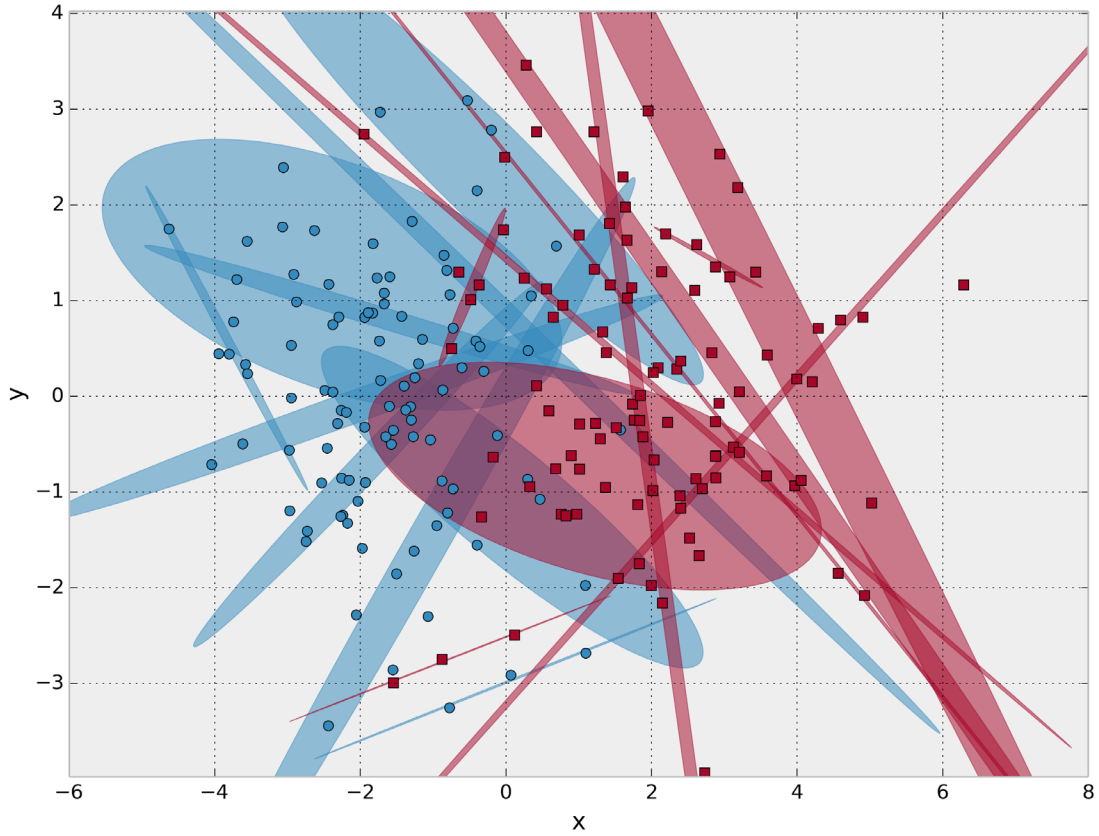
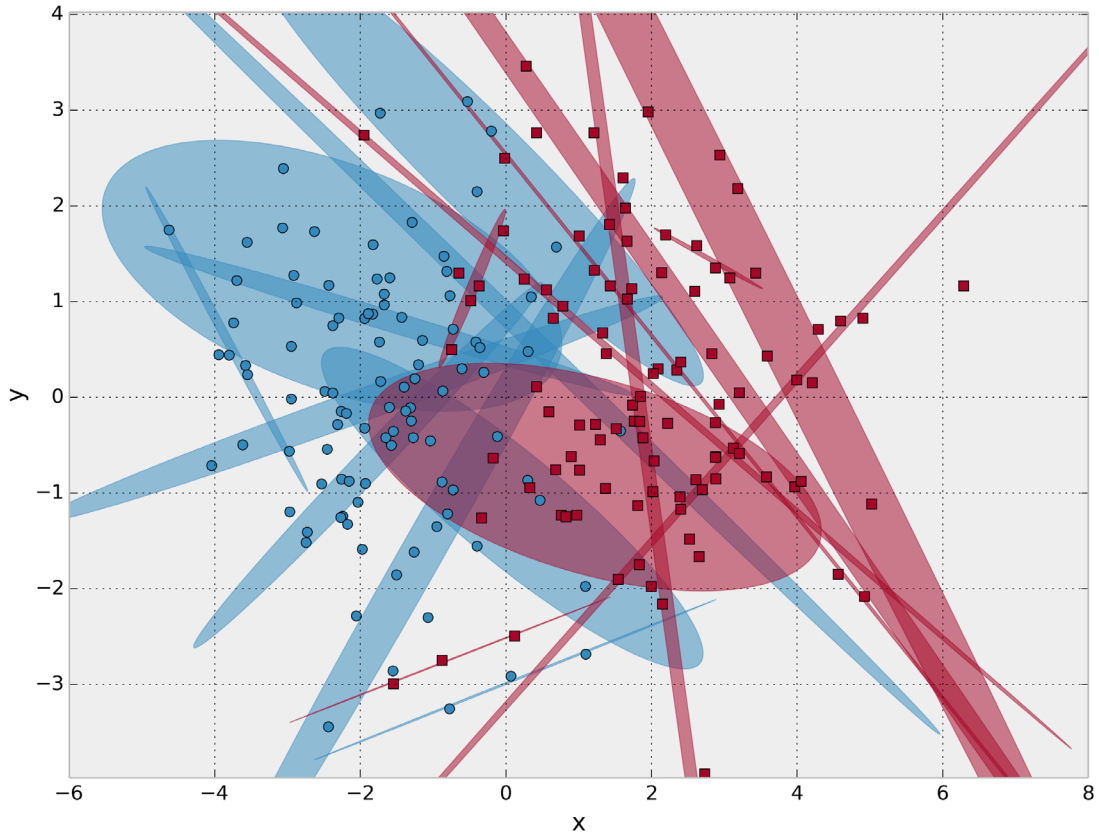
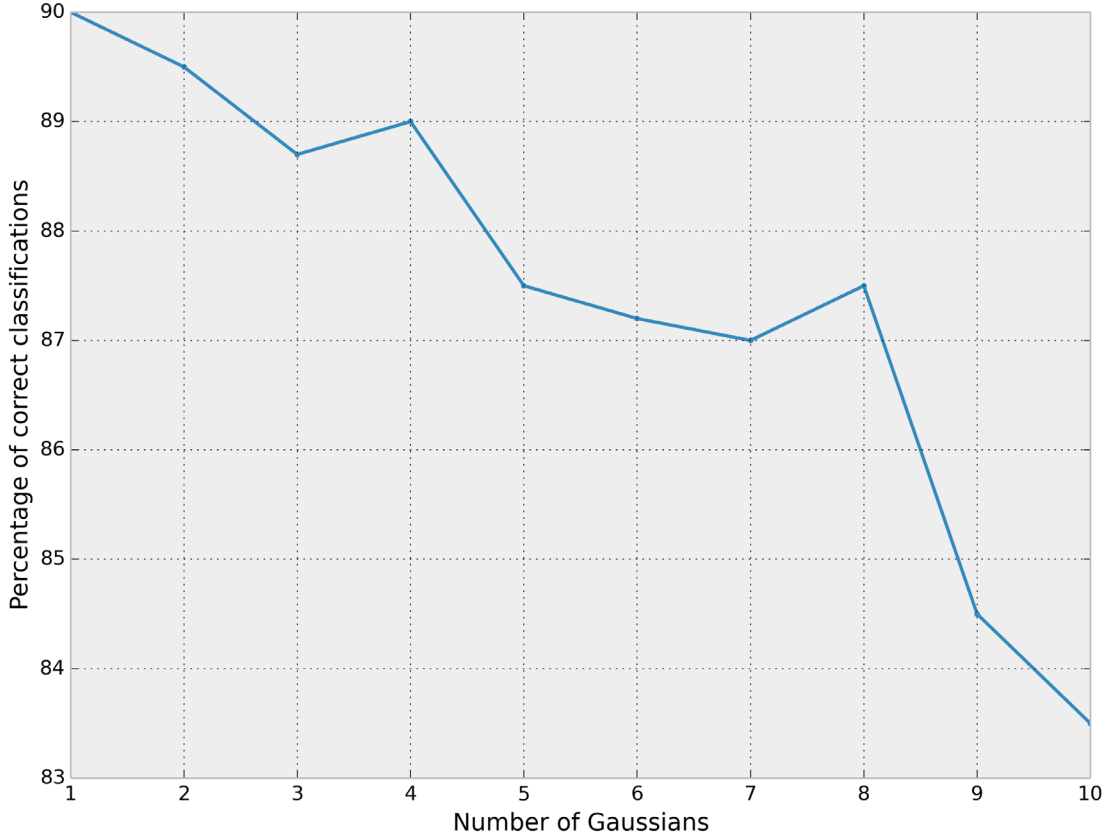
- Risk of overfitting.



Q2.A

- Risk of overfitting.
- Proper usage of K-fold cross-validation.





Q2.B

- An example dataset and choice of GMM that leads to overfitting.

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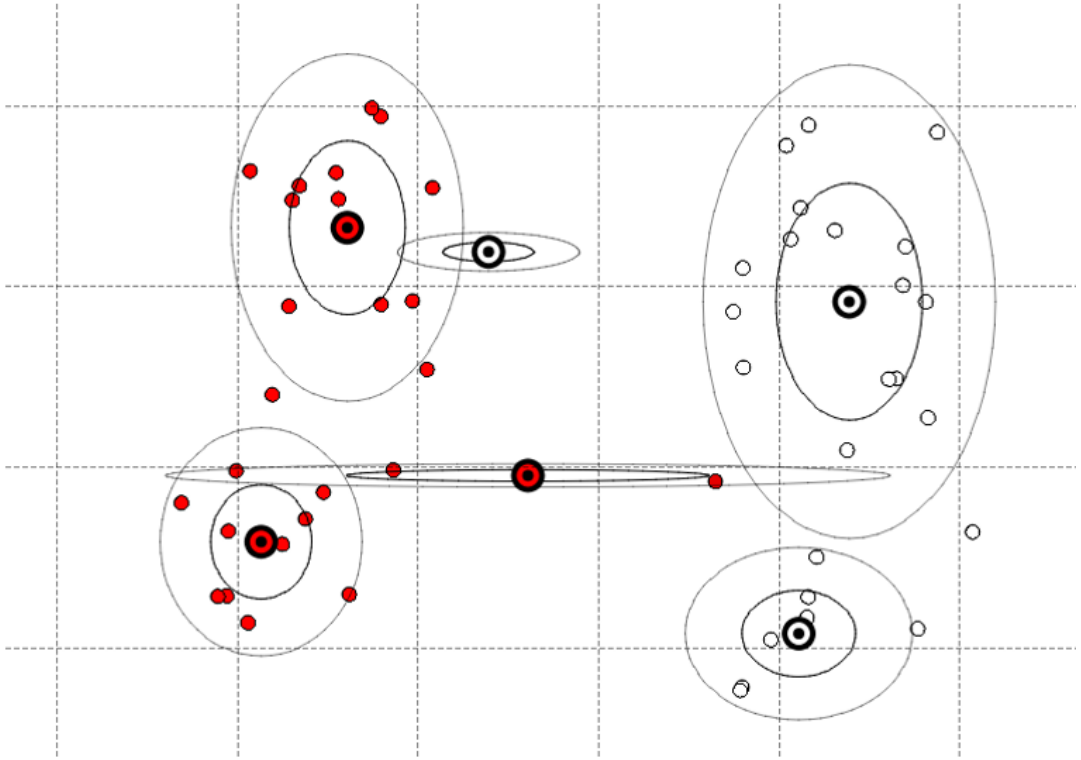

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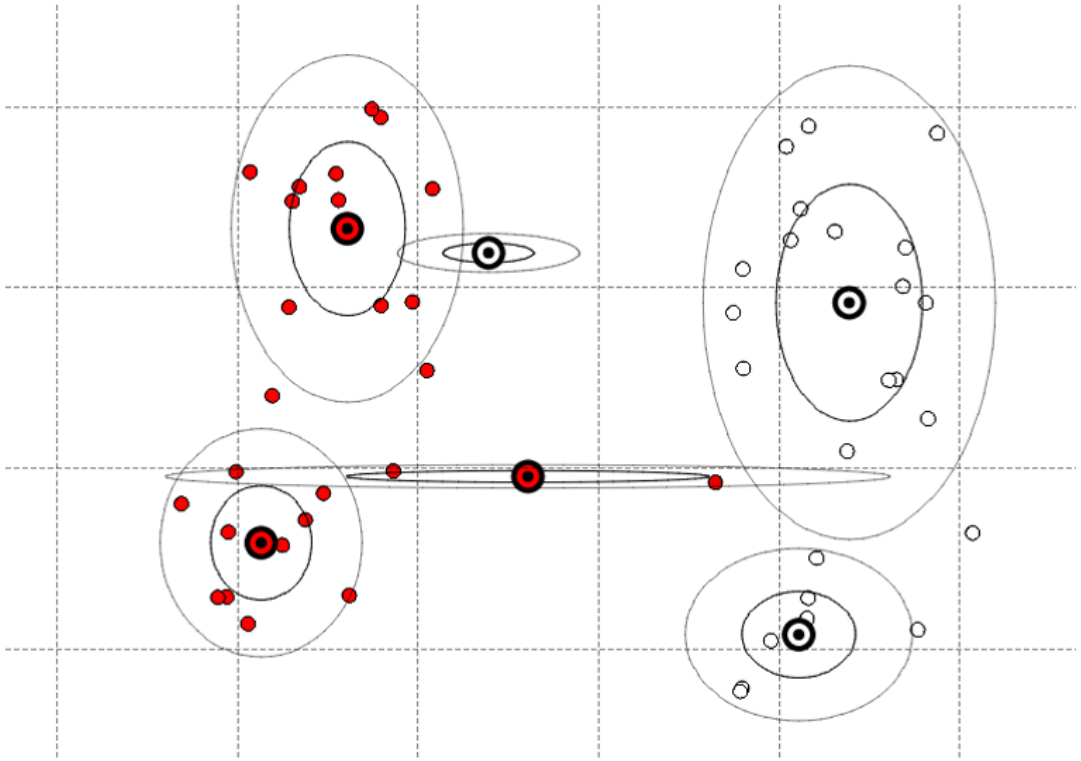

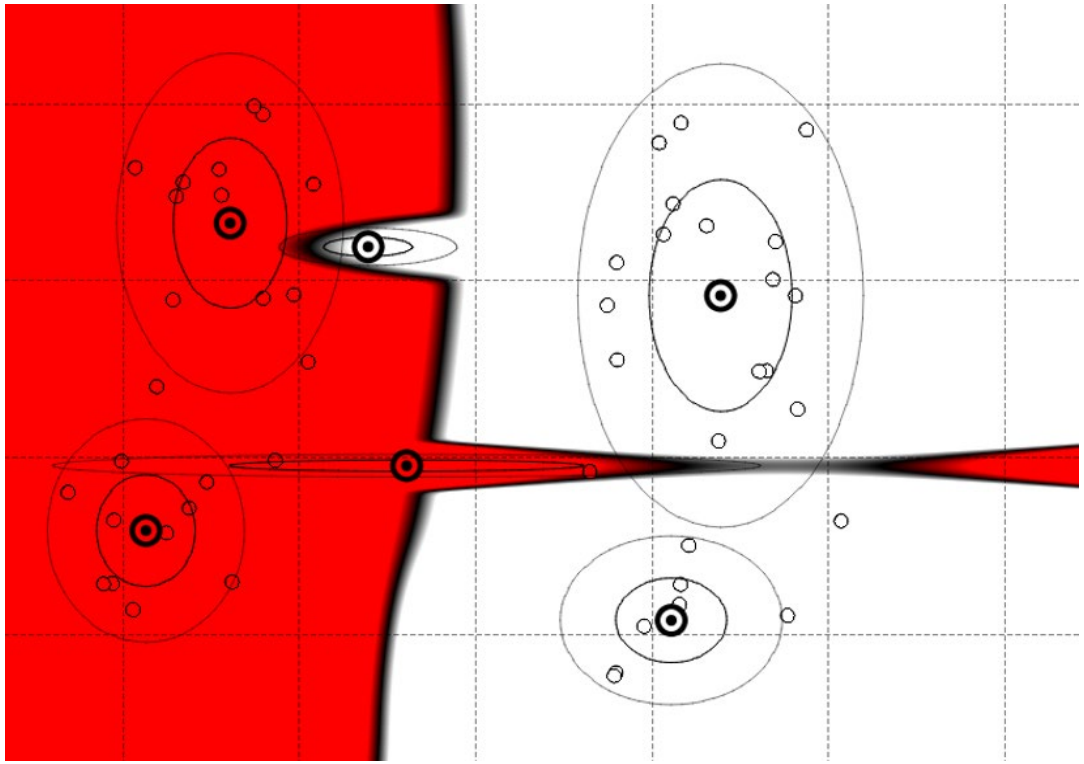

Q2.C

- What is the number of parameters to be estimated for GMM?
- What is the computational cost per iteration of the update step for GMM?

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covariance matrix mean vector

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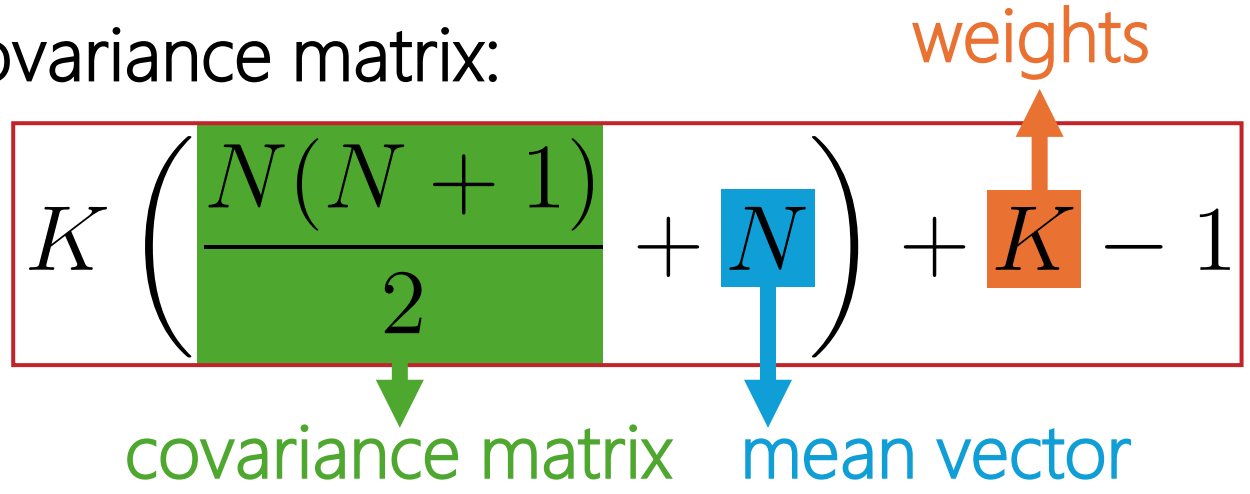

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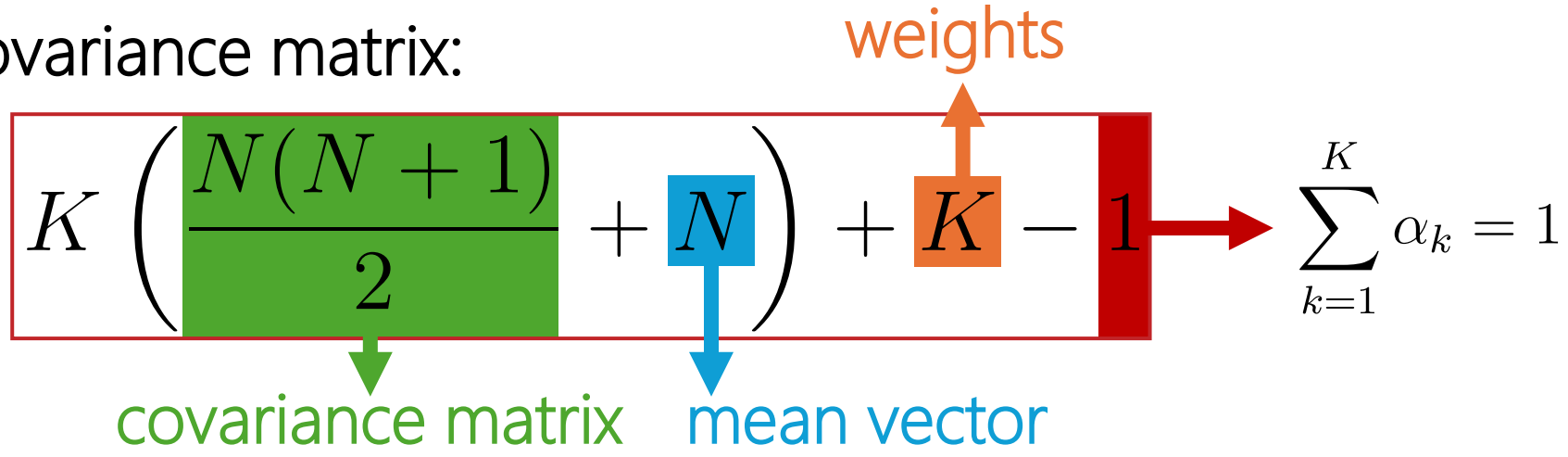

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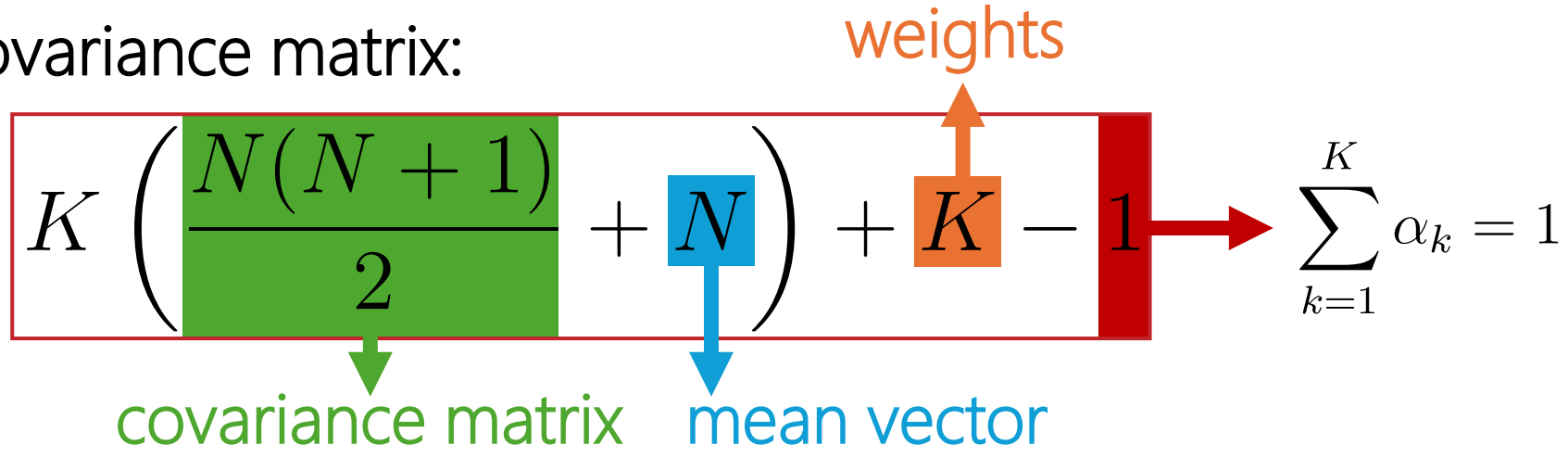

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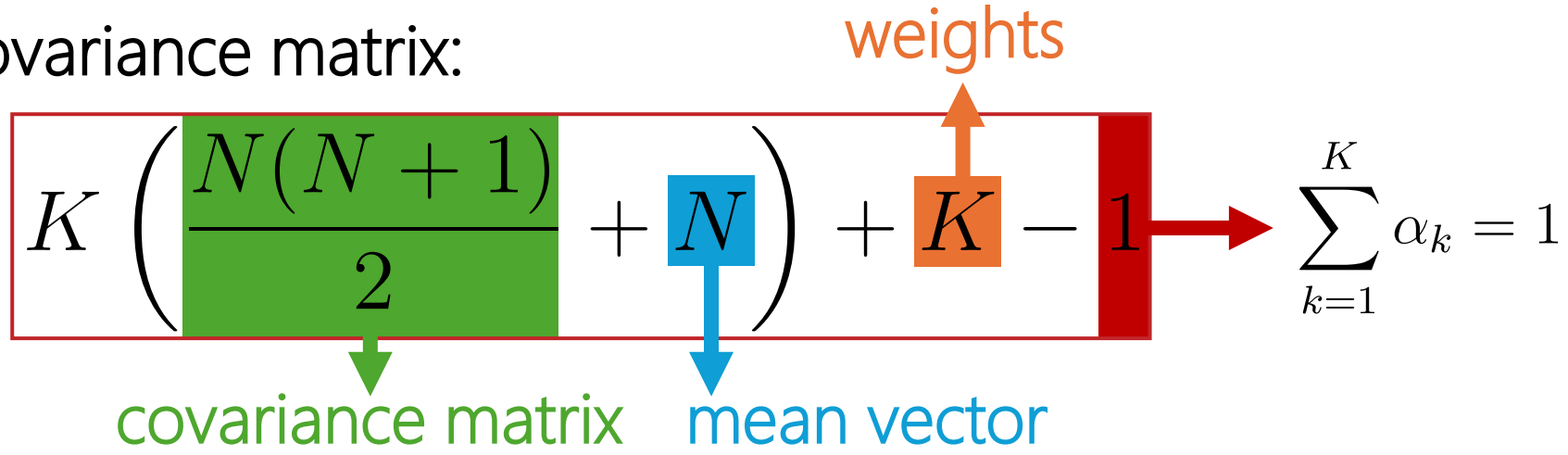

- Diagonal covariance matrix: $K(N+N)+K-1$
- Spherical covariance matrix: $K(1+N)+K-1$

Q2.C > Computational cost of the update step

- Update of the covariance matrices.

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$$\Sigma_{\text{dia}}^{k\ (t+1)} = \text{diag}((\sigma_1^{k(t+1)})^2, \ldots, (\sigma_N^{k\ (t+1)})^2)$$

$$\Sigma_{\text{iso}}^{k\ (t+1)} = \text{diag}((\sigma^{k(t+1)})^2)$$

where

$$(\sigma_i^{k(t+1)})^2 = \frac{\sum_j p(k|x^j, \Theta^{(t)})(x_i^j - \mu_i^{k(t+1)})^2}{\sum_j p(k|x^j, \Theta^{(t)})} \quad \forall i = 1, \ldots, N$$

are the variances along each dimension i and

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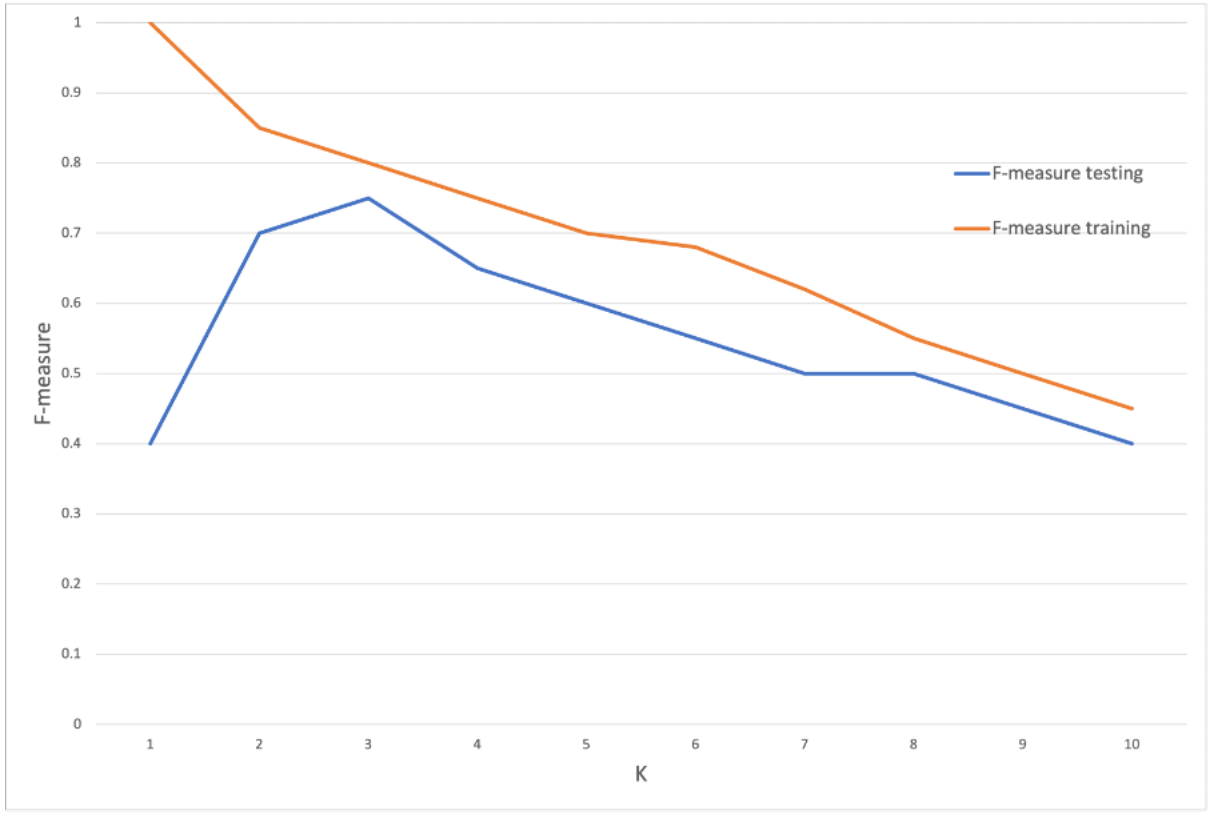
Type	Complexity
Spherical	$\mathcal{O}(KM)$
Diagonal	$\mathcal{O}(KMN)$
Full	$\mathcal{O}(KMN^2)$

Q2.D

- Choosing hyperparameter K in KNN classification based on F-measure.



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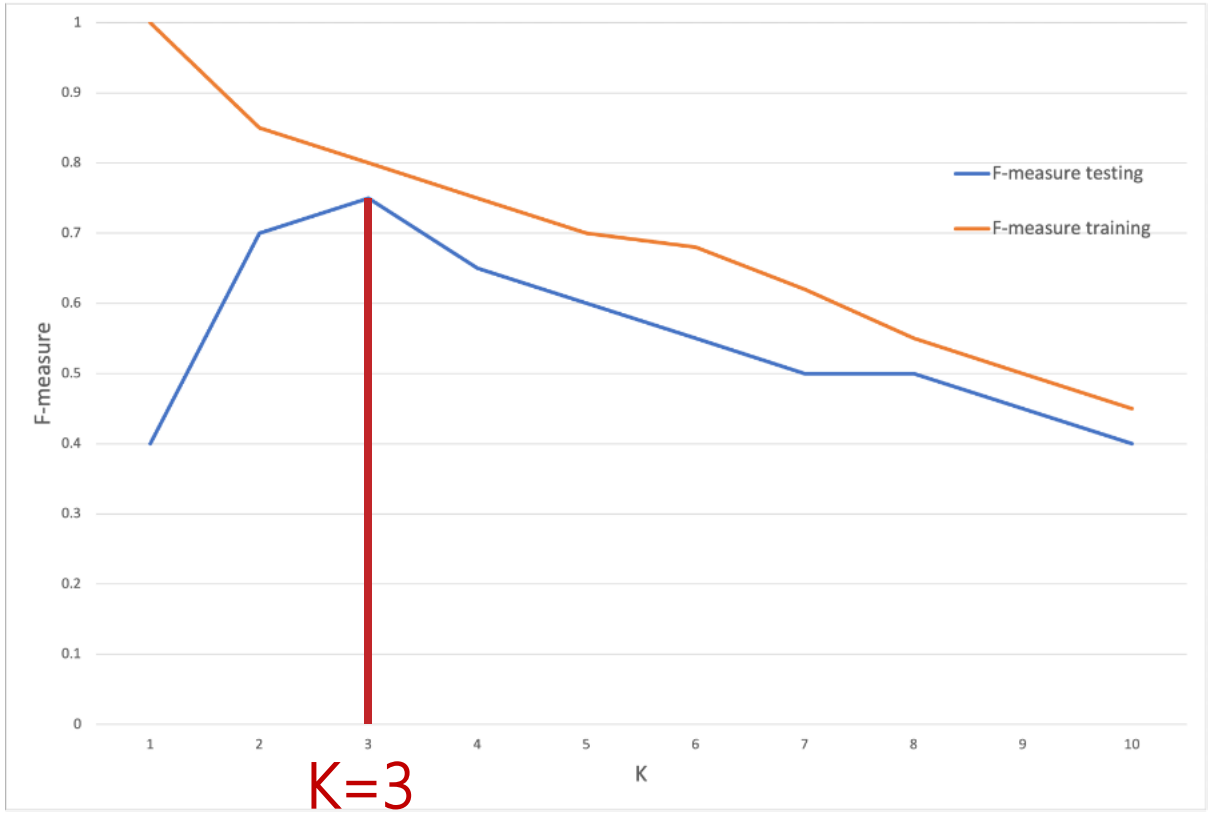

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