

# **Applied Data Science**

## **Machine Learning Lecture 3**

**John Tsitsiklis  
June 14, 2024**

# Today's agenda — Classification

---

- The general problem
  - formulation
  - types of error
- Model-based (Gaussian and Bayesian)
  - linear discriminant analysis
  - quadratic discriminant analysis
- Logistic regression
- Other approaches
  - Nearest-neighbor methods

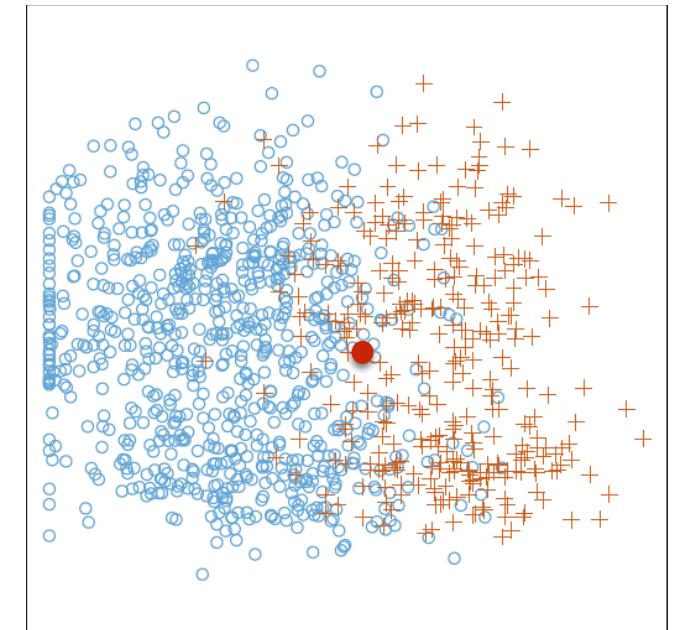
## The general context — applications

$X_1$	$Y_1$
$\vdots$	$\vdots$
$X_n$	$Y_n$
<hr/>	
$X$	$Y?$

- Classify a data record into one of multiple categories, based on examples

$Y = 0, 1$  (binary)

$Y = 1, \dots, m$  ( $m$ -ary)



$X$ : symptoms, test results

$Y$ : cancer?

$X$ : an email message

$Y$ : spam?

$X$ : image of a digit  $Y$

$Y$ : which digit is it? ( $m = 10$ )

$X$ : image of an animal  $Y$

$Y$ : cat, dog, cow, ...

## Example: prediction of loan default

---

$Y$	$X_1$	$X_2$	$X_3$
default	student	balance	income
No	No	729.5265	44361.63
No	Yes	817.1804	12106.13
No	No	1073.549	31767.14
No	No	529.2506	35704.49
No	No	785.6559	38463.5
No	Yes	919.5885	7491.559
No	No	825.5133	24905.23
No	Yes	808.6675	17600.45
No	No	1161.058	37468.53

- 10,000 samples
  - 3.33% of the samples represent defaults
- encoding: “No” = 0, “Yes” = 1”

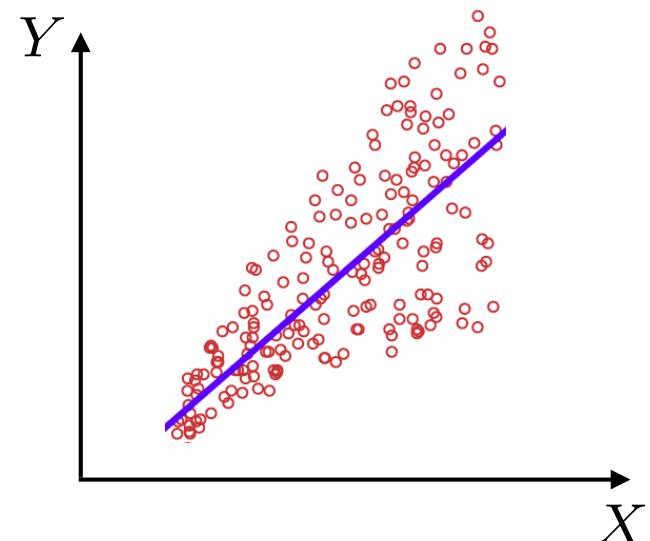
## Predictors and classifiers

---

- In regression:

predictor  $\hat{Y} = g(\mathbf{X})$

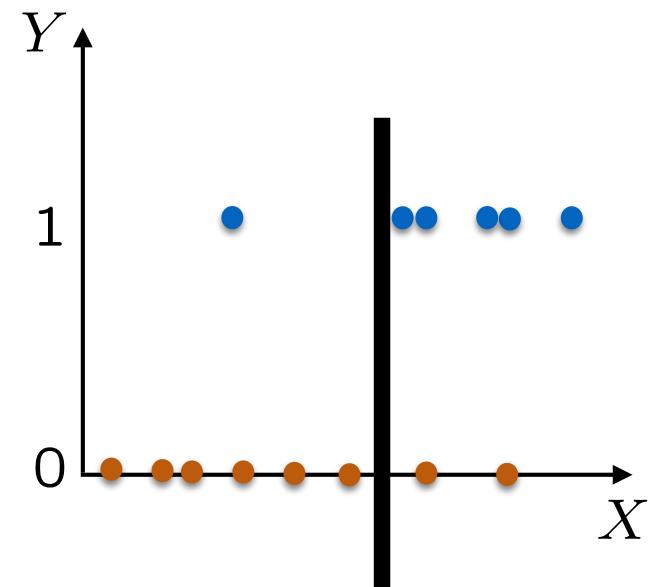
metric  $\mathbb{E}[(\hat{Y} - Y)^2]$



- In classification:

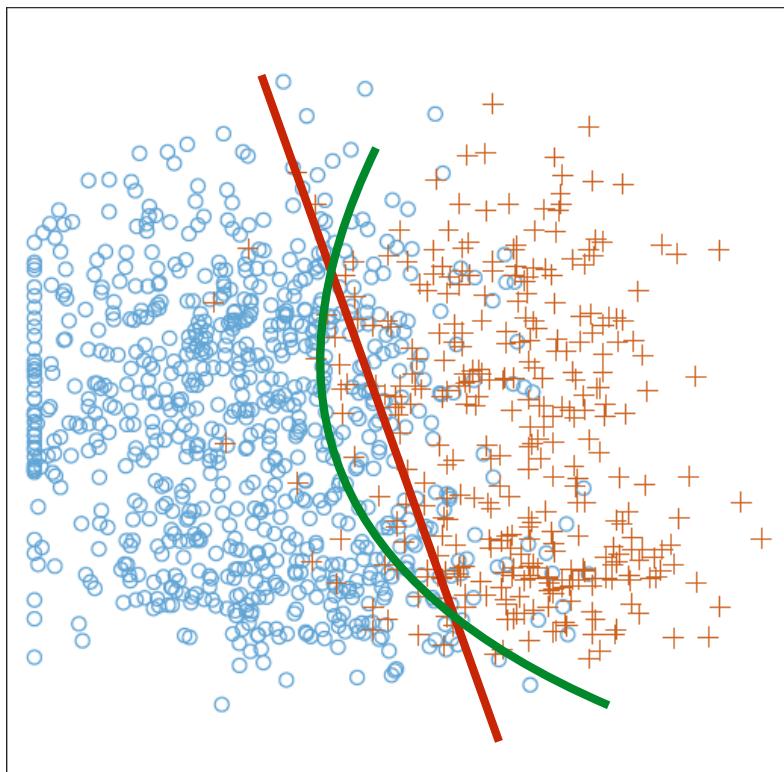
classifier  $\hat{Y} = g(\mathbf{X}) \in \{1, \dots, m\}$

metric  $\mathbb{P}(\text{mistake})$



## Types of classifiers

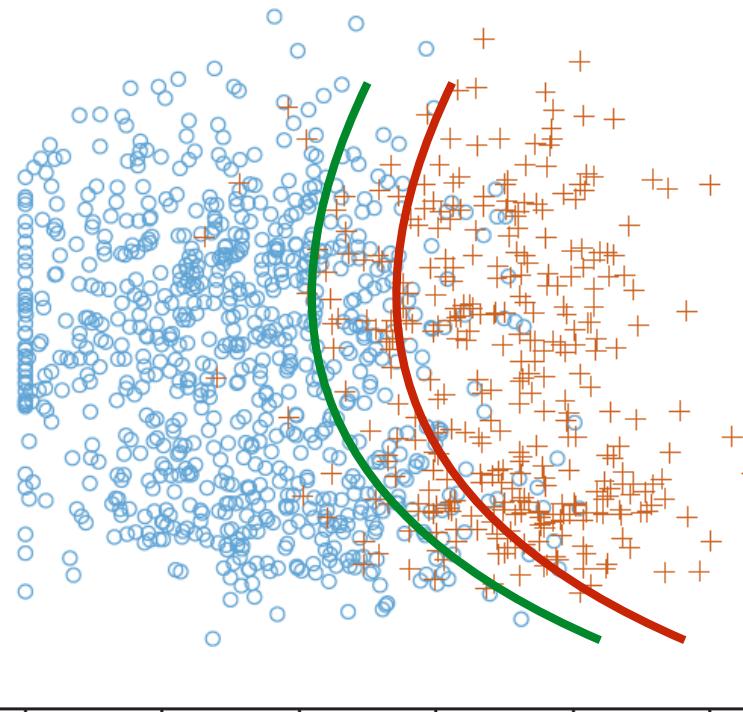
---



- **Linear classifiers:** compare  $\theta^T \mathbf{X}$  to a threshold
  - learn “good” vector  $\theta$  and threshold
- **Nonlinear classifiers:** compare  $h(\mathbf{X})$  to a threshold
  - learn “good” function  $h$  and threshold

- Nonlinear classifier  $\theta_1 X_1 + \theta_2 X_2 + \theta_{12} X_1 X_2$  is actually **linear** if we redefine  $\mathbf{X} = (X_1, X_2, X_1 X_2)$
- **Feature-based linear classifier:** compare  $\theta^T \phi(\mathbf{X})$  to a threshold

# Error types and confusion matrix



- Interested in having few errors on new data records
- Aim at few errors on training set
- Tradeoff between the two error types
- Similar **confusion matrix**, for  $m$ -ary classification

- Binary classification, two error types:  
truth is “blue”, decide  $\hat{Y} = “brown”$   
truth is “brown”, decide  $\hat{Y} = “blue”$

		True labels	
		blue	brown
Predicted labels	blue	✓	✗
	brown	✗	✓

		True labels	
		good	default
Predicted labels	good	9644	252
	default	23	81

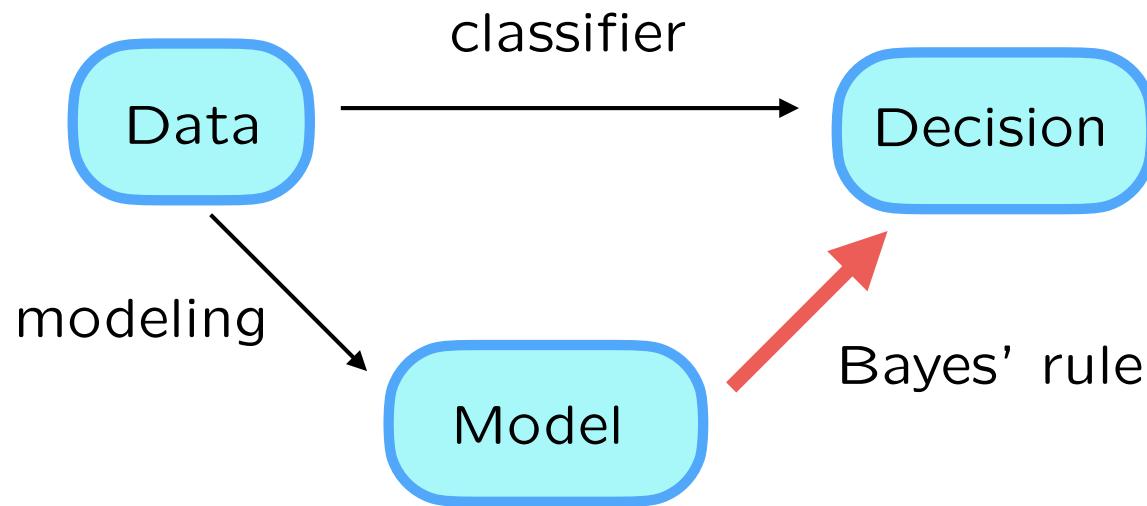
Jargon: accuracy, precision, recall, sensitivity, specificity, false alarm,...

## **(GAUSSIAN) MODEL-BASED APPROACH**

This file is meant for personal use by patgrinwald@gmail.com only.  
Sharing or publishing the contents in part or full is liable for legal action.

## The model-based approach

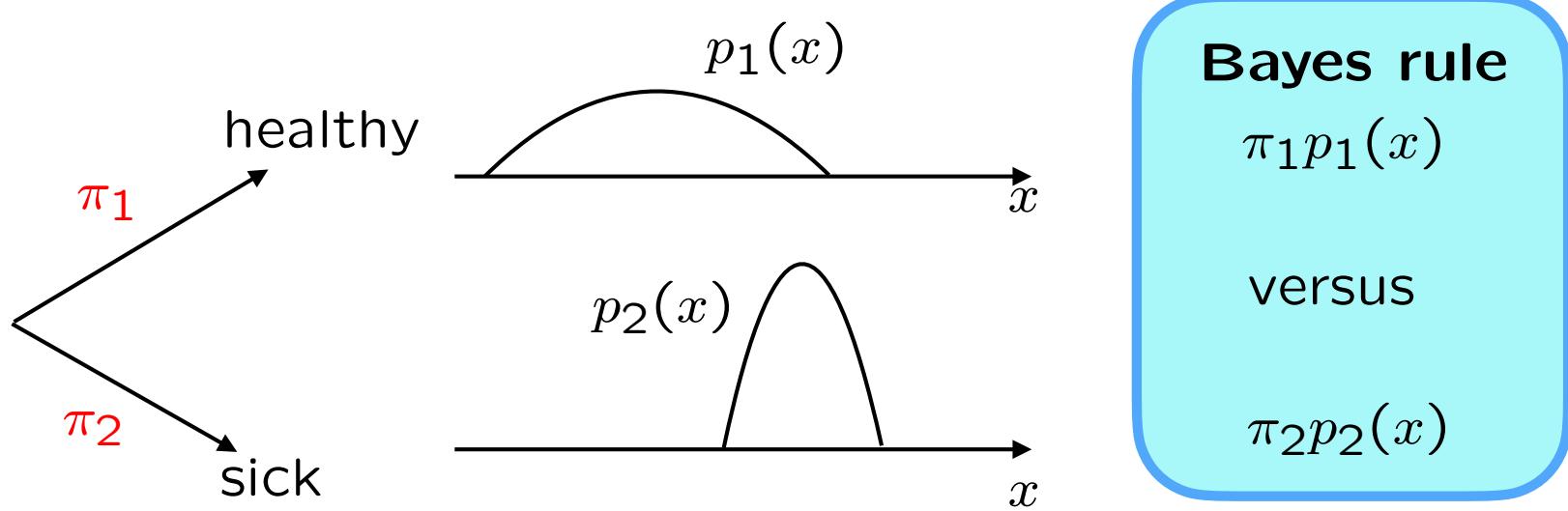
---



Gaussian “generative” model

Apply (and exemplify) the Bayes’ rule, in this context

# The Bayesian model-based approach in pictures



**example/data-driven method**

assume

$$N(\mu_1, \sigma_1^2) \longrightarrow \mu_1, \sigma_1^2$$
$$N(\mu_2, \sigma_2^2) \longrightarrow \mu_2, \sigma_2^2$$

- Generalize
  - more classes
  - higher-dimensional feature vectors  $\mathbf{X}$

# Gaussian model

- $\mathbb{P}(Y = k) = \pi_k \quad (k = 1, \dots, m)$  “prior” probabilities

- $\mathbb{P}(\mathbf{X} | Y = k) \sim N(\boldsymbol{\mu}_k, C_k)$

$$\gamma_k \cdot \exp \left\{ -\frac{(X - \mu_k)^2}{2\sigma_k^2} \right\}$$

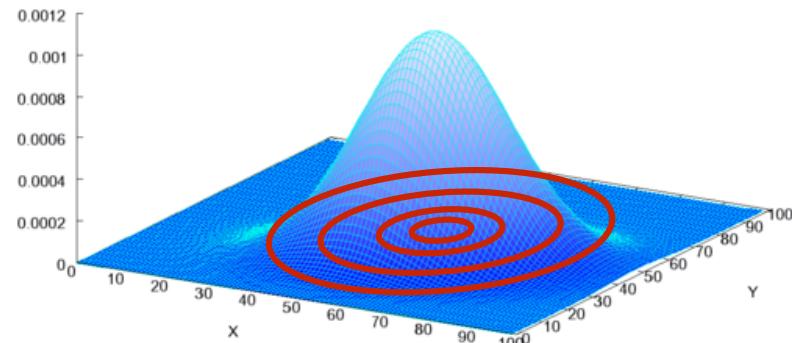
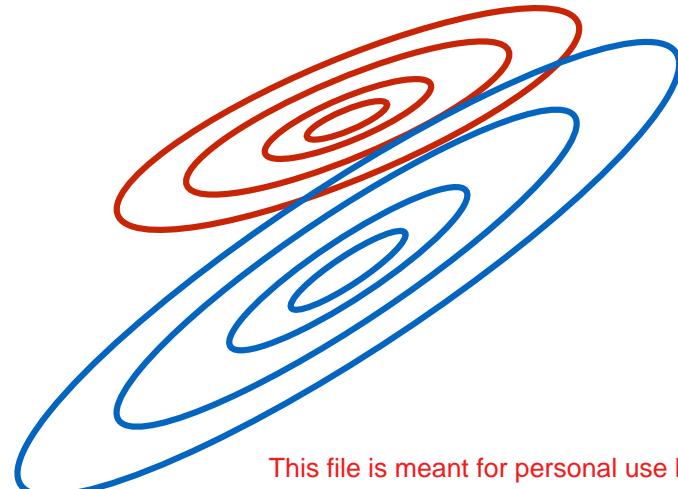
$\boldsymbol{\mu}_k$ : mean vector  $\mathbb{E}[\mathbf{X} | Y = k]$

$$\gamma_k \cdot \exp \left\{ -\frac{1}{2}(\mathbf{X} - \boldsymbol{\mu}_k)^T C_k^{-1} (\mathbf{X} - \boldsymbol{\mu}_k) \right\}$$

$C_k$ : covariance matrix  $[\text{Cov}(X_i, X_j)]$   
for class  $k$

$$\text{Cov}(Y, Z) = \rho \cdot \sigma_Y \cdot \sigma_Z$$

correlation



## The modeling part — for class $k$

---

- $\mathbb{P}(Y = k) = \pi_k$

$$\hat{\pi}_k = \frac{\text{\# samples of class } k}{\text{total \# of samples}}$$

- $\mu_k = \mathbb{E}[\mathbf{X} | Y = k]$

$\hat{\mu}_k$  = average value of  $\mathbf{X}$   
over all samples of class  $k$

- $C_k = \mathbb{E}[(\mathbf{X} - \mu_k)(\mathbf{X} - \mu_k)^T | Y = k]$

$\hat{C}_k$  = average value of  $(\mathbf{X} - \hat{\mu}_k)(\mathbf{X} - \hat{\mu}_k)^T$ ,  
over all samples of class  $k$

“plugin estimates”

(replace expectations with averages)

## Bayes' rule

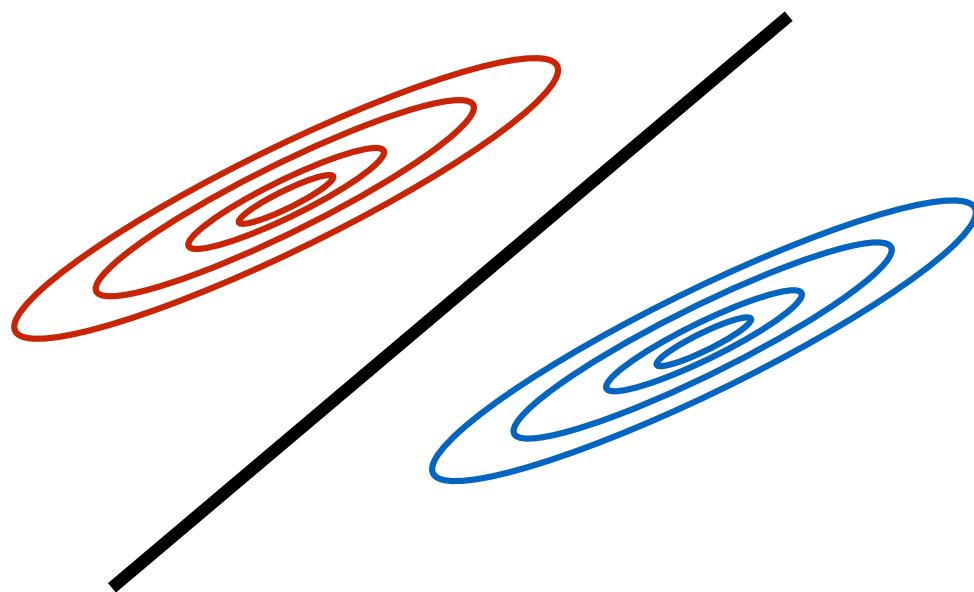
---

$$\mathbb{P}(Y = k | \mathbf{X}) = \frac{\pi_k \cdot \mathbb{P}(\mathbf{X} | Y = k)}{\mathbb{P}(\mathbf{X})} \quad (\text{posterior})$$

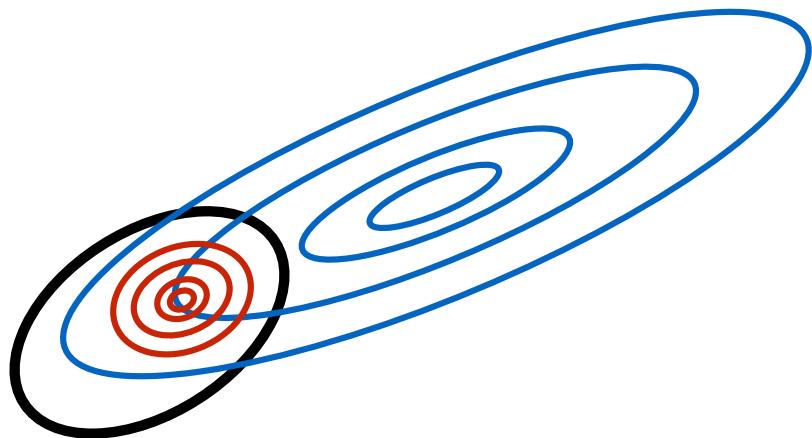
- Given value  $\mathbf{X}$ , choose  $k$  with largest posterior
  - minimizes  $\mathbb{P}(\text{error})$   $\pi_k \cdot \gamma_k \cdot \exp \left\{ -\frac{1}{2}(\mathbf{X} - \boldsymbol{\mu}_k)^T C_k^{-1}(\mathbf{X} - \boldsymbol{\mu}_k) \right\}$
- Quadratic discriminant analysis (QDA)  
Boundaries between regions described by quadratic functions
  - Compare  $\log(\pi_k \cdot \gamma_k) - \frac{1}{2}(\mathbf{X} - \boldsymbol{\mu}_k)^T C_k^{-1}(\mathbf{X} - \boldsymbol{\mu}_k)$ , for different classes  $k$ 
    - boundary: when same value for some  $k, k'$   $\rightarrow$  quadratic in  $\mathbf{X}$
- Linear discriminant analysis (LDA) all  $C_k = C$  (same)  
Boundaries are linear
  - When all  $C_k = C$  (same), second-order terms in  $\mathbf{X}$  are all the same
    - compare  $\log(\pi_k \cdot \gamma_k) - (\boldsymbol{\mu}_k)^T C^{-1}\mathbf{X} - \frac{1}{2}(\boldsymbol{\mu}_k)^T C^{-1}\boldsymbol{\mu}_k$ , for different  $k$ 
      - boundary: when same value for some  $k, k'$   $\rightarrow$  linear in  $\mathbf{X}$

## LDA versus QDA

---



different means  
same covariances



different means  
**different** covariances

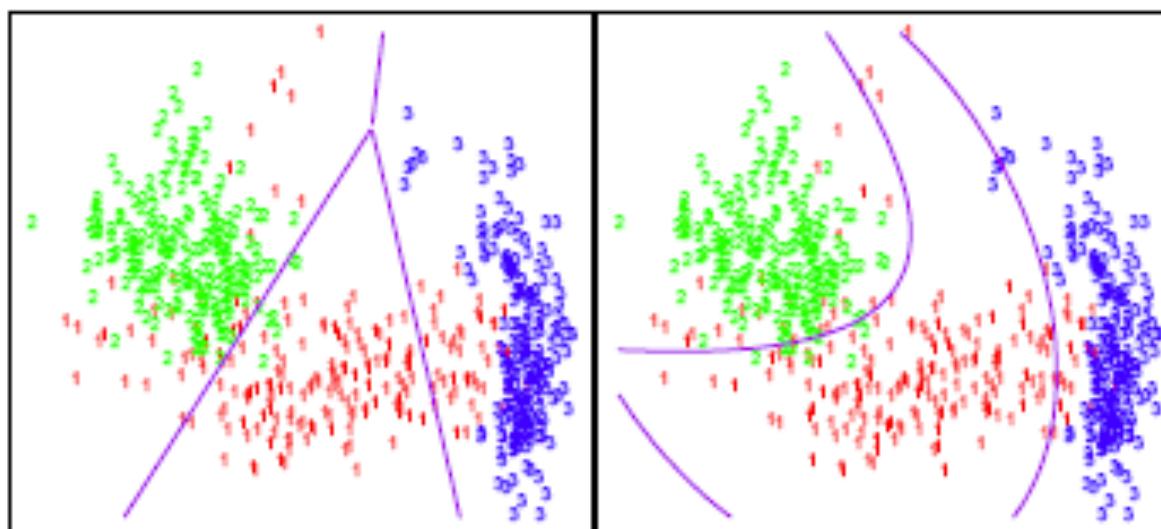
# LDA versus QDA

---

Assume

same versus different

covariances



LDA

QDA

## Prediction default example

---

- Performance on the training set
- Recall that only 3.33% of the records correspond to defaults
  - **Always decide "no default:"** Miss-classification rate 3.33%
- Make predictions using only one component of  $\mathbf{X}$  ("balance")
  - LDA: 2.81%
  - QDA: 2.73%
- Make predictions using all of  $\mathbf{X}$ 
  - LDA: 2.75%
  - QDA: 2.70%
- Should validate performance on a holdout set or through cross-validation 2.76%

		True labels	
		good	default
Predicted labels	good	9644	252
	default	23	81

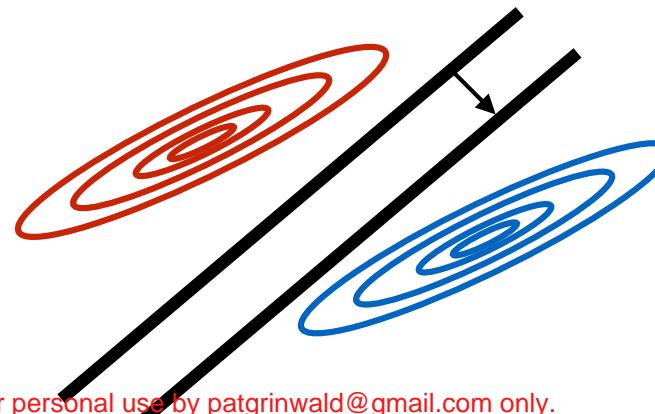
## Unbalanced costs

- some error types may be more costly

$$c_{\text{def}} \gg c_{\text{lost}}$$

		True labels	
		good	default
Predicted labels	good	9644	252 $c_{\text{def}}$
	default	23 $c_{\text{lost}}$	81

- $c_{\text{def}}$ : cost if  $\hat{Y} = \text{good}$  (give the loan) and  $Y = \text{default}$
- $c_{\text{lost}}$ : cost if  $\hat{Y} = \text{default}$  and  $Y = \text{good}$  (lost customer)
- Minimize probability of error versus **expected cost**:  
compare  $c_{\text{def}} \cdot \mathbb{P}(Y = \text{default} | \mathbf{X})$  to  $c_{\text{lost}} \cdot \mathbb{P}(Y = \text{good} | \mathbf{X})$
- Shifts the thresholds



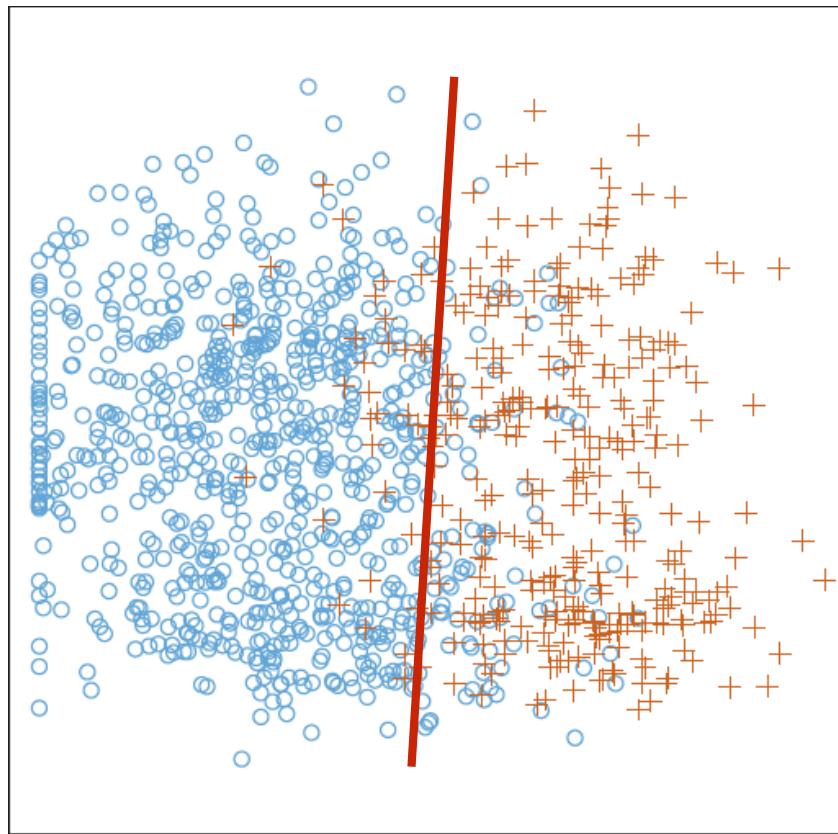
# **LEARNING/REGRESSION METHODS FOR CLASSIFICATION**

This file is meant for personal use by patgrinwald@gmail.com only.  
Sharing or publishing the contents in part or full is liable for legal action.

## An approach that does not work

---

- Restrict to special family of classifiers (e.g., linear)
  - find classifier with **fewest missclassified samples**
  - computationally intractable



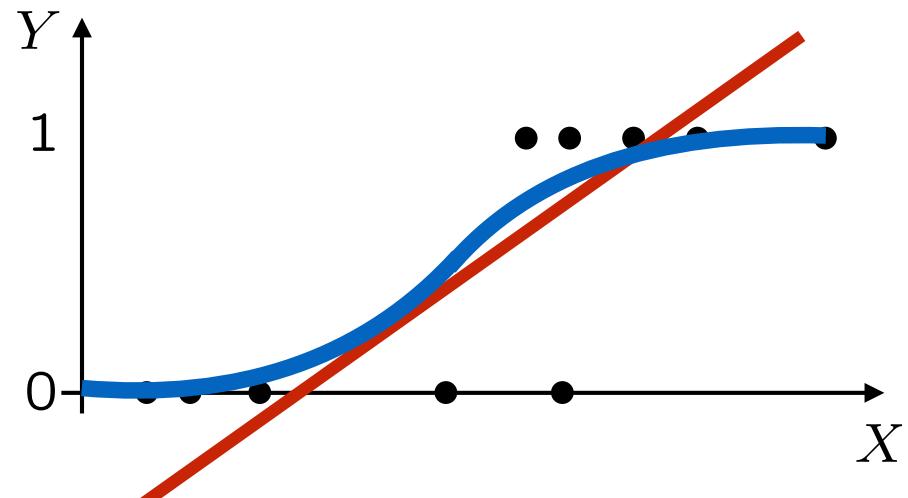
## An attempt to use regression

---

- Regress  $Y$  on  $\mathbf{X}$

$$\min_{\theta} \sum_i (Y_i - \theta^T \mathbf{X}_i)^2$$

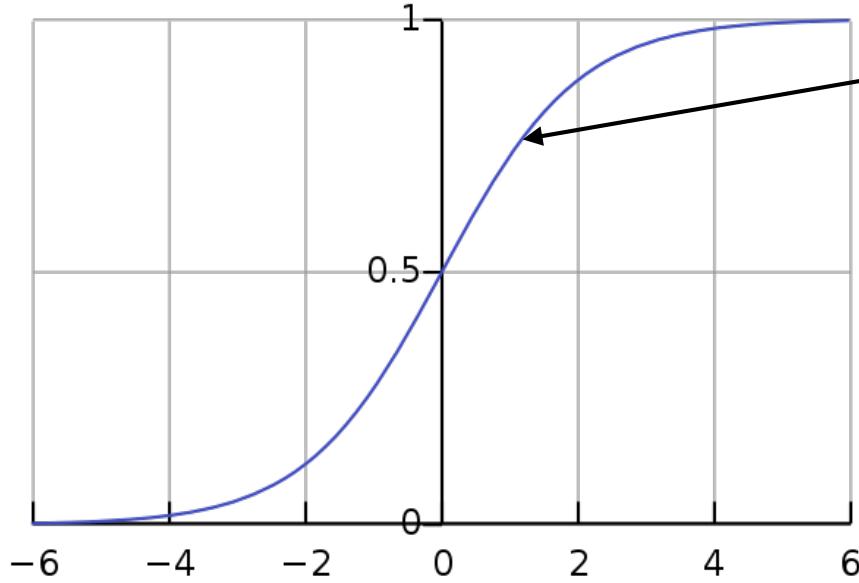
- predict  $\hat{Y} = 1$  if  $\hat{\theta}^T \mathbf{X} \geq 0.5$



- error criterion is not meaningful

- **A better idea:** Fit a curve that ranges between 0 and 1 (must be nonlinear)
- interpret as (estimated) probability  $\mathbb{P}(Y = 1 | \mathbf{X})$

# The logistic model



$$\frac{e^x}{e^x + e^{-x}}$$

shift and scale

$$\frac{e^{\theta_1 x}}{e^{\theta_0 x} + e^{\theta_1 x}}$$

$$\mathbb{P}(Y = 1 | x)$$

$$\frac{e^{\theta_0 x}}{e^{\theta_0 x} + e^{\theta_1 x}}$$

$$\mathbb{P}(Y = 0 | x)$$

$$\mathbb{P}(Y = k | \mathbf{X}) \sim e^{\theta_k x}$$

- Assume model of the form

$$\mathbb{P}(Y = k | \mathbf{X}) = \frac{\exp\{\boldsymbol{\theta}_k^T \mathbf{X}\}}{\sum_s \exp\{\boldsymbol{\theta}_s^T \mathbf{X}\}}$$

- Use the data to find “best-fitting” vectors  $\hat{\boldsymbol{\theta}}_1, \dots, \hat{\boldsymbol{\theta}}_m$
- Decision rule: choose class  $k$  with biggest  $\hat{\boldsymbol{\theta}}_k^T \mathbf{X}$  **linear!**
- But we do not have training data for these **probabilities**

## Training the logistic model: maximum likelihood $\max_{\theta} L(\text{data}; \theta)$

---

- Assume the  $\mathbf{X}_i$  are somehow set (random or otherwise)
- Assume the model structure  $\mathbb{P}(Y = k | \mathbf{X}) = \frac{\exp\{\boldsymbol{\theta}_k^T \mathbf{X}\}}{\sum_s \exp\{\boldsymbol{\theta}_s^T \mathbf{X}\}}$   
(+ independence)
- Likelihood function of the observed data  $L(\text{data}; \theta) = \prod_i \mathbb{P}(Y_i | \mathbf{X}_i)$
- Example data:  $(\mathbf{X}_1, 1), (\mathbf{X}_2, 0), (\mathbf{X}_3, 1)$   
$$L(\text{data}; \theta) = \mathbb{P}(Y = 1 | \mathbf{X}_1) \cdot \mathbb{P}(Y = 0 | \mathbf{X}_2) \cdot \mathbb{P}(Y = 1 | \mathbf{X}_3)$$
- $\log L(\text{data}; \theta) = \sum_{i \text{ of class 0}} \log \mathbb{P}(Y = 0 | \mathbf{X}_i) + \sum_{i \text{ of class 1}} \log \mathbb{P}(Y = 1 | \mathbf{X}_i)$
- “Messy, but:
  - convex
  - gradients are easy to calculate
  - efficient algorithms

## Comments, caveats

---

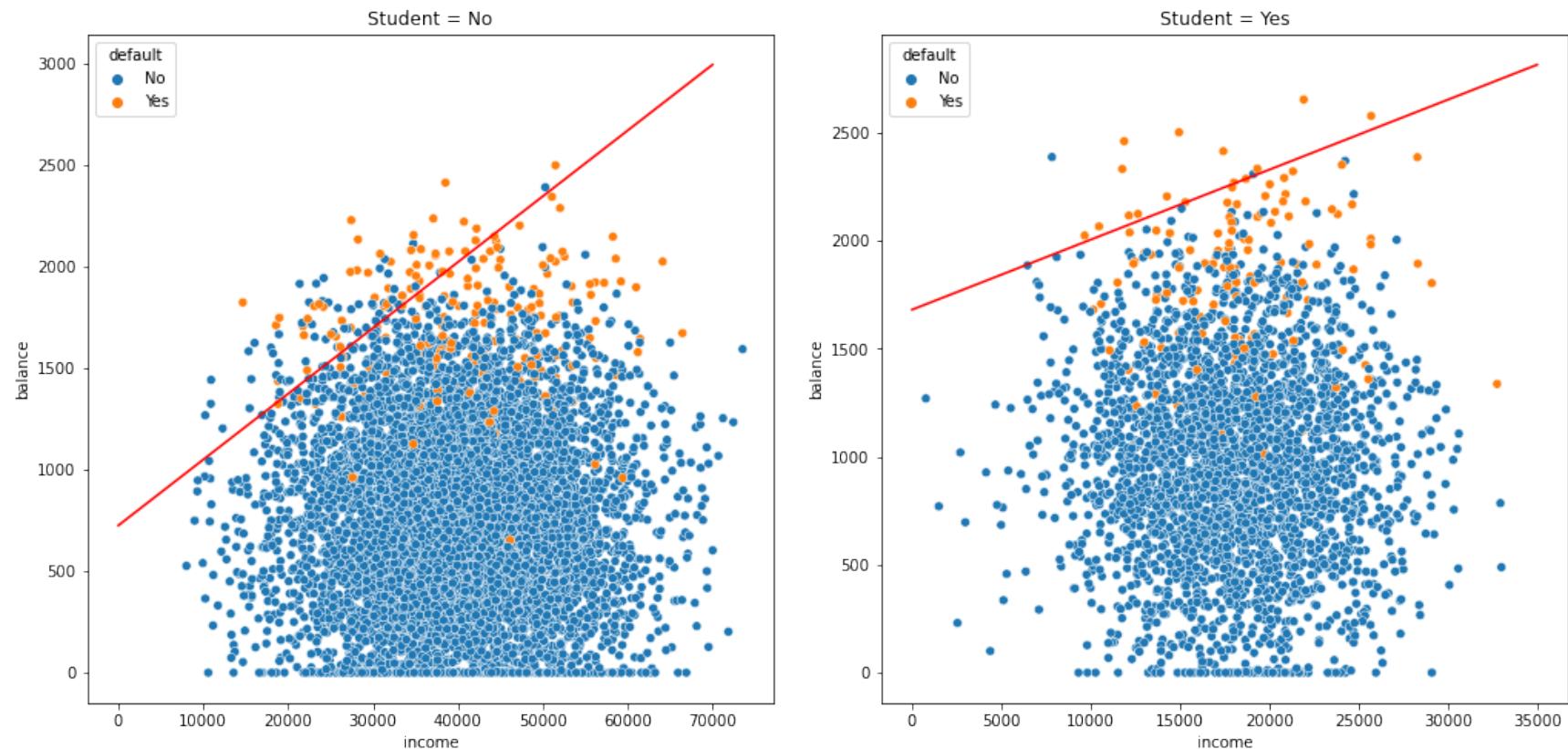
- Much from linear regression applies here too
- Good predictions do not imply causality
- Can use features  $\exp\{\boldsymbol{\theta}_k^T \mathbf{X}\} \longrightarrow \exp\{\boldsymbol{\theta}_k^T \phi(\mathbf{X})\}$
- Can add regularization terms
  - $\log L(\text{data}; \boldsymbol{\theta}) - \gamma \cdot \|\boldsymbol{\theta}\|^2$   
or sum of absolute values
  - tune hyperparameter  $\gamma$  “experimentally”
- Evaluating performance on the training set is not enough
  - use separate validation set
- Confidence intervals, various tests,...

## Results

- Recall that only 3.33% of the records correspond to defaults
    - **Always decide "no default:"** Miss-classification rate 3.33%
  - Make predictions using only one component of  $\mathbf{X}$  10-fold CV
    - LDA: 2.81% 2.79%
    - QDA: 2.73% 2.77%
    - **Logistic: 2.73%** 2.77%
  - Make predictions using all of  $\mathbf{X}$  10-fold CV
    - LDA: 2.75% 2.76%
    - QDA: 2.70% 2.72%
    - **Logistic: 3.33%** 3.25%
    - **Logistic with absolute value regularization: 2.66%** 2.71%

# Results

---



- Logistic: 3.33%

## Unbalanced data sets and/or costs

- $\log L(\text{data}; \theta) = \sum_{i \text{ of class 0}} \log \mathbb{P}(Y = 0 | \mathbf{X}_i) + w \sum_{i \text{ of class 1}} \log \mathbb{P}(Y = 1 | \mathbf{X}_i)$
- Solution pays less attention to classes with few samples
  - always declaring “class 0” does pretty well
- Problem is exacerbated if errors on defaulting customers are much more **costly**
- Solution: increase weight of “red” sum
  - equivalent to adding to the data set replicas of the “class 1” samples

defaulting customers in the data set

too few

Predicted labels

good  
default

True labels	
good	default
good	9644
default	23
	81

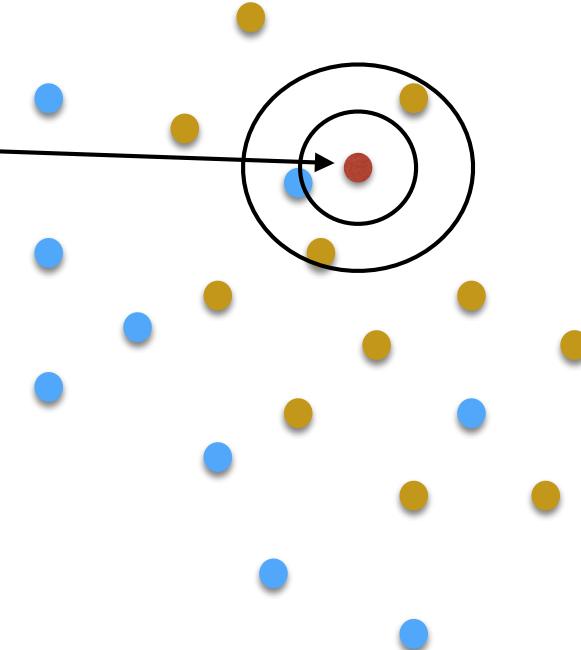
# NEAREST-NEIGHBOR CLASSIFIERS

This file is meant for personal use by patgrinwald@gmail.com only.  
Sharing or publishing the contents in part or full is liable for legal action.

## The $k$ -NN classifier

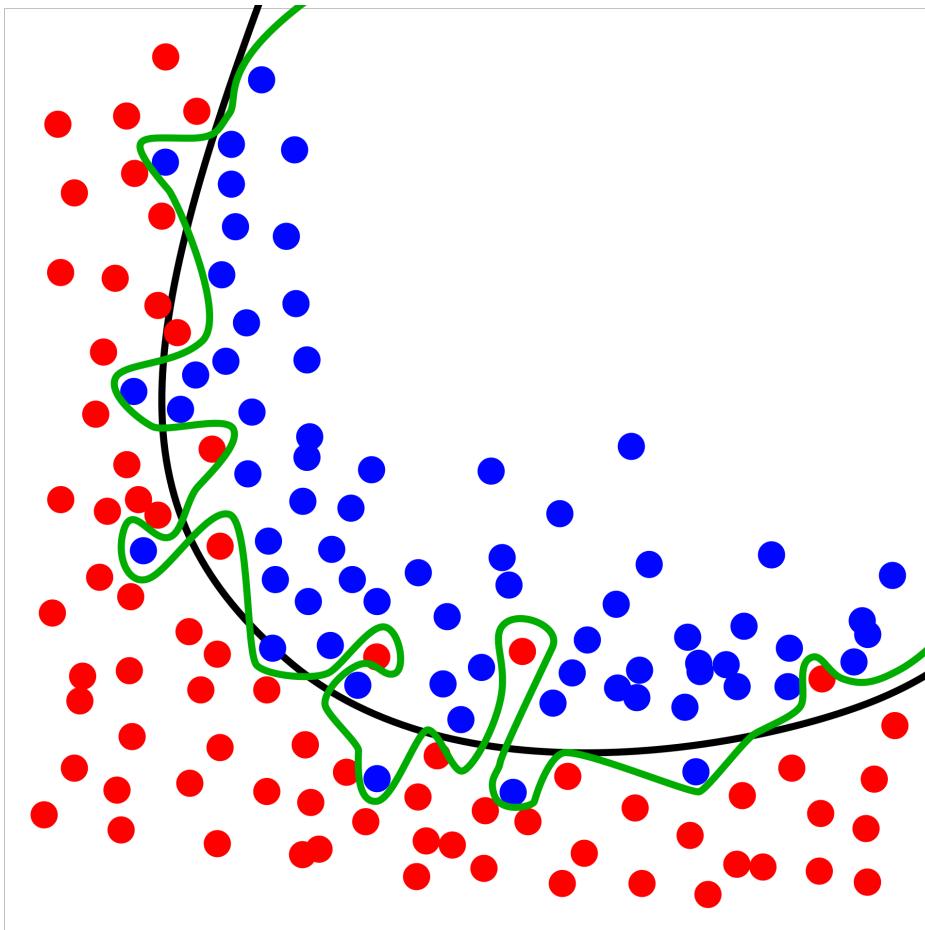
---

- The nearest-neighbor classifier:
  - given new  $\mathbf{X}$
  - find closest  $\mathbf{X}_i$  in the data set  
(with smallest  $\|\mathbf{X} - \mathbf{X}_i\|$ )
  - prediction: the label  $Y_i$  of  $\mathbf{X}_i$
- The  $k$ -NN classifier:
  - given new  $\mathbf{X}$
  - find  $k$  closest  $\mathbf{X}_i$  in the data set
  - prediction: majority vote of the  $k$  labels
- Simple, no training required



## Illustration

---



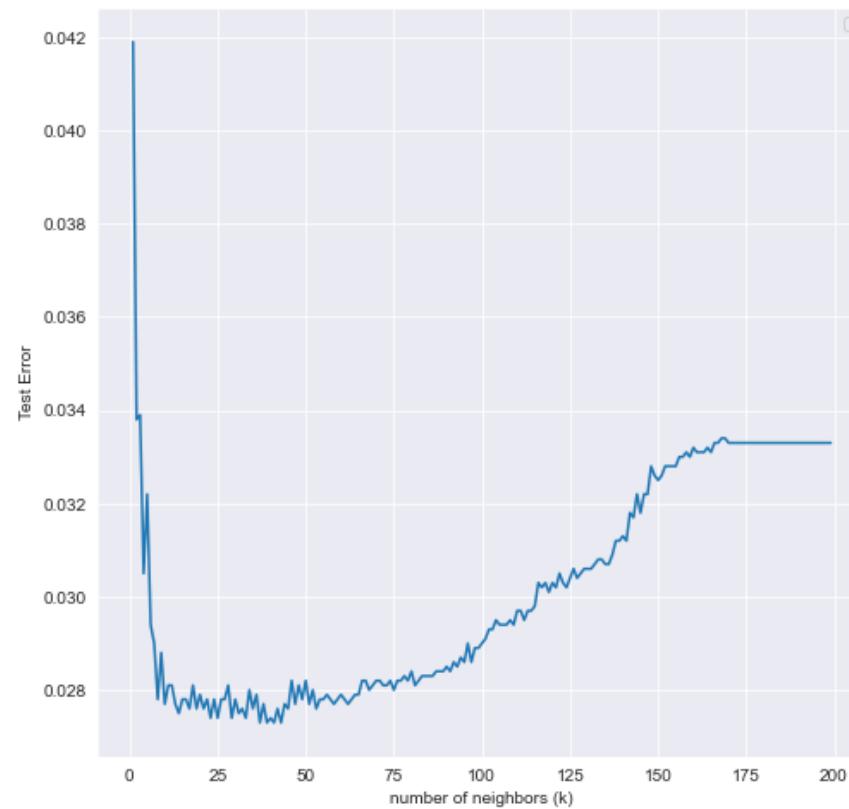
<https://commons.wikimedia.org/wiki/File:Overfitting.svg#/media/File:Overfitting.svg>

## Selecting $k$

---

- Default data
  - LOOCV: classify a record, based on the remaining ones

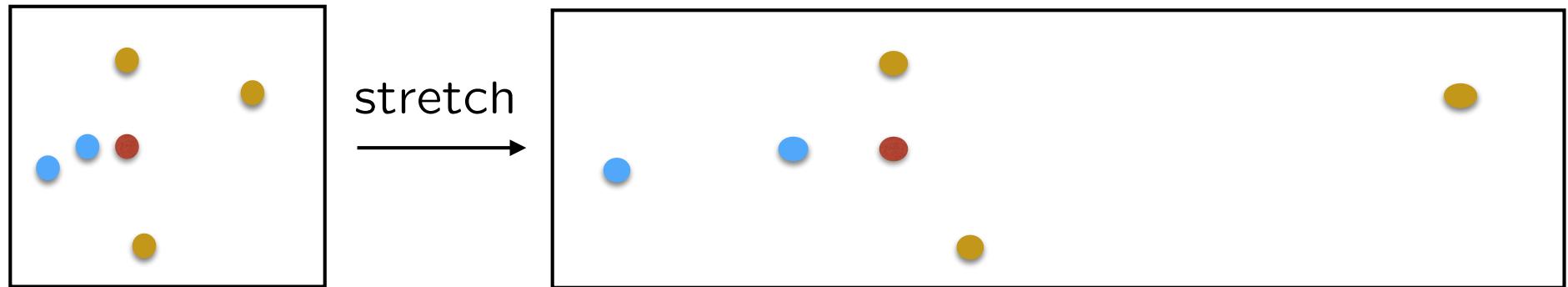
Value of K	Error
5-NN	3.22
6-NN	2.94
7-NN	2.9
8-NN	2.78
9-NN	2.88
10-NN	2.77
11-NN	2.81
12-NN	2.81
13-NN	2.77
14-NN	2.75
15-NN	2.78



- This is an example of **hyperparameter search** to choose between models/algorithms

# Scaling matters

---



$$k = 3$$

decide “blue”

$$k = 3$$

decide “brown”

- Scale so that the components of  $\mathbf{X}$  have comparable ranges
- equivalently: use a weighted distance metric,

$$\text{e.g. } \|\mathbf{x}\| = \sqrt{x_1^2 + \mathbf{w} \cdot \mathbf{x}_2^2}$$

## Some other classification algorithms

---

- **Weighted NN**
  - $k$ -NN: majority vote between  $k$  neighbors
  - Consider weighting the votes, as a function of the distance
  - every point could vote, far away points would have little weight
    - Similar idea applies to standard regression problems
      - estimate  $\mathbb{E}[Y | \mathbf{X}]$  by weighing the  $Y_i$ 's of nearby  $\mathbf{X}_i$ **(kernel regression)**
- **Support vector machines**
- **Decision trees**
- **Neural networks**

## Interpretability of models; explainability of predictions

---

- A generic issue in machine learning
- In regression, coefficients  $\theta$  allow us to interpret the “logic” behind particular predictions

$$\widehat{\text{Sales}} = 2.94 + 0.046 \cdot (\text{TV}) + 0.19 \cdot (\text{Radio}) - 0.001 \cdot (\text{NewsP})$$

- Similarly in logistic regression  $\mathbb{P}(Y = k | \mathbf{X}) = \frac{\exp\{\boldsymbol{\theta}_k^T \mathbf{X}\}}{\sum_s \exp\{\boldsymbol{\theta}_s^T \mathbf{X}\}}$
- Nearest neighbor methods do not yield an interpretable model
  - but allow us to explain the predictions

“Beth’s profile is similar to that of Barbara, Beatrice, and Bo...”
- A challenge for more complex machine learning models

## Wrapping up

---

- Saw a number of methods
  - for prediction and “model-building”
- Encountered the main general methodologies
  - empirical risk minimization
  - maximum likelihood
  - plugin estimates
  - Bayesian
- “Classical” methods (regression, LDA, QDA, NN, etc.) form the starting point for more complex methods
- General toolbox for performance assessment (validation, bootstrap)
- Need care to avoid misinterpretations