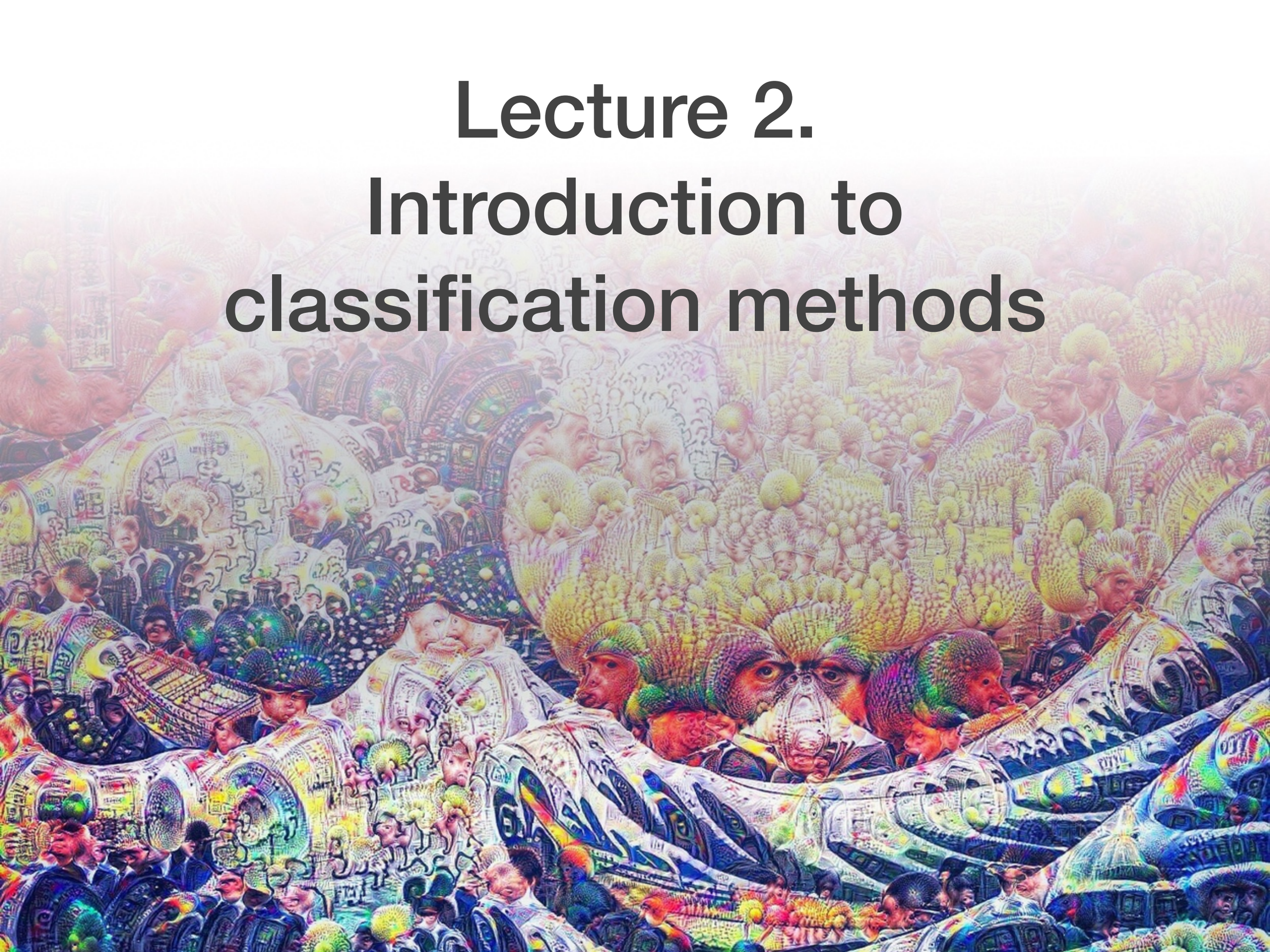
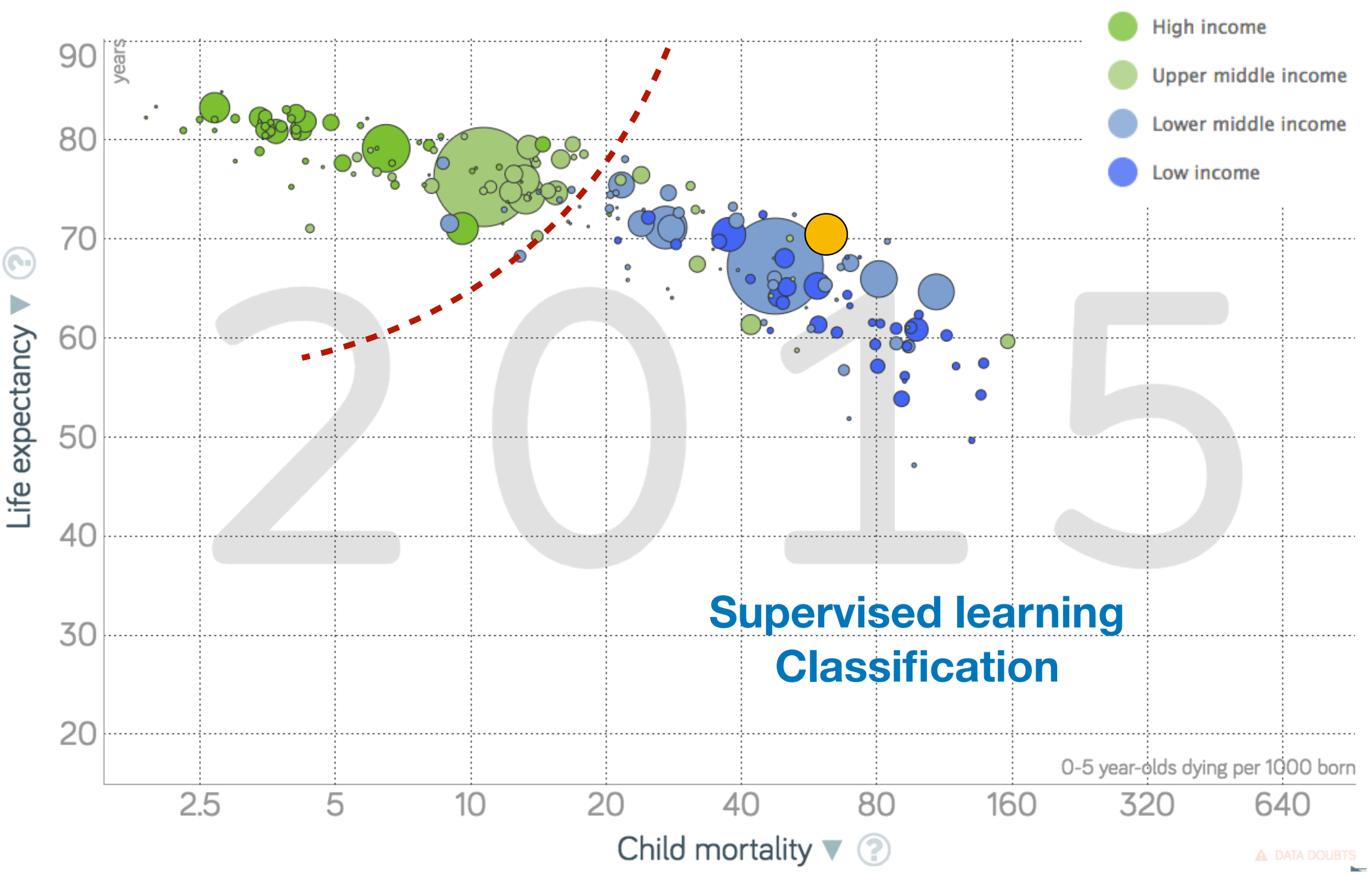
Lecture 2.
Introduction to classification methods



Taxonomy through examples



Supervised learning
Classification

Maximum likelihood method and logistic regression

Logistic regression

$y_i = 0$

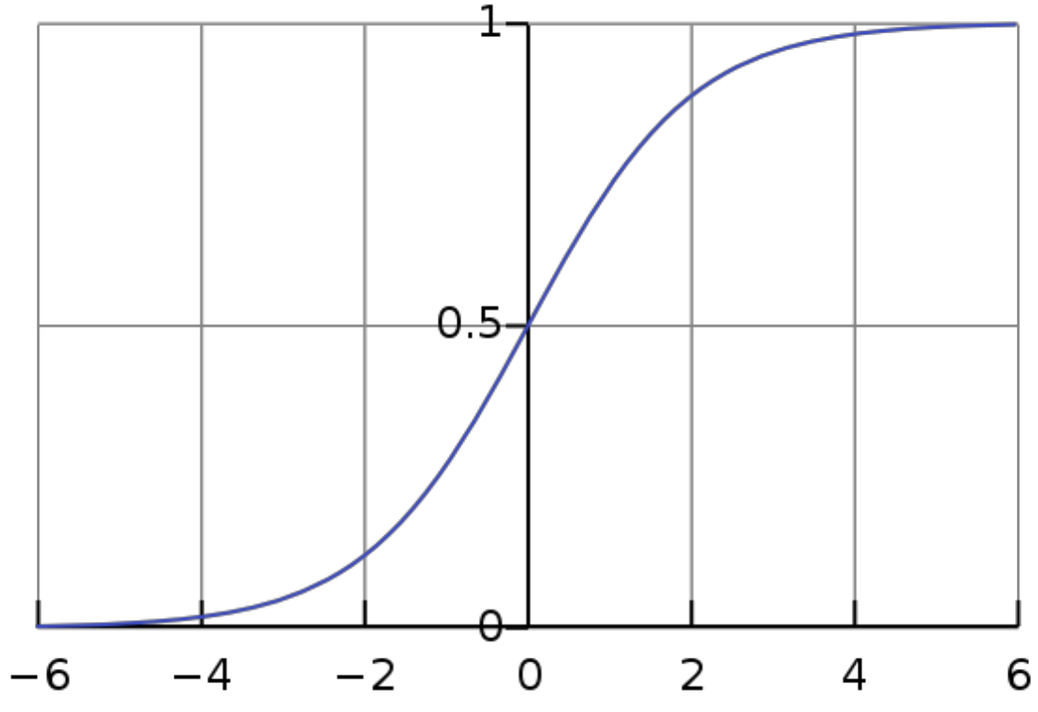
$y_j = 1$

Learn the probability

based on categorical and

continuous features

$$\hat{P}\left(y_i = 1 | x_{i,1}, x_{i,2}, \ldots\right)$$



$$\hat{P}_i \equiv \frac{1}{1 + \exp\left(-\beta_0 - \beta_1 x_{i,1} - \beta_2 x_{i,2} - \ldots\right)}$$

Last lecture -logistic regression

(Multiple) Logistic regression - a classification problem

$$y_j = 1$$

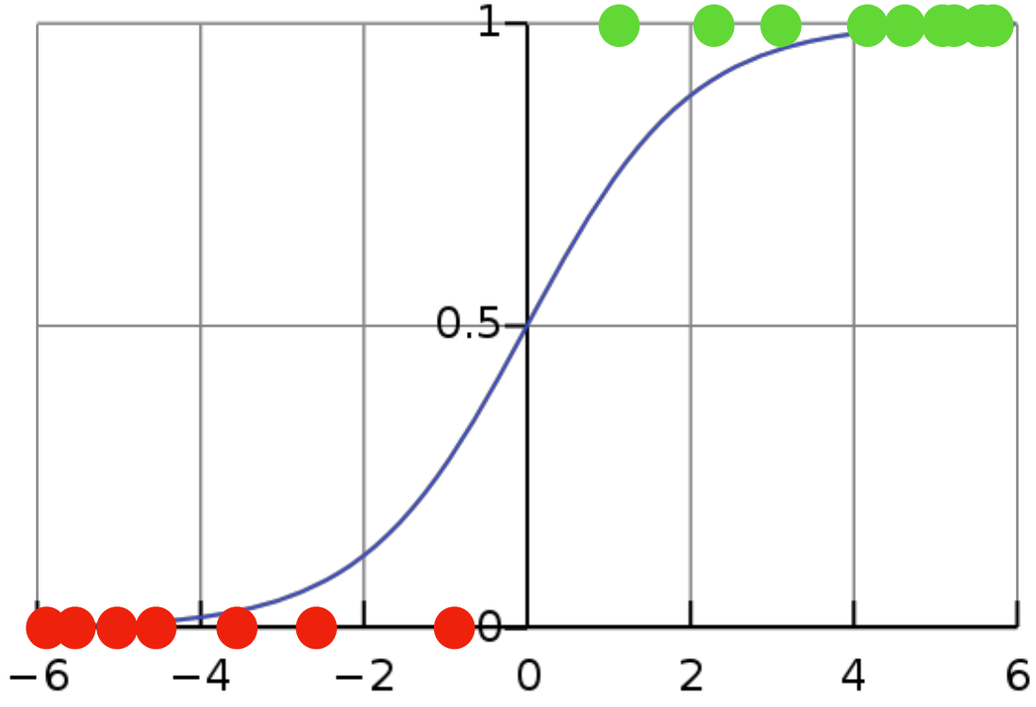
$$y_i = 0$$

Learn the probability

based on categorical and

continuous features

$$\hat{P}\left(y_i = 1 | x_{i,1}, x_{i,2}, \ldots\right)$$



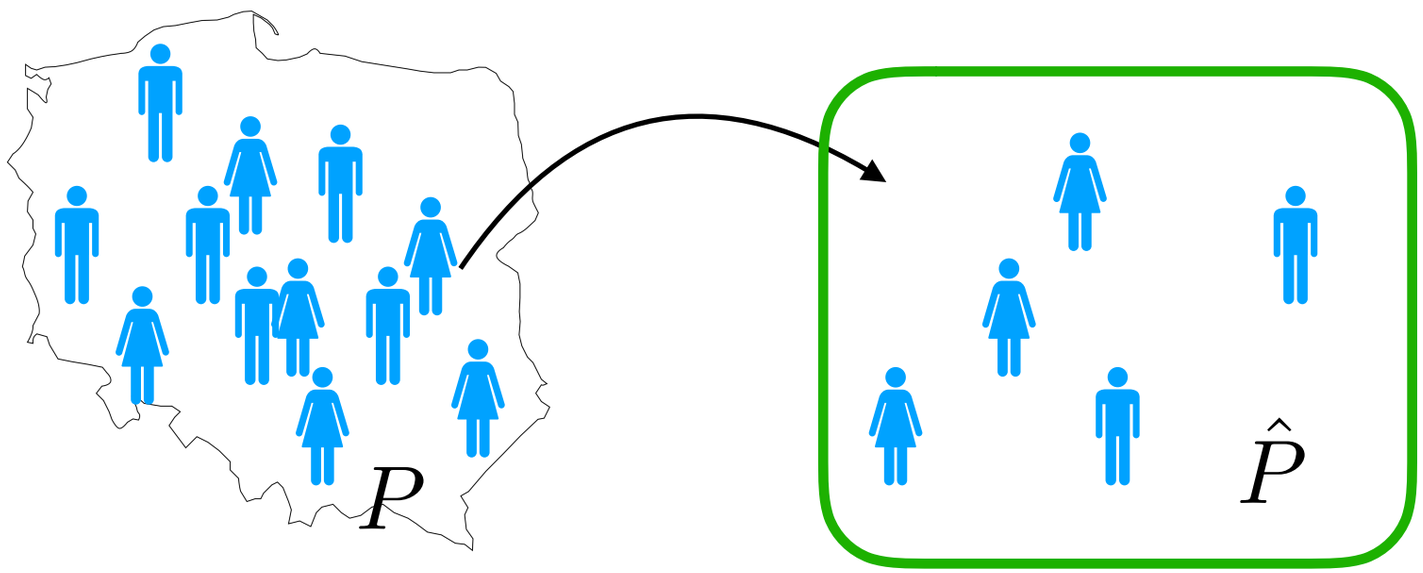
$$\log \frac{P(x)}{1 - P(x)} = \beta_0 + \beta_1 x_1 + \ldots$$

log-odds or logit

$$\hat{P}_i \equiv \frac{1}{1 - \exp\left(-\beta_0 - \beta_1 x_{i,1} - \beta_2 x_{i,2} - \ldots\right)}$$

Logistic regression with maximum likelihood method

Maximum Likelihood method



Estimate the probability of randomly choosing a male from the population of PL

$y_i = 0$

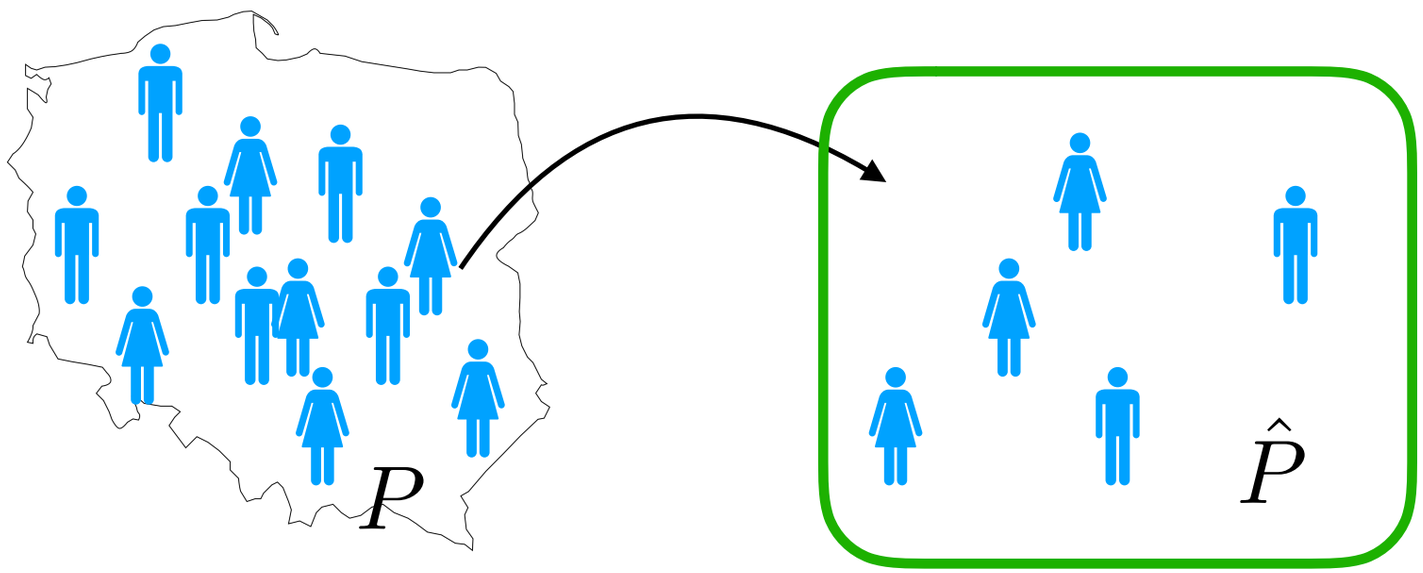
$y_j = 1$

$$L = \prod_i P^{y_i} (1 - P)^{1 - y_i}$$

$$\frac{\partial L}{\partial P}|_{P=\hat{P}} = 0$$

Logistic regression with maximum likelihood method

Maximum Likelihood method



Estimate the probability of randomly choosing a male from the population of PL, given some some features of the person

Sample

$y_i = 0$

$y_j = 1$

$$\hat{P}_i \equiv \frac{1}{1 + \exp\left(-\beta_0 - \beta_1 x_{i,1} - \beta_2 x_{i,2} - \ldots\right)}$$

$$L = \prod_i P_i^{y_i} \left(1 - P_i\right)^{1 - y_i}$$

For each j:

$$\frac{\partial L}{\partial \beta_j}|_{\beta=\hat{\beta}} = 0$$

Last lecture -logistic regression

(Multiple) Logistic regression - a classification problem

$$y_j = 1$$

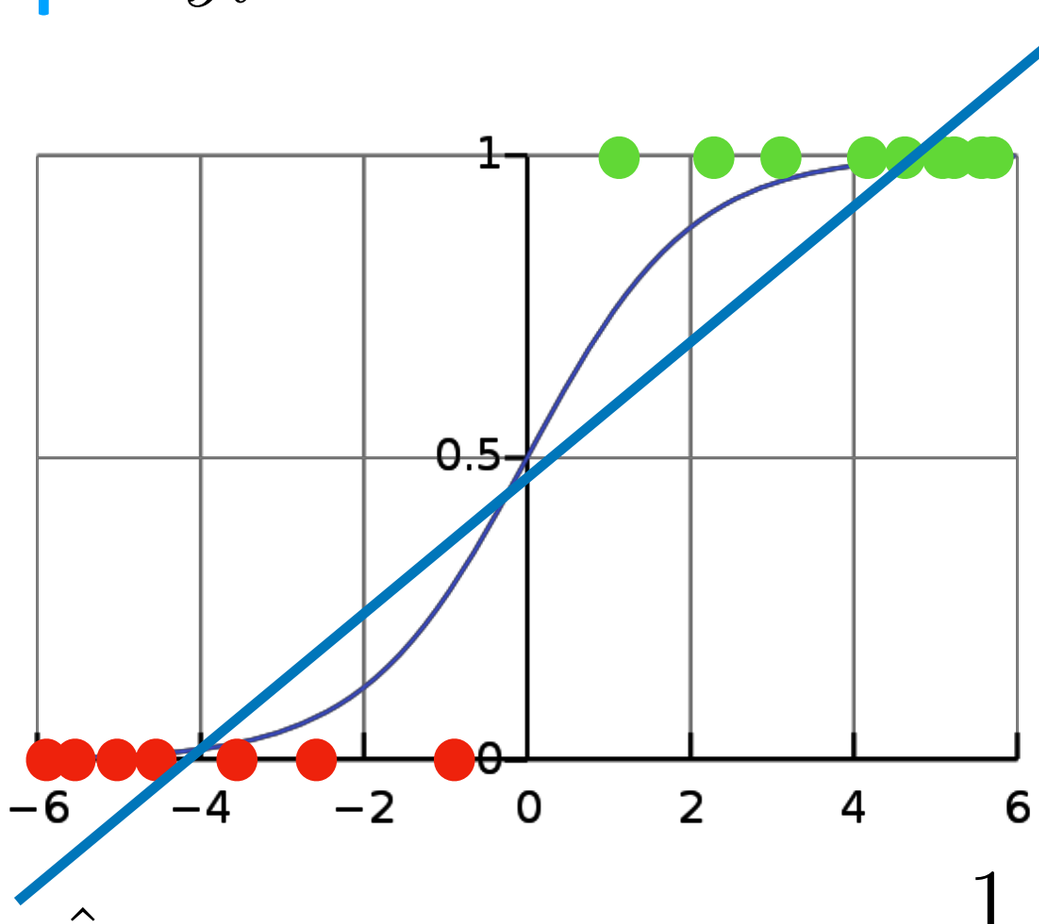
$$y_i = 0$$

Learn the probability

based on categorical and

continuous features

$$\hat{P}\left(y_i = 1 | x_{i,1}, x_{i,2}, \ldots\right)$$



$$\log \frac{P(x)}{1 - P(x)} = \beta_0 + \beta_1 x_1 + \ldots$$

log-odds or logit

$$y(x) = \beta_0 + \beta_1 x_1 + \ldots$$

$$\hat{P}_i \equiv \frac{1}{1 - \exp\left(-\beta_0 - \beta_1 x_{i,1} - \beta_2 x_{i,2} - \ldots\right)}$$

Another reason not to use linear regression for classification

Predict medical condition of a patient in the emergency room

1 if stroke

2 if drug overdose

3 if epileptic seizure

- But this imposes arbitrary order
- and suggests that the differences are the same between some pairs

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1 if epileptic seizure

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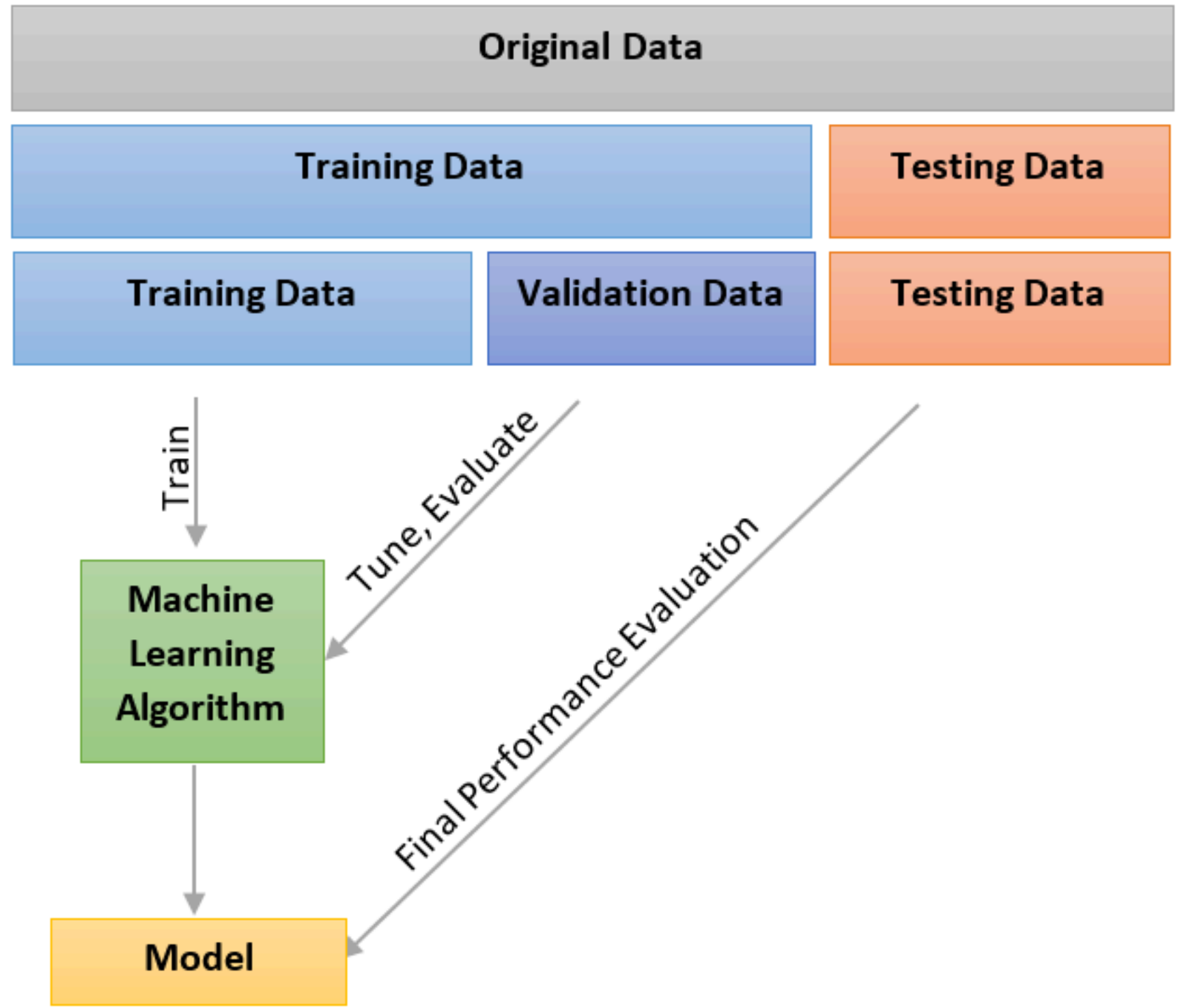
With linear regression, this would lead to three different models with different predictions

1 if epileptic seizure

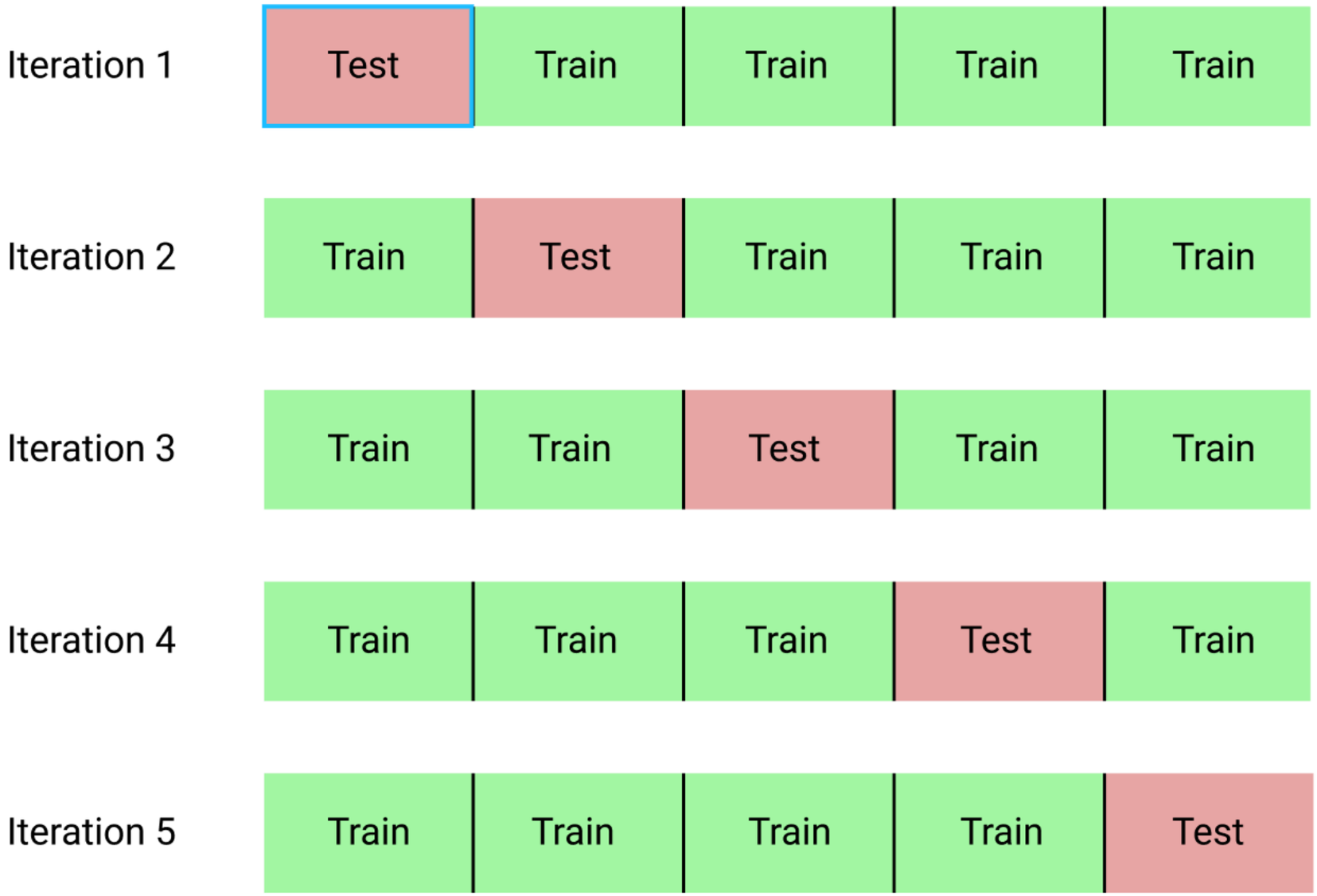
3 if stroke

9 if drug overdose

How to measure the quality of predictions (in binary Classification)



How to measure the quality of predictions (in binary Classification)



k-fold cross validation (for example when little data)

- watch out for bias and stationarity (this would look different for time series prediction)

Quality of predictions - Bayes rule

Seek estimate of f (call it $\hat{f}$) on the basis of observations (from the training ds): $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$

- **Training error rate** $= \frac{1}{n} \sum_{i=1}^{n} I(y_i, \hat{y}_i)$

$$I(y_i \neq \hat{y}_i) = 1$$

$$I(y_i = \hat{y}_i) = 0$$

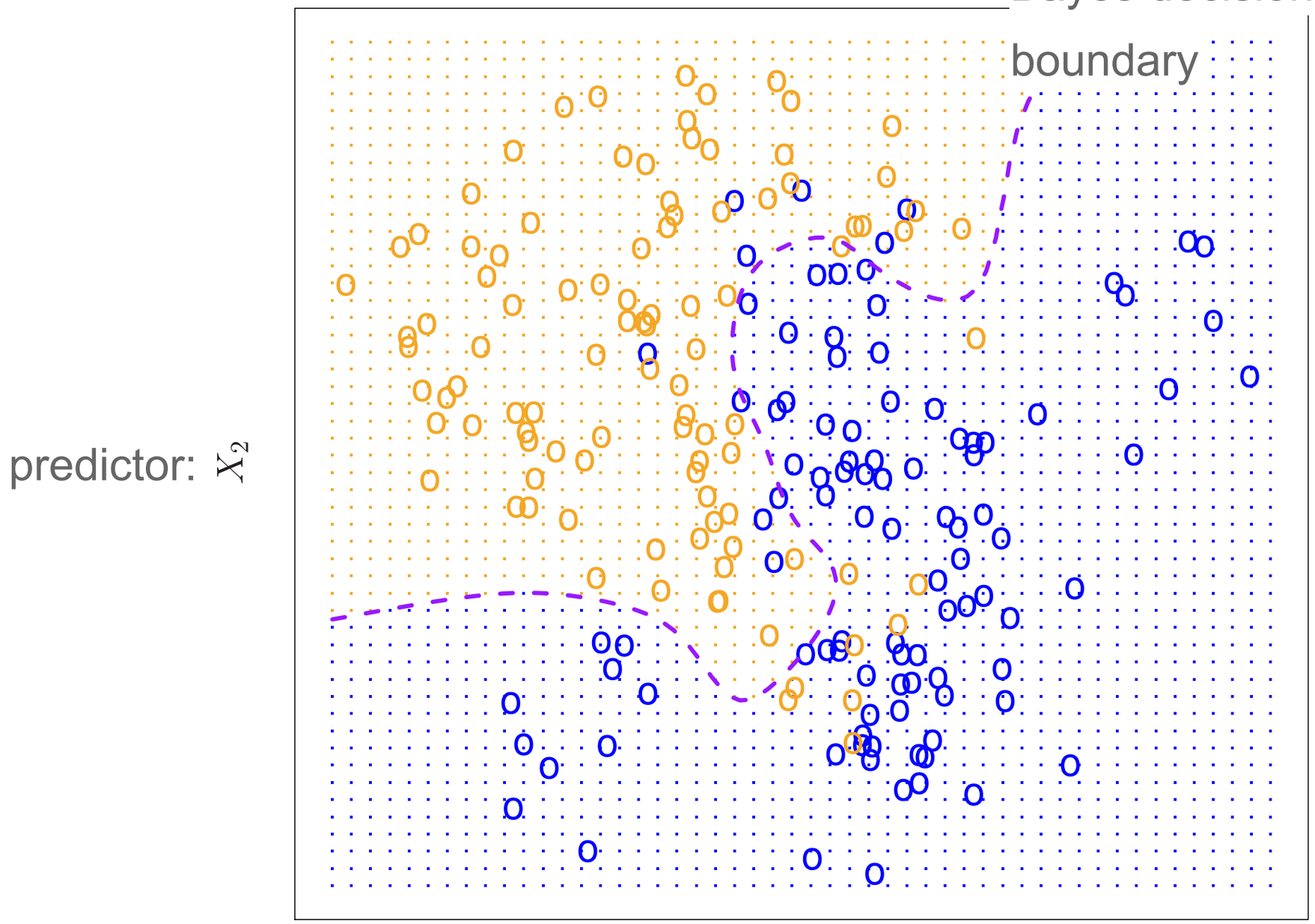
$\{(x_{n+1}, y_{n+1}), \ldots, (x_{n+m}, y_{n+m})\}$ (test ds)

- **Test error rate** $= \frac{1}{m-n} \sum_{i=n}^{m} I(y_i, \hat{y}_i)$

Theorem: Test error is minimized, on average, by the so-called Bayes classifier, that assigns the observations to the most likely class, given the predictor (x) values. In other words: to minimize test error, assign class to maximize the conditional probability: $P(Y = j | X = x)$

Quality of predictions - Bayes rule

In binary classification (simulated data)



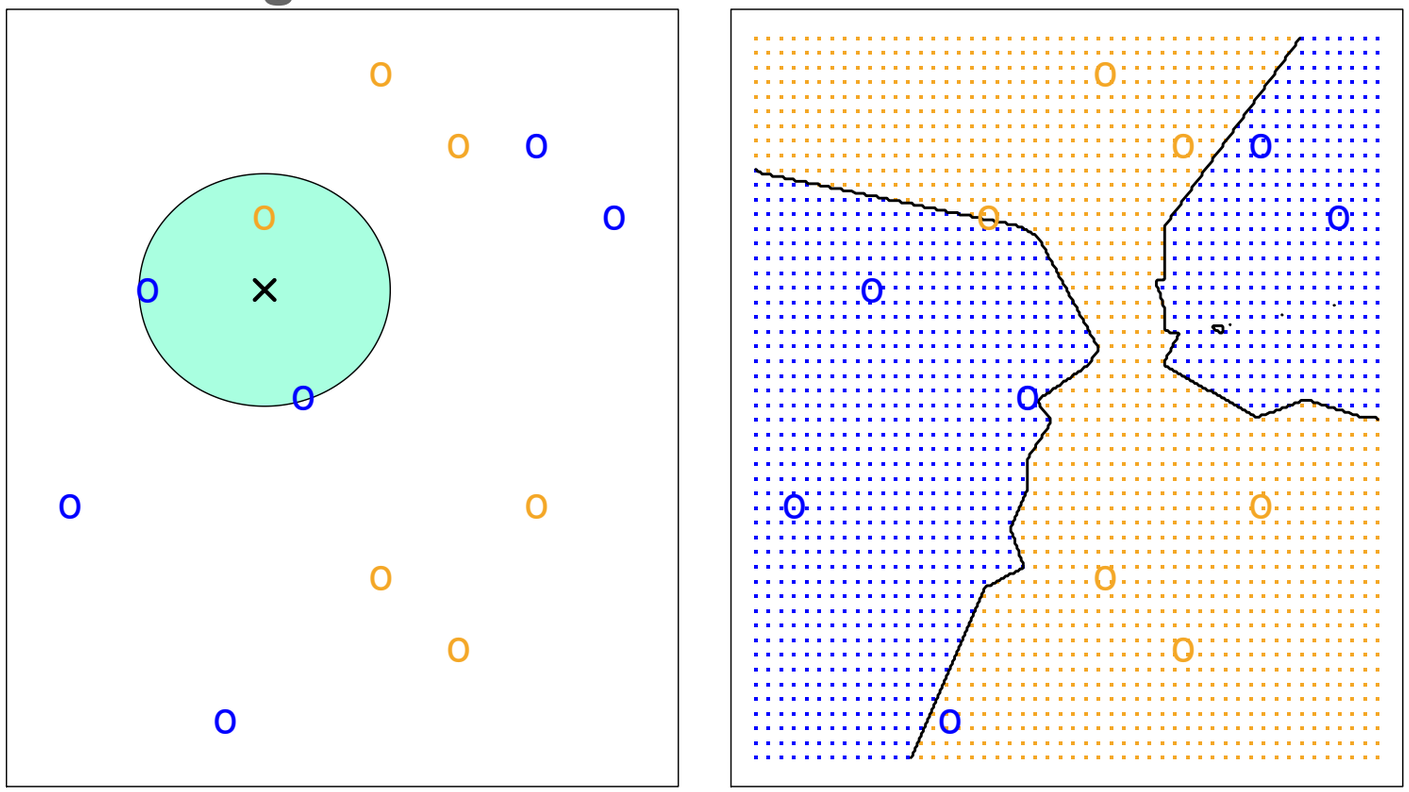
$P(Y = 1|X = x) > 0.5$ $P(Y = 0|X = x) > 0.5$

In reality, we never know the conditional probability distribution of Y given X!

Quality of predictions - K-Nearest Neighbor example

Thus some methods attempt to estimate the conditional probability distribution of Y given X.

Example: K-Nearest Neighbor classifier



Given an integer K, and test observation x_0, the KNN classifier identifies the points in the training data that are closest to x_0 (represented by N_0), and estimates the conditional probability for class j as the fraction of points in N_0 whose response values equal j:

$$P(Y = j|X = x_0) = \frac{1}{K} \sum_{i \in N_0} I(y_i = j)$$

Then applies the Bayes rule (our theorem) to classify x_0 to the class with highest probability

Quality of predictions - K-Nearest Neighbor example

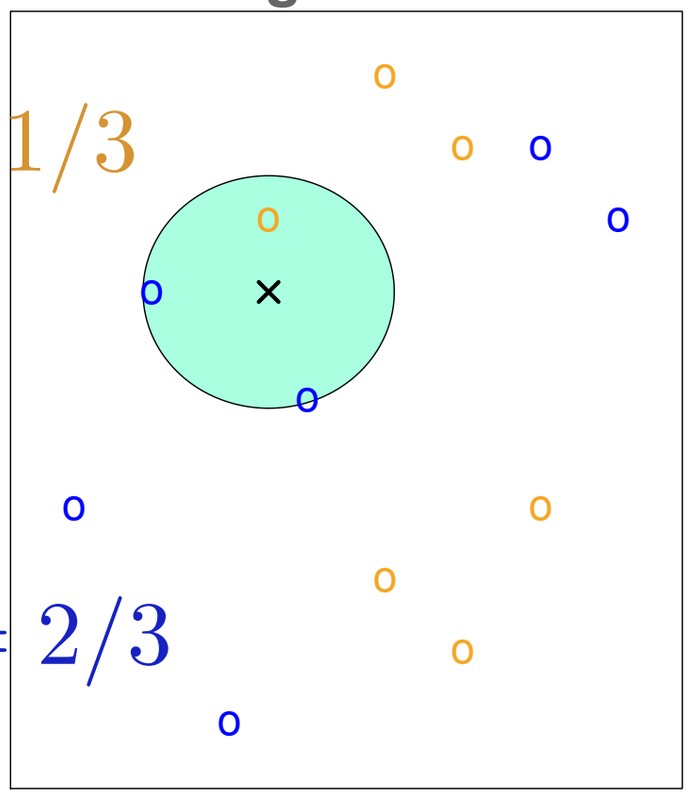
Thus some methods attempt to estimate the conditional probability distribution of Y given X.

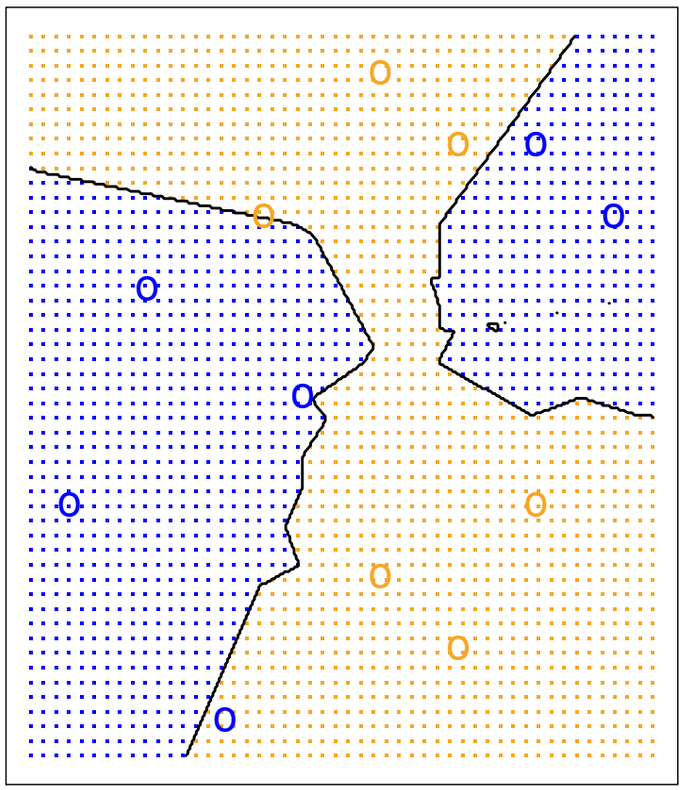
Example: K-Nearest Neighbor classifier

$P = 1/3$

$K = 3$

$P = 2/3$





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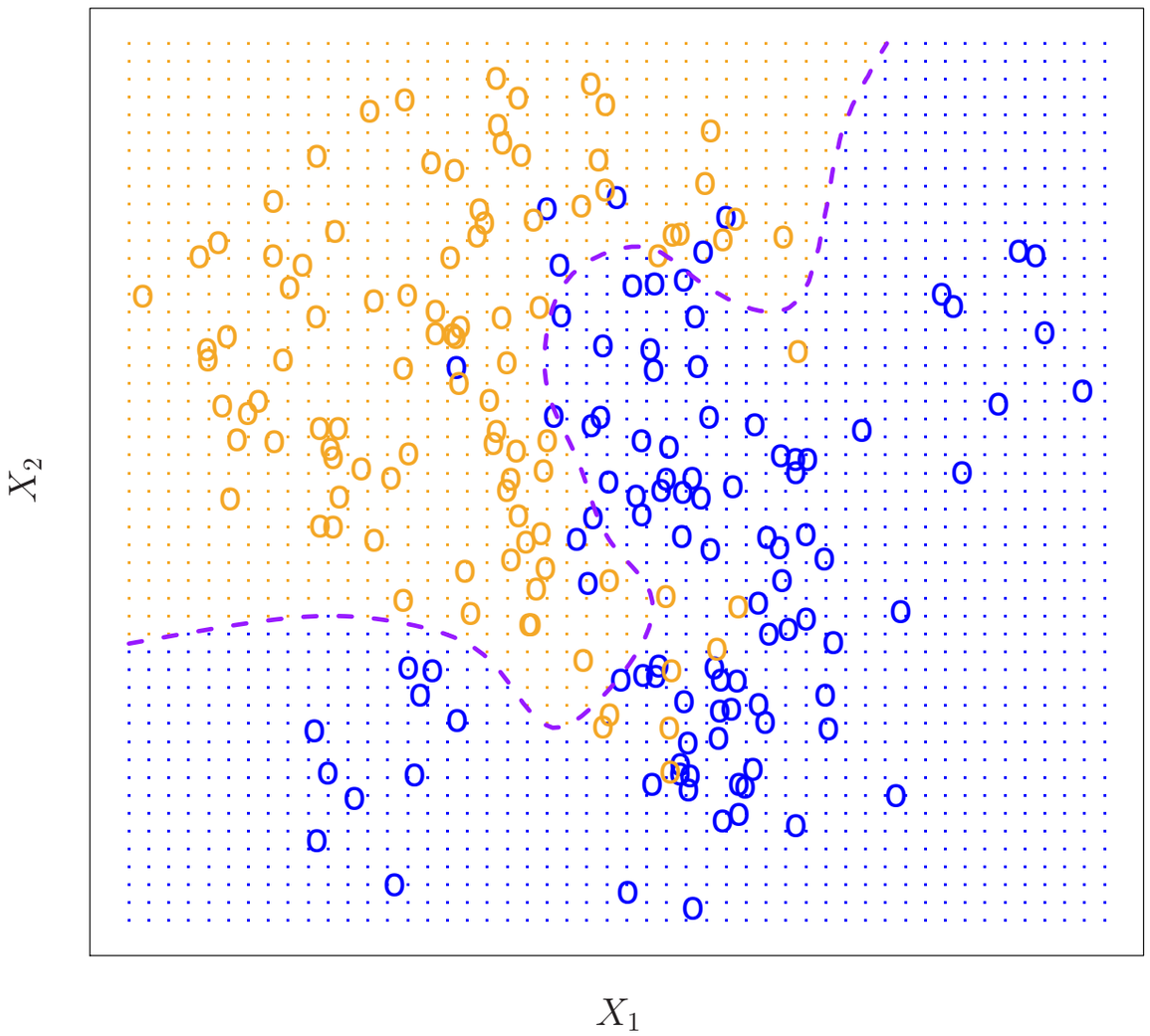
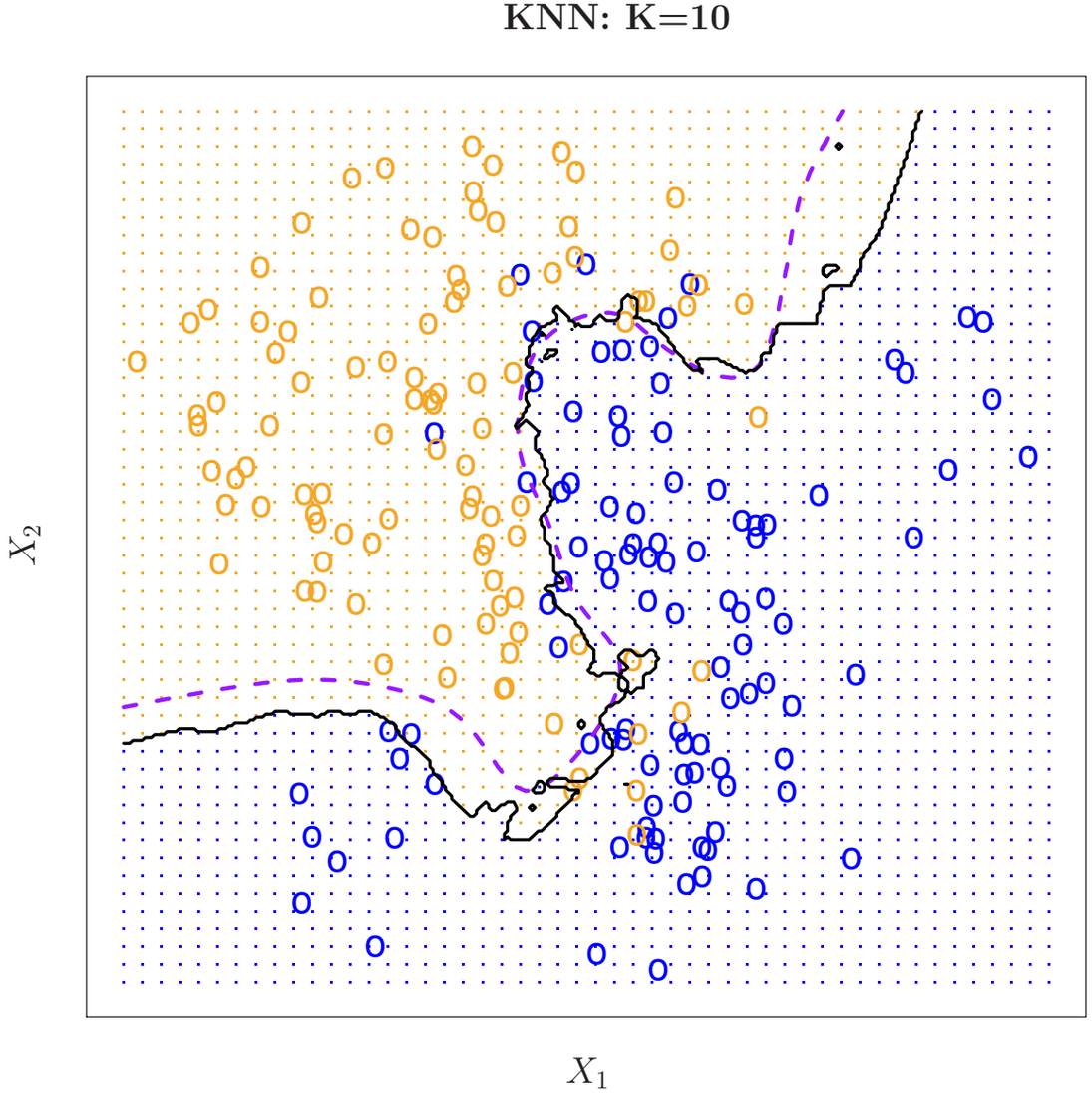
Quality of predictions - K-Nearest Neighbor example



Bayes error rate: 0.1304

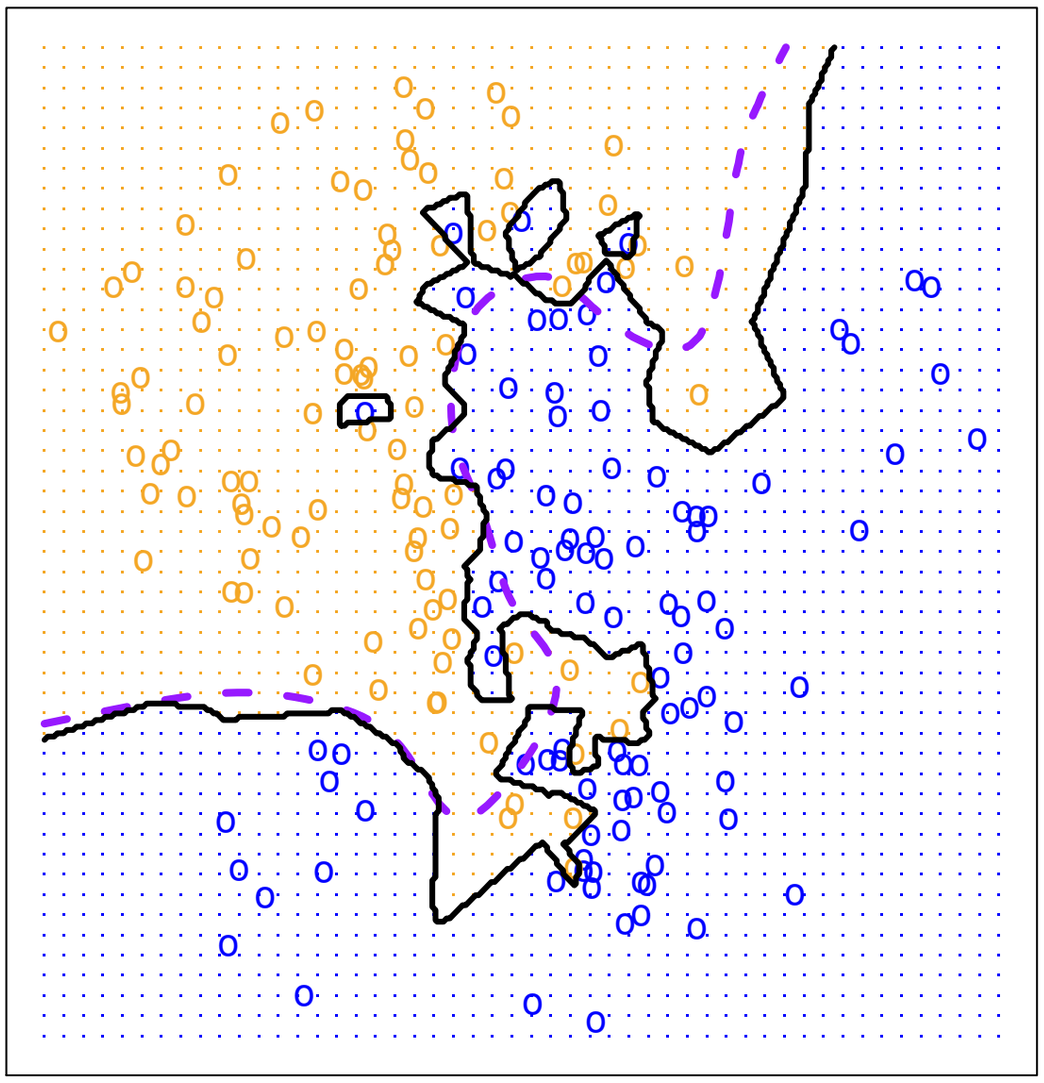
(>0 due to class overlap

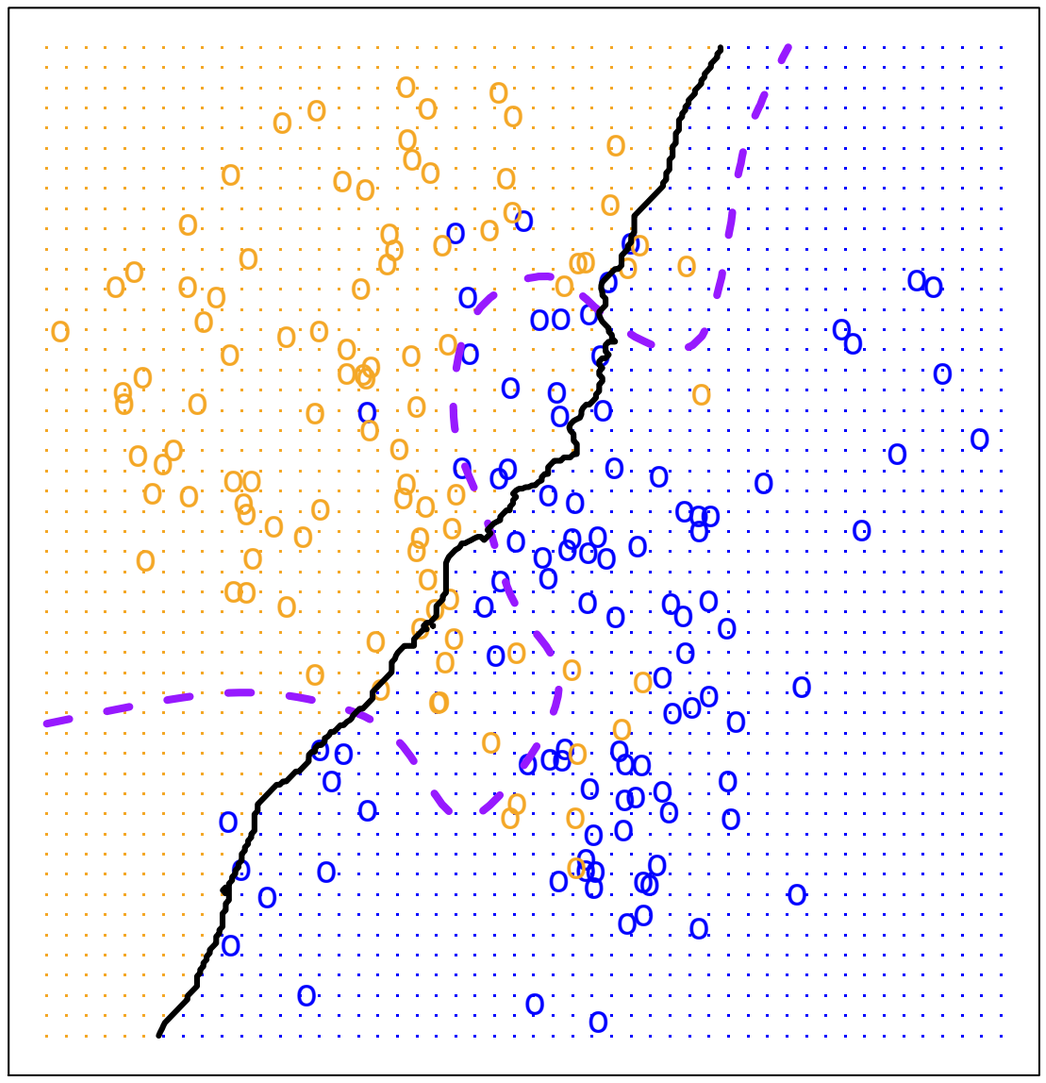
in real population)



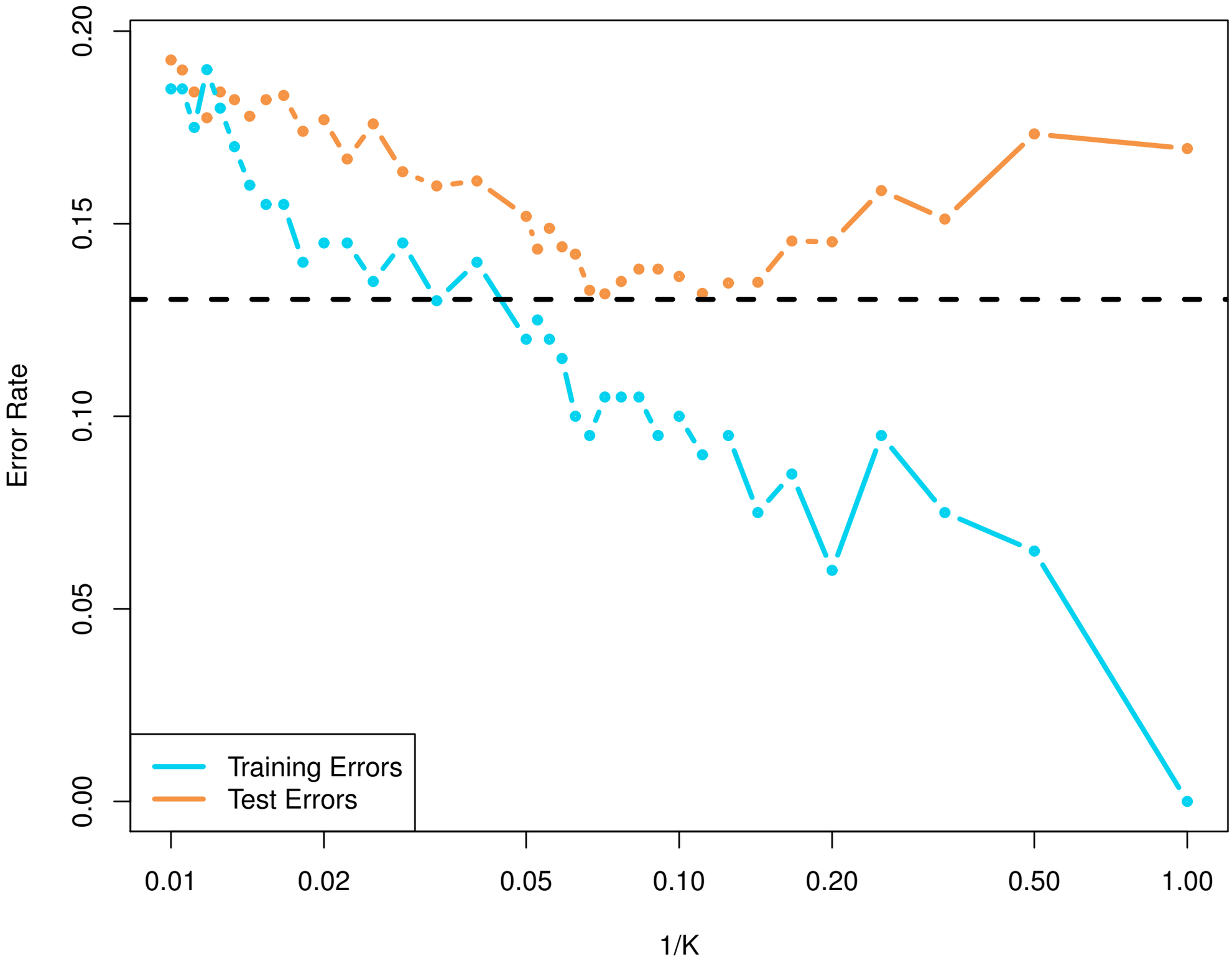
K=10-NN error rate 0.1363

Quality of predictions - K-Nearest Neighbor example





Quality of predictions - K-Nearest Neighbor example



Approximating the Bayes classifier

- KNN is a method for approximating the conditional probability and using the Bayes classifier. $P\left(Y=j|X=x_0\right)=\frac{1}{K}\sum_{i\in N_0}I(y_i=j)$

- **another way to this is Bayes theorem:** $P(A|B)P(B)=P(B|A)P(A)$

$$\pi_k \equiv P(Y=k) \quad \textbf{- prior}$$

$$f_k(X) \equiv P(X=x|Y=k) \quad \textbf{- likelihood}$$

$$p_k(X) \equiv P(Y=k|X=x) \quad \textbf{- posterior}$$

$$p_k(X)=\frac{\pi_k f_k(x)}{\sum_{l=1}^{K}\pi_l f_l(x)}$$

Approximating the Bayes classifier

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- **another way to this is Bayes theorem:** $P(A|B)P(B)=P(B|A)P(A)$

$\pi_k \equiv P(Y=k)$ **- prior - easy to estimate**

$f_k(X)\equiv P(X=x|Y=k)$

$p_k(X)\equiv P(Y=k|X=x)$ **- posterior - we need some assumptions on the form**

$$p_k(X)=\frac{\pi_k f_k(x)}{\sum_{l=1}^{K}\pi_l f_l(x)}$$

Approximating the Bayes classifier - Linear Discriminant Analysis

- assume only one predictor (p=1) and $f_k(X)$ is a Gaussian.

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2}(x-\mu_k)^2\right)$$

- let (for simplicity): $\sigma \equiv \sigma_1 = \sigma_2 = \ldots = \sigma_K$

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x-\mu_k)^2\right)}{\sum_{l=1}^{K} \pi_l \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(x-\mu_l)^2\right)}$$

Independent <- of k

- our rule is that, given predictor x we assign class k with highest $p_k(x)$. This is the one with largest:

$$\delta_k(x) = x\,\frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{(2\sigma^2)} + \log \pi_k$$

Linear Discriminant Analysis - example 1

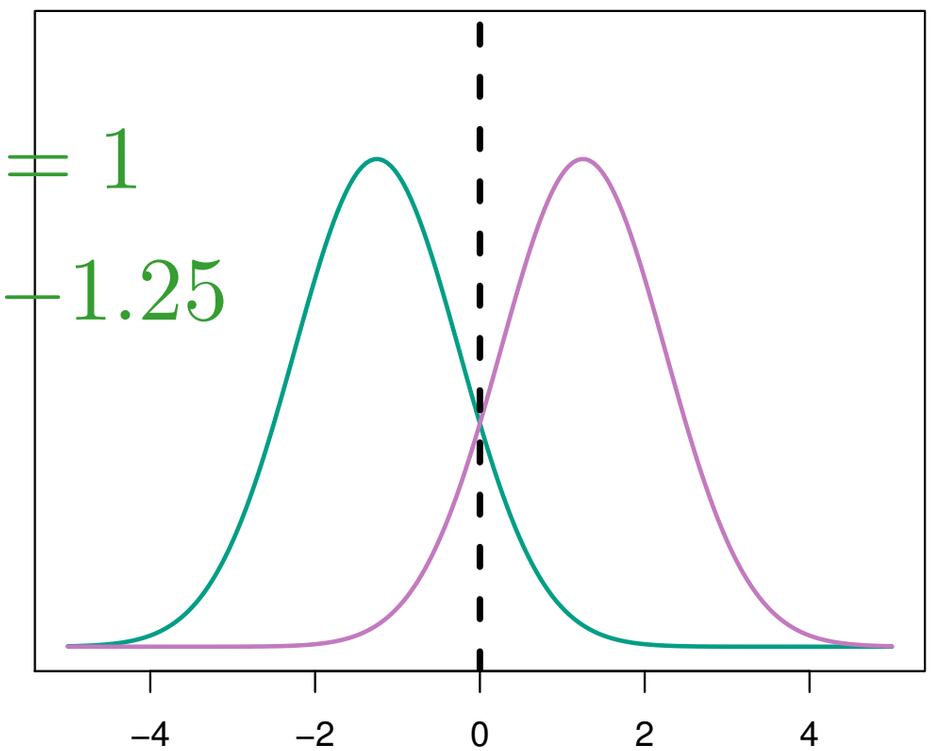
- assume 2 classes - $K = 2$
- represented in the same amount in the sample - $\pi_1 = \pi_2$ = 0.5
- Then the Bayes classifier assigns an observation to class 1 if:

$$2x(\mu_1 - \mu_2) > \mu_1^2 - \mu_2^2$$

- and the decision boundary is the average of the means $\frac{\mu_1 + \mu_2}{2}$

$$\sigma = 1$$

$$\mu_1 = -\mu_2 = -1.25$$



But, usually, we don't know the parameters of the distribution!

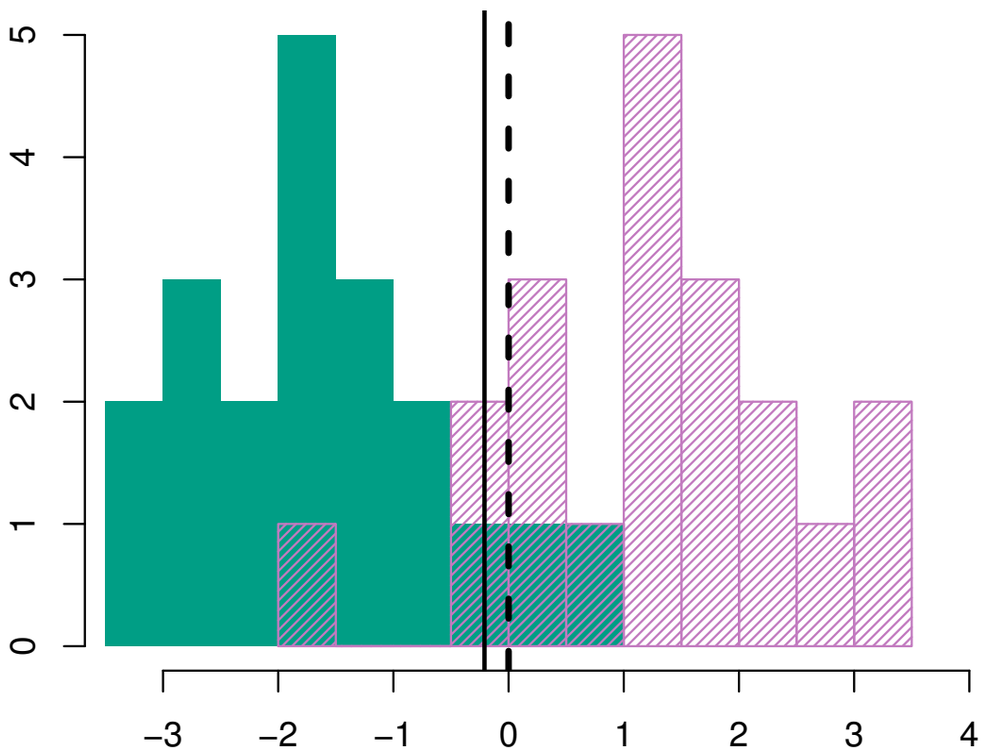
Linear Discriminant Analysis - example 2

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i \qquad \hat{\pi}_k = \frac{n_k}{n}$$

$$\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2$$

- compute estimates of the parameters of the distribution

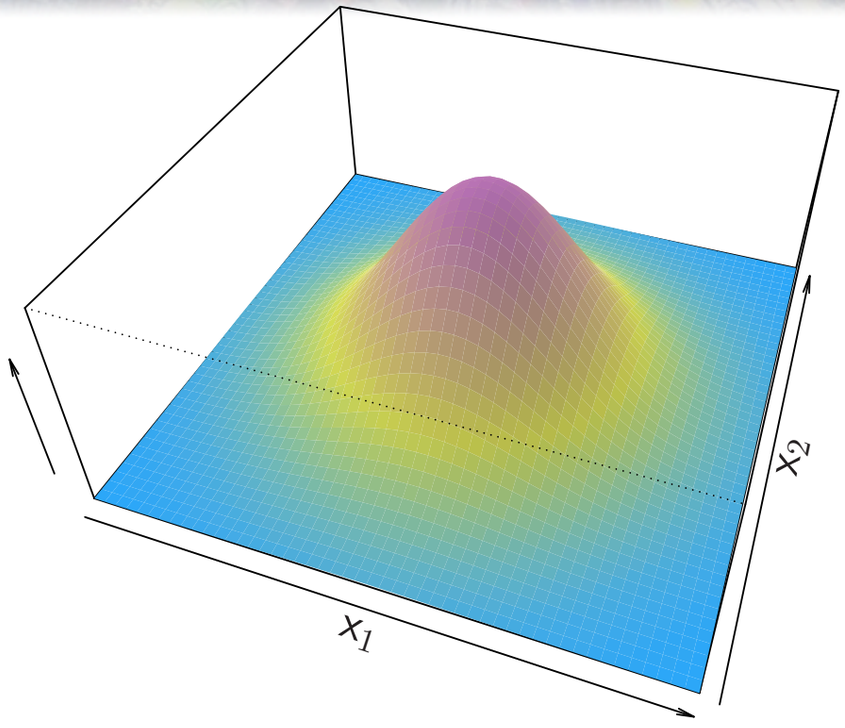
$$\hat{\delta}_k(x) = x \frac{\hat{\mu}_k}{\hat{\sigma}^2} - \frac{\hat{\mu}_k^2}{(2\hat{\sigma}^2)} + \log \hat{\pi}_k$$

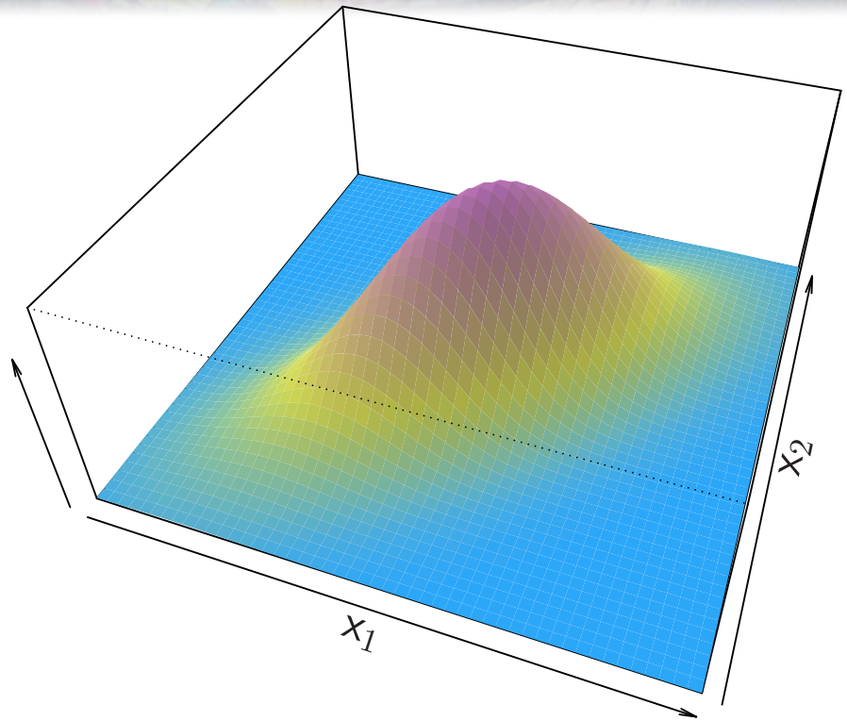


example 2 - based on 20 data point for each of the distribution from example 1

Bayes error rate = 0.106
LDA error rate = 0.111

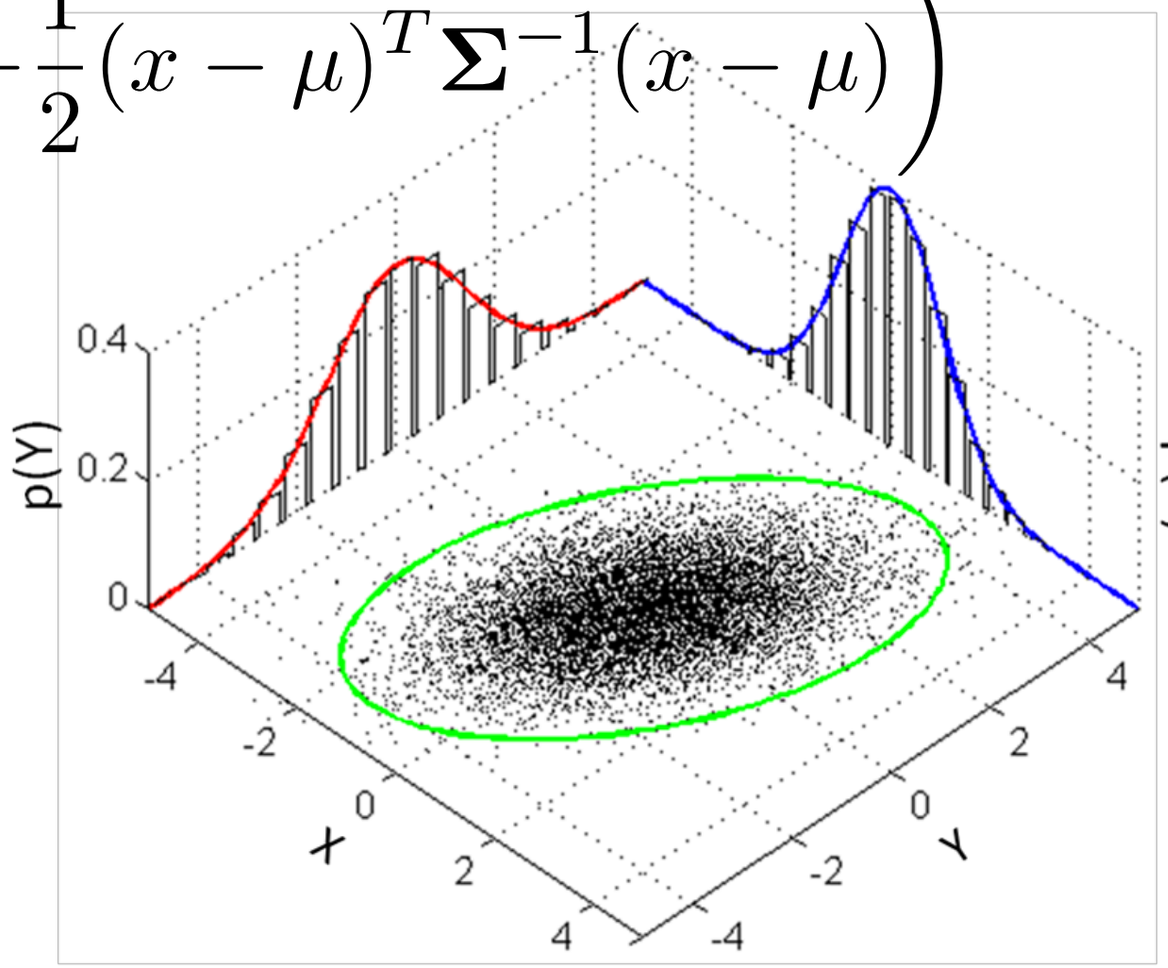
Linear Discriminant Analysis - multiple predictors - p>1



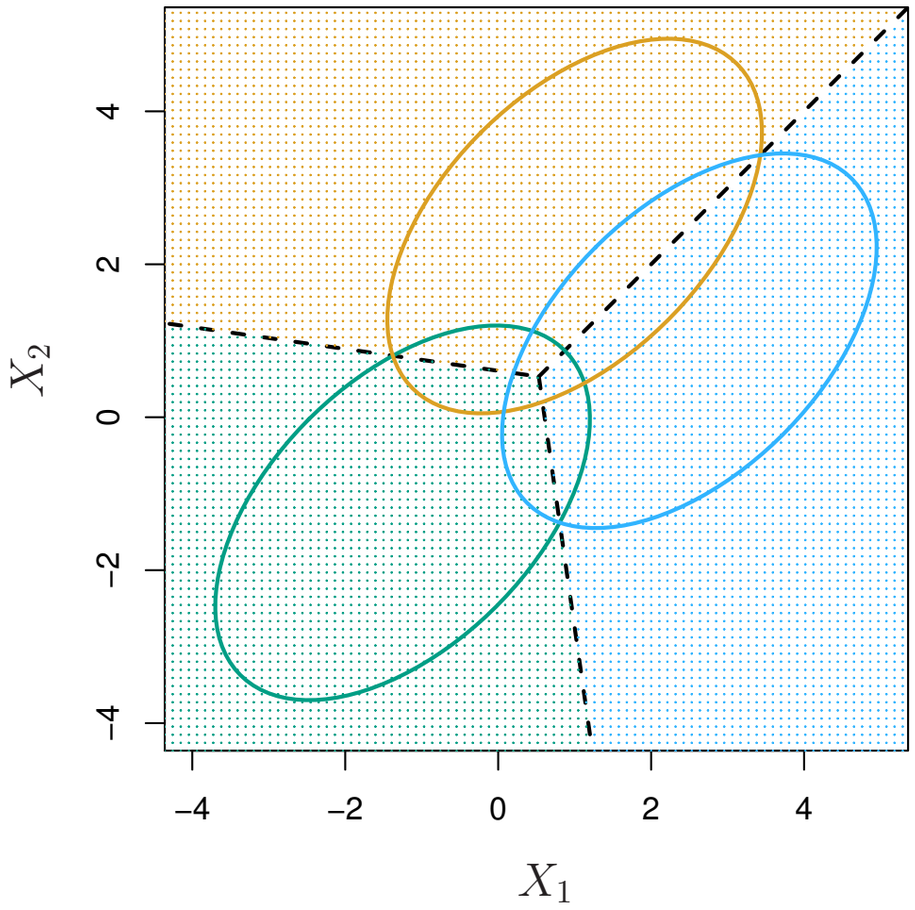


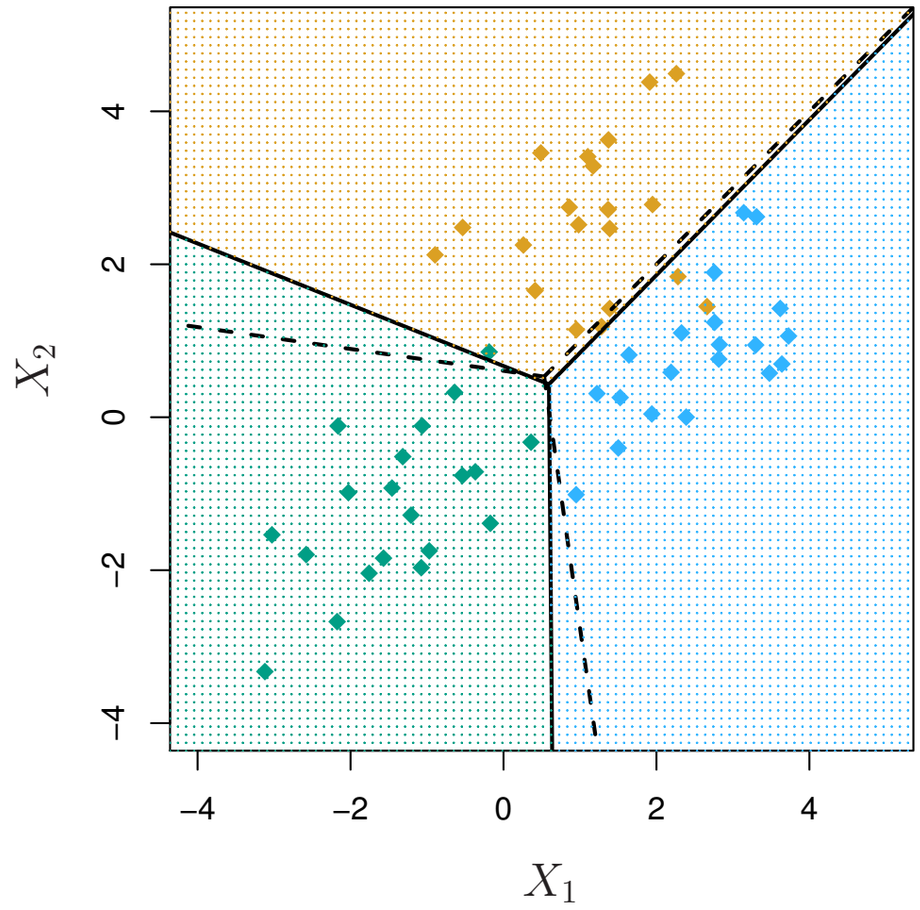
$$f_k(x) = \frac{1}{\sqrt{(2\pi)^p \det \mathbf{\Sigma}}} \exp\left(-\frac{1}{2}(x-\mu)^T \mathbf{\Sigma}^{-1}(x-\mu)\right)$$

- multivariate Gaussian distribution



Linear Discriminant Analysis - multiple predictors - p>1



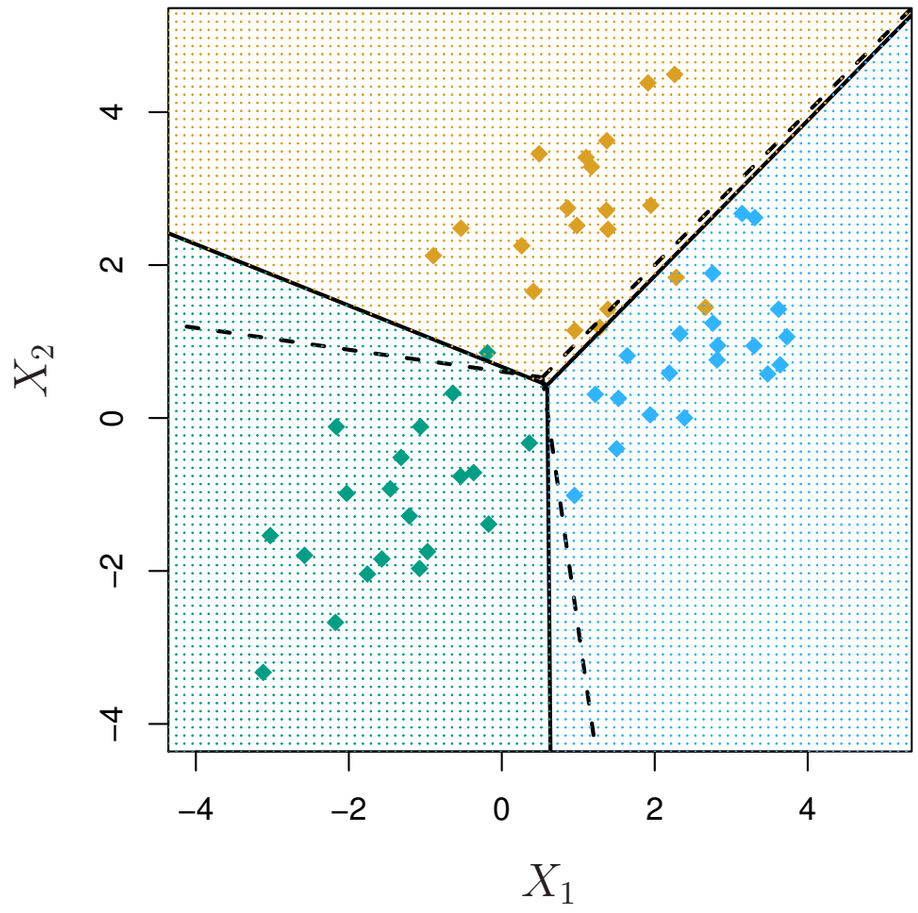


- our rule is that, given predictor x we assign class k with highest $p_k(x)$. This is the one with largest:

$$\hat{\delta}_k(x) = x^T \hat{\mathbf{\Sigma}}^{-1} \mu_k - \frac{1}{2} \mu_k^T \hat{\mathbf{\Sigma}}^{-1} \mu_k + \log \hat{\pi}_k$$

and the decision boundaries for: $\hat{\delta}_k(x) = \hat{\delta}_l(x)$

Linear Discriminant Analysis - multiple predictors - p>1



Bayes error rate = 0.0746
LDA error rate = 0.0770

- our rule is that, given predictor x we assign class k with highest $p_k(x)$. This is the one with largest:

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and the decision boundaries for: $\hat{\delta}_k(x) = \hat{\delta}_l(x)$

What if the classes are not balanced?

- example: default data - consider weather an individual will default on his credit card payment (based on income, credit card balance, student or not) for a sample of 10 000

p=3, K=2

With LDA -> for training data

		True deafault status		
		No	Yes	Total
Predicted default status	No	9 644	252	9 896
	Yes	23	81	104
	Total	9 667	333	10 000

- training error rate 2,75 % (= (252 +23)/10000) low, but:
- only 3,33 % defaulted, so if we always say no, we achieve almost the same result!
- Two types of error here: **False Positive error rate 23 / 9667 ~ 0,24%** and **False Negative 252 / 333 ~ 75,7%** **!**
- The cost of different types of errors needs to be considered
- The Bayes classifier has the lowest **TOTAL** error rate

What if the classes are not balanced?

- Instead of assigning class for which posterior is greatest, for K=2:

$$P(\text{default} = \text{Yes}|X = x) > 0.5$$

- we assign when

$$P(\text{default} = \text{Yes}|X = x) > 0.2$$

Now **False Negative error rate 138 / 333 ~ 41,4%**

		True deafault status		
		No	Yes	Total
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	Yes	23	81	104
	Total	9 667	333	10 000

		True deafault status		
		No	Yes	Total
Predicted default status	No	9 432	138	9 570
	Yes	235	195	430
	Total	9 667	333	10 000

What if the classes are not balanced? -tresholds

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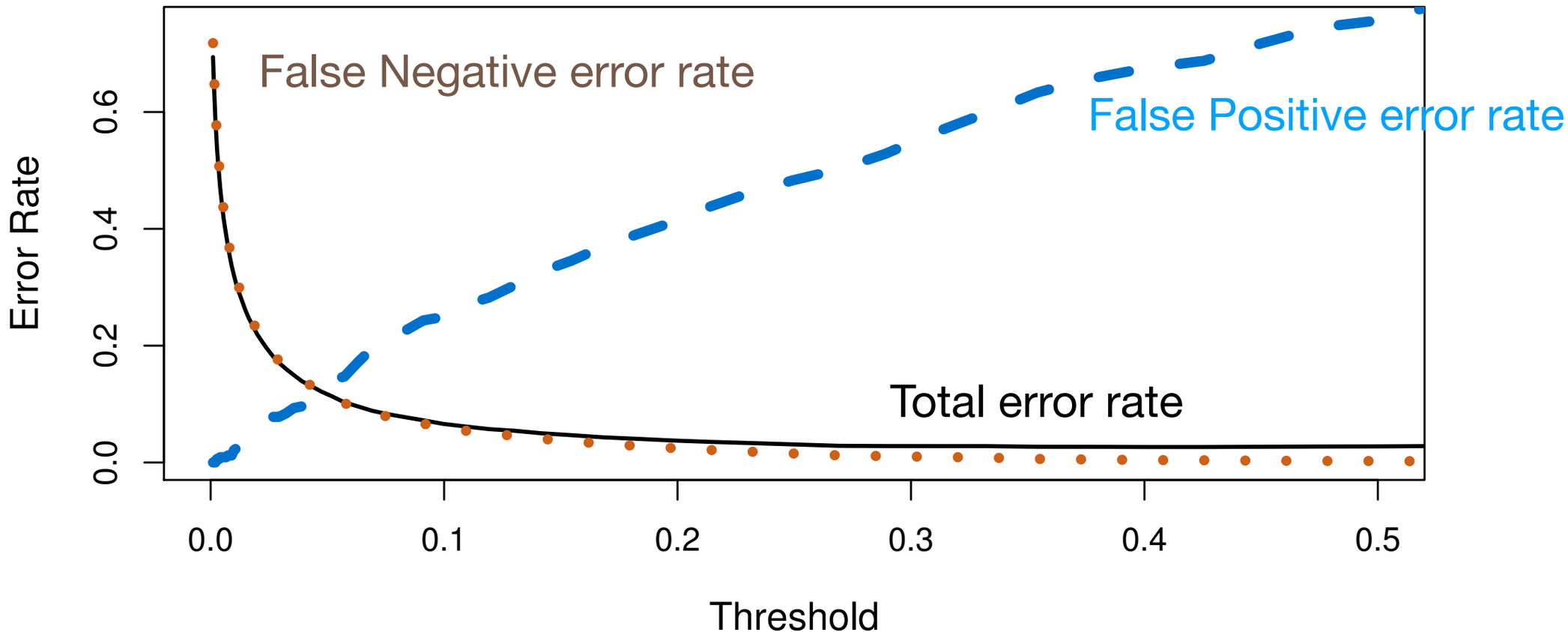
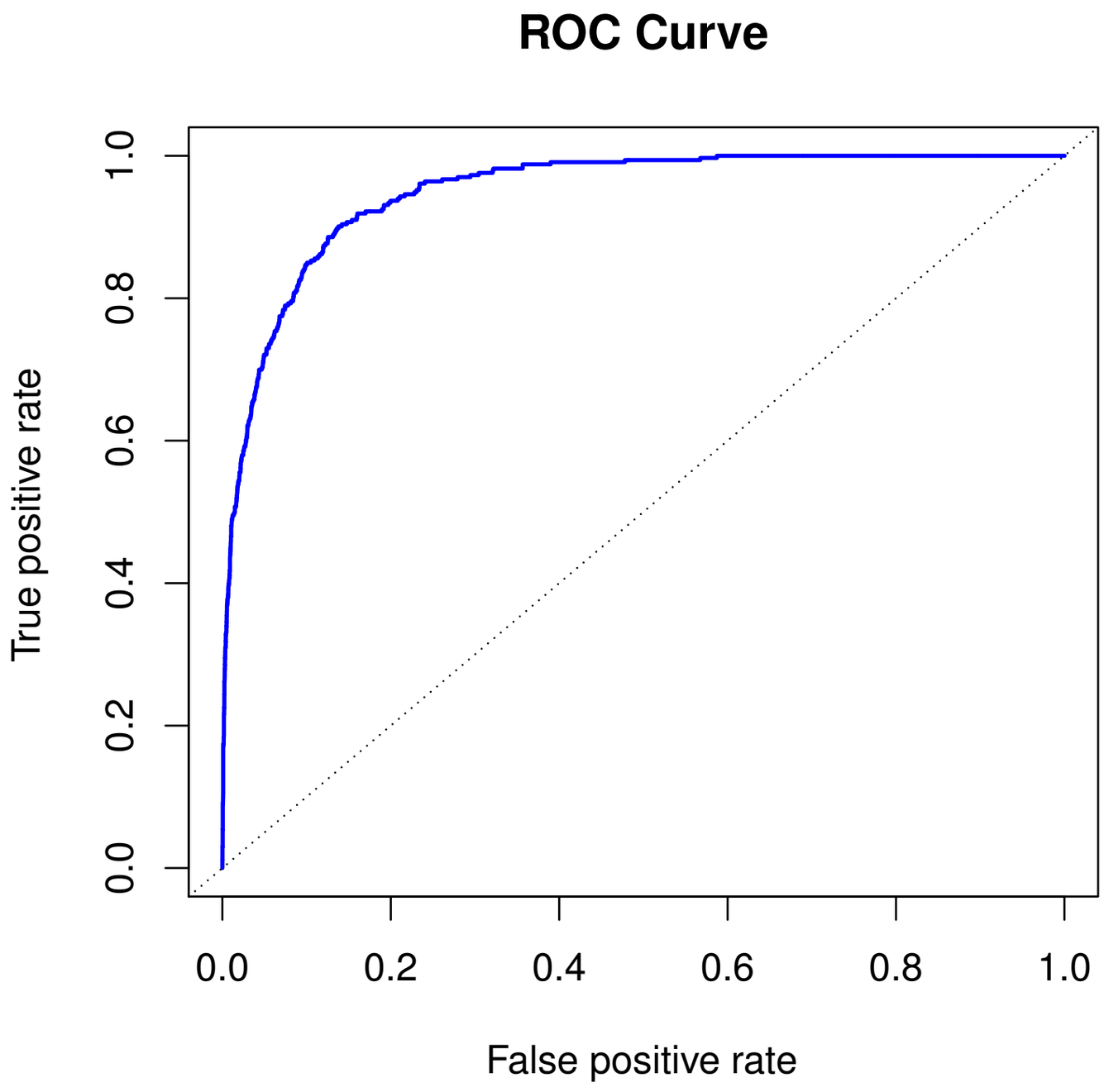


What if the classes are not balanced? - naming and measures

		Predicted class		
		- or Null	+ or Non-null	Total
True class	- or Null	True Neg. (TN)	False Pos. (FP)	N
	+ or Non-null	False Neg. (FN)	True Pos. (TP)	P
	Total	N*	P*	

Name	Definition	Synonyms
False Pos. Rate	FP/N	Type I error
True Pos. Rate	TP/P	Type II error, power, sensitivity, recall
Pos. Pred. value	TP/P*	Precision
Neg. Pred. value	TN/N*	
Specificity	1-FP/N	
False discovery proportion	1-TP/P*	
F1 score	2 TP/ (P* + P)	
Accuracy	(TP+TN)/(N+P)	

What if the classes are not balanced? - ROC curve



- ROC curve (receiver operating characteristics -historic name)
- AUC - area under curve, hear 0.95 for LDA, train data. 0.5 for random - measure of accuracy independent of threshold
- Calculate both for training and test data

Quadratic Discriminant Analysis

- LDA - (probabilities of x in specific class) multivariate Gaussians with class specific mean and common covariance matrix

- what if we make covariance class specific?

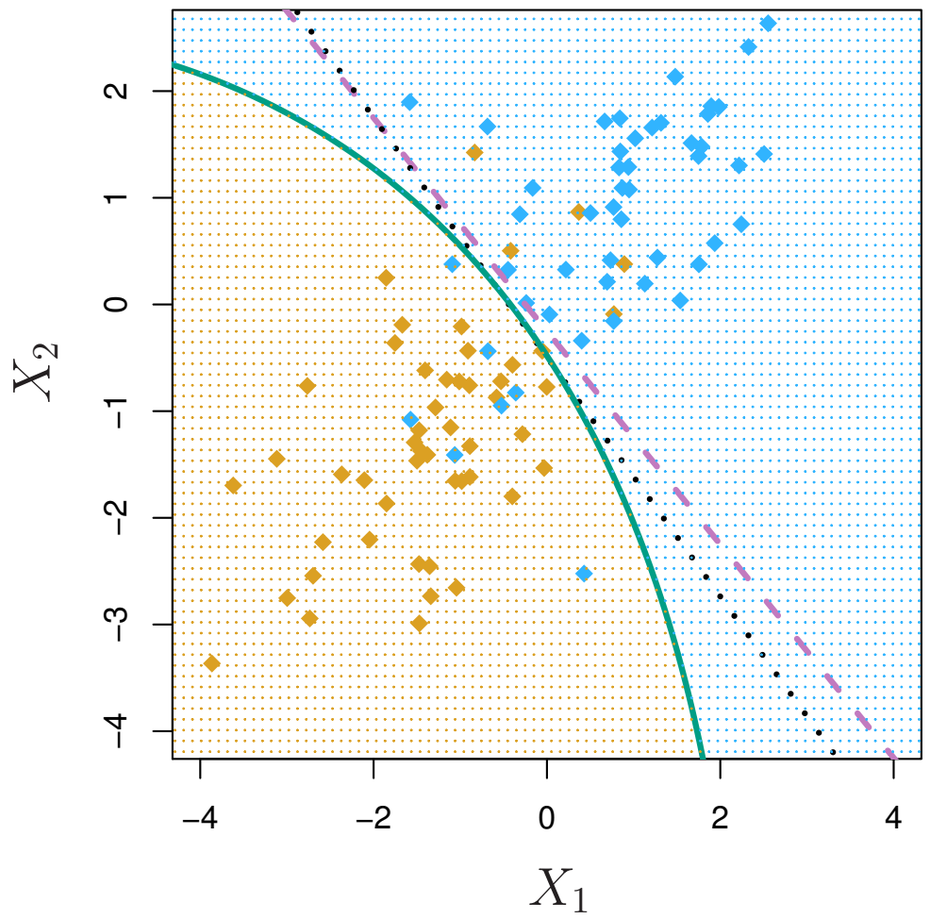
$$\hat{\delta}_k(x) = -\frac{1}{2}x^T\hat{\mathbf{\Sigma}}_k^{-1}x + x^T\hat{\mathbf{\Sigma}}_k^{-1}\mu_k - \frac{1}{2}\mu_k^T\hat{\mathbf{\Sigma}}_k^{-1}\mu_k - \frac{1}{2}\log|\det\hat{\mathbf{\Sigma}}_k| + \log\hat{\pi}_k$$

- QDA - Quadratic discriminant analysis

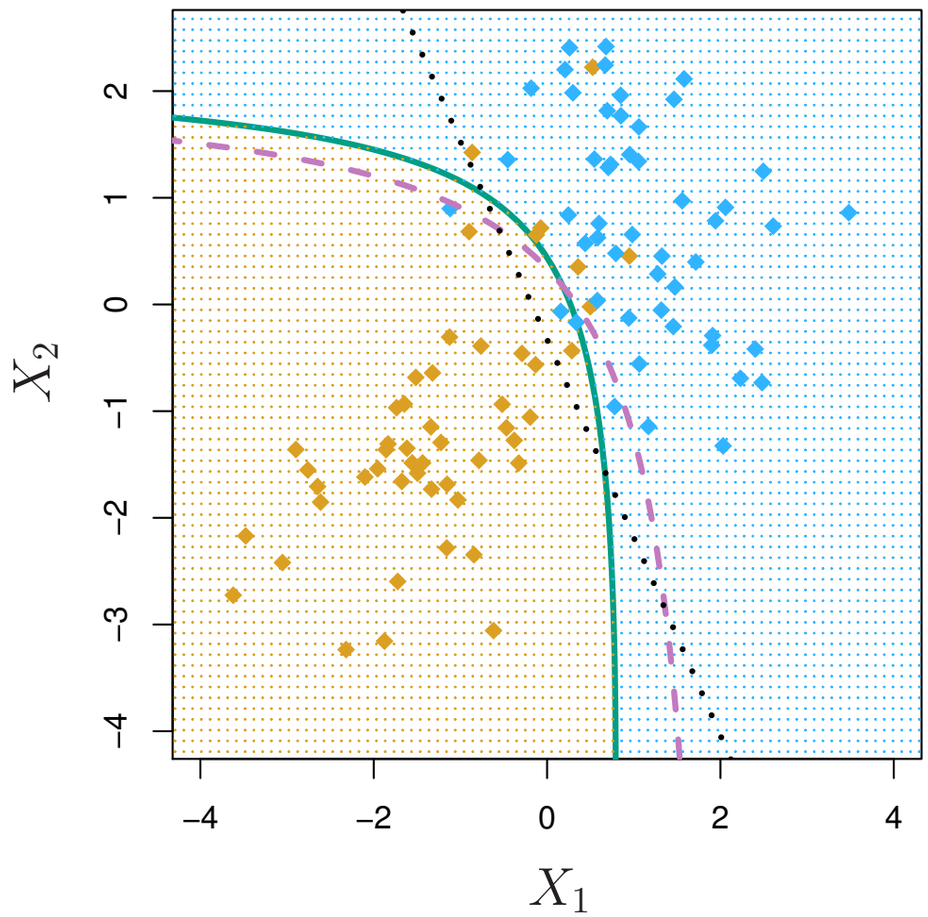
- note, for p predictors, p(p+1)/2 parameters for covariance matrix, times K for classes. LDA, a lot less.

- This translates into more flexibility but more likely overfitting if the p large and n comparably not so

Quadratic vs. Linear Discriminant Analysis



- same cov. of 0.7
- Bayes dec. boundary linear (in violet)
- QDA inferior



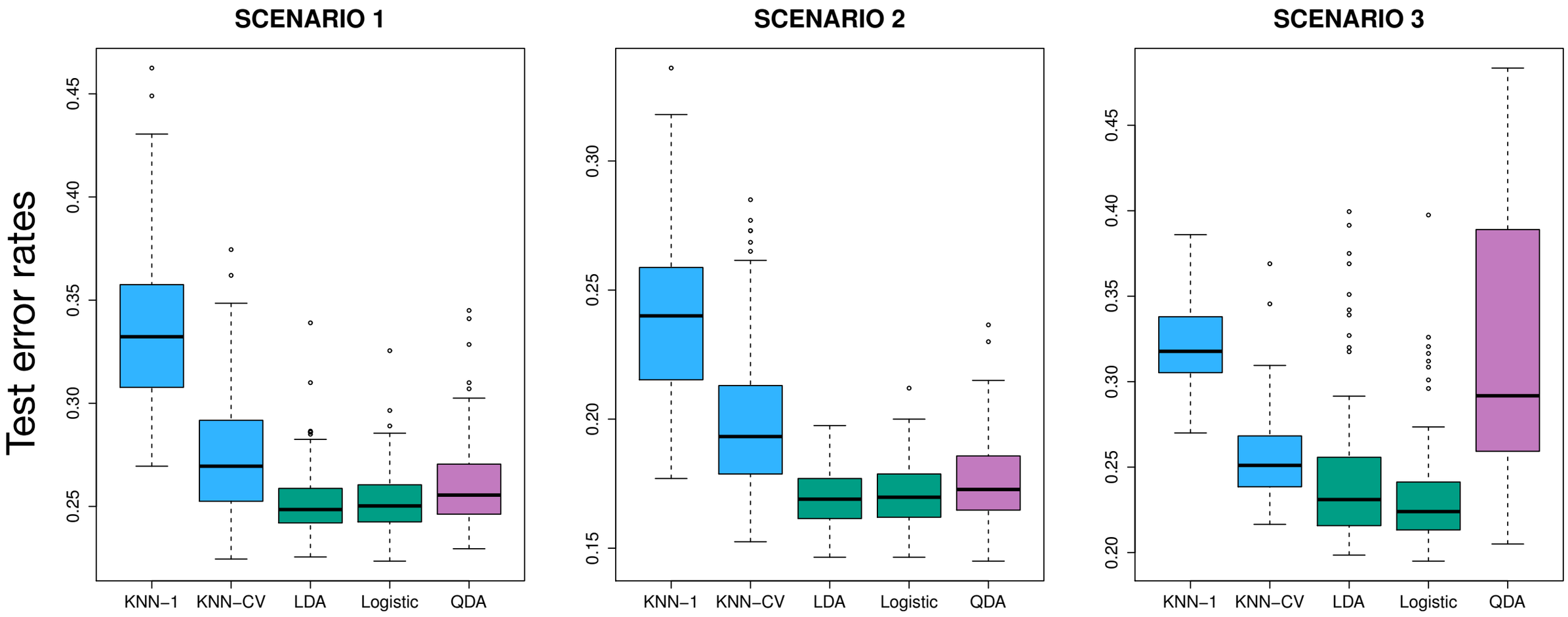
- cov. 0.7 and -0.7
- Bayes dec. boundary quadratic
- QDA superior

Comparison of KNN, Logistic Reg., LDA and QDA

- LDA and Log Reg - linear boundaries, different fitting.
- But, LDA Gaussianity assumption
- KNN completely non-parametric - no assumption about shape of decision boundary - dominates if db highly nonlinear
- but, we don’t now which predictors important like with Log reg.
- QDA a compromise between KNN and linear approaches

- 6 scenarios
- 100 random training data sets each
- 3 linear db
- 3 nonlinear db
- KNN with K=1 and based on a validation approach
- p=2 predictors

Comparison of KNN, Logistic Reg., LDA and QDA

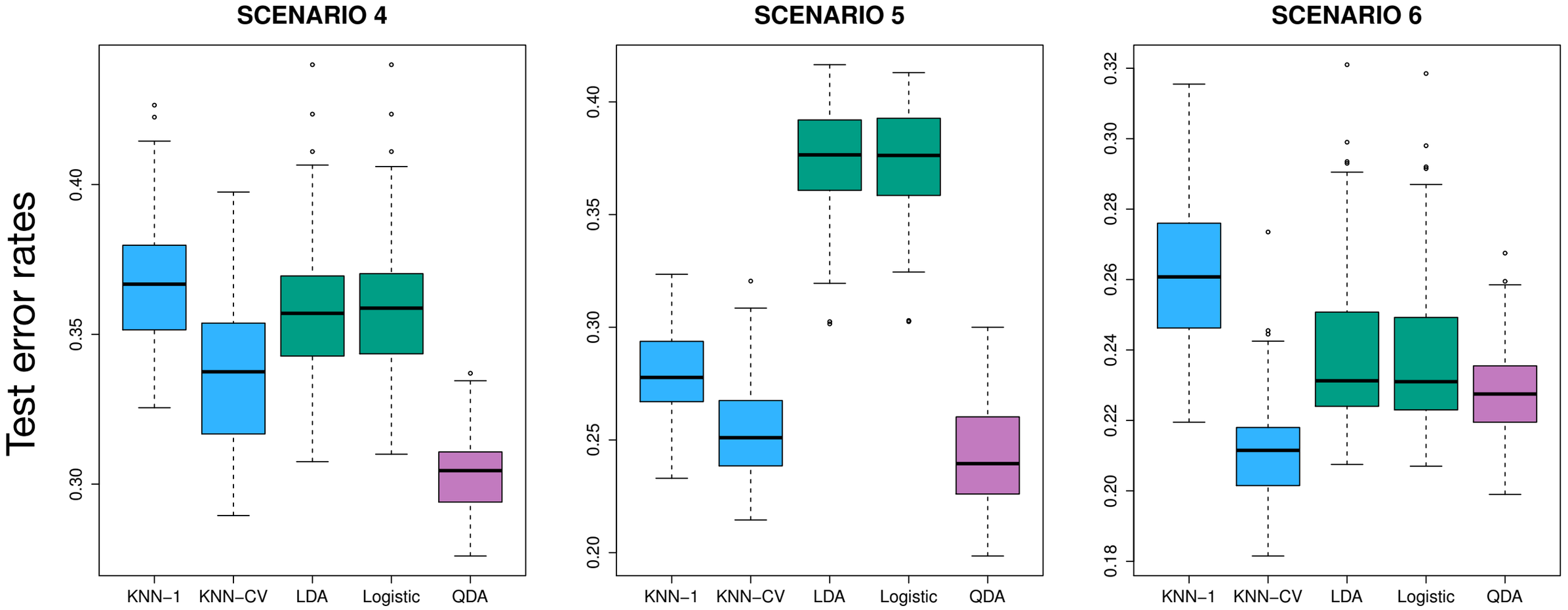


- 20 observation in each class
- uncorrelated normal
- different mean

- same, but
- predictors correlated with -0.5

- 50 observation in each class
- heavier distribution tails (non-normality)

Comparison of KNN, Logistic Reg., LDA and QDA



- normal
- correlations 0.5 and -0.5

- x1 and x2 normal
- uncorrelated
- but predictors x1^2, x2^2 and x1 x2

- highly non-linear db

One final model - Naive (or Simple, Independence) Bayes

- **strong assumption: predictors are uncorrelated (independent)**

$$p_k(x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}$$

- look for k such that max

$$f_k(X) \equiv P(X = x|Y = k) = \prod_{i=1}^{p} P(x_i|Y = k)$$

discrete case: $$P(x_i|Y = k) = \frac{\sharp D\{X = x_i \wedge Y = k\}}{\sharp D\{Y = k\}}$$

- Fast, also for K>2, scales well to high n, requires small amount of data
- When assumption of independence holds, a Naive Bayes classifier performs better compare to other models like logistic regression and you need less training data.
- Good for high dimensional data when model complexity not important
- For continuous predictors use independent continuous distributions (ex.: Gaussian (NB)) (and estimate its parameters)
- in applications, smoothing (Laplace j=1) required to get reasonable results if the training data doesn't include any points from some class(es)

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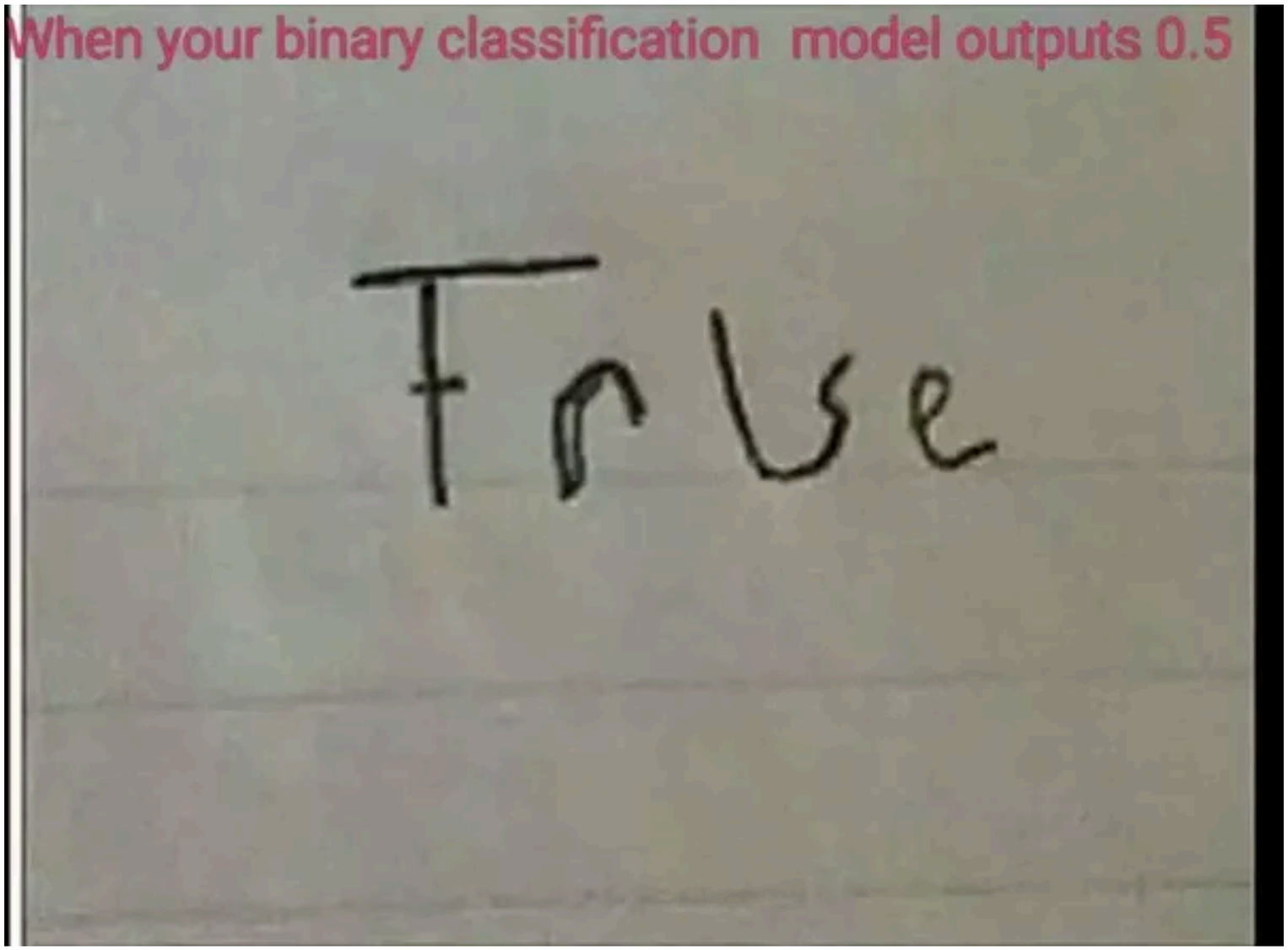

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