Introduction to Machine Learning
Topic 1: Basic concepts

Lecture 1a

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Course outline

- Nine **topics**:
  - Basic concepts in machine learning. Software for ML.
  - Regression, regularization and model selection
  - Classification methods
  - Dimensionality reduction and uncertainty estimation
  - Support vector machines and kernel methods
  - Gaussian processes and mixture models
  - Splines and additive models
  - Neural networks and deep learning
  - Ensemble methods and high-dimensional problems

Course outline

- **Course structure:**
  - **Lectures.**
    - Approx 2 per topic.
    - Concepts and theory.
  - **Labs.**
    - One per topic.
    - Practical implemenations of methods.
    - Individual report + aggregate group report
    - Reports submission via LISAM
  - **Seminars.**
    - Two labs discussed at one seminar.
    - Presentation of group reports. Randomly selected persons.
- **Teachers**: Mattias Villani, Oleg Sysoev and Isak Hietala.

Overview of Lecture 1a

- What is machine learning?
- Motivating examples
- Unsupervised vs Supervised learning
- Regression vs Classification
- Generative vs Discriminative models
- Parametric vs nonparametric models
- Overfitting and Regularization
- Prediction and Model evaluation

Overview of Lecture 1b

- Introduction to Bayesian learning
- Bernoulli model with beta prior
- Normal model with normal prior
- Multinomial model with Dirichlet prior

Overview of Lecture 1c

- R programming.

What is machine learning?

Machine learning is a subfield of ***computer science*** *that evolved from the study of* ***pattern recognition*** *and computational learning theory in* ***artificial intelligence****.*

Machine learning explores the study and construction of ***algorithms*** *that can* ***learn*** *from and make* ***predictions*** *on* ***data****. Such algorithms operate by building a model from example inputs in order to make data-driven predictions or* ***decisions****, rather than following strictly static program instructions.*

Machine learning is closely related to and often overlaps with ***computational statistics****; a discipline that also specializes in prediction-making.*

Wikipedia (Oct 11, 2015).

What is machine learning?

- Machine learning is an area in the **intersection** of **computer science**, **statistics** and **artificial intelligence**. It is closely related to **data mining**, **knowledge discovery** and **data science**.
- Machine learning uses mainly **statistical** **(probabilistic)** **models** **for analyzing** **data**. Data mining and knowledge discovery tend to use less rigorous, but often effective, algorithms.
- Machine learning differs from traditional statistics by a **heavier focus on prediction**, and lesser focus on interpretation.
- Models in machine learning are often **more** **flexible** (more parameters) than those in traditional statistics, and **regularization** to **avoid over-fitting** is therefore a much bigger concern.
- Machine learning applications often involve large data data sets (**big data**), and **computational complexity** of estimation algorithms is therefore important.

Statistics or Computer Science? Both!

I keep saying the sexy job in the next ten years will be statisticians.

Hal Varian, Chief Economist, Google.

But the challenges for massive data go beyond the storage, indexing, and querying . . . and, instead, hinge on the ambitious goal of inference. ***Inference*** *is the problem of* ***turning data into knowledge*** *. . . Statistical rigor is necessary to justify the inferential leap from data to knowledge . . .”*

from the report “Frontiers in Massive Data Analysis”, US National Research Council.

Computer scientists involved in building big-data systems must develop a deeper awareness of inferential issues, while statisticians must concern themselves with scalability, algorithmic issues, and real-time decision-making.

from the report “Frontiers in Massive Data Analysis”, US National Research Council.

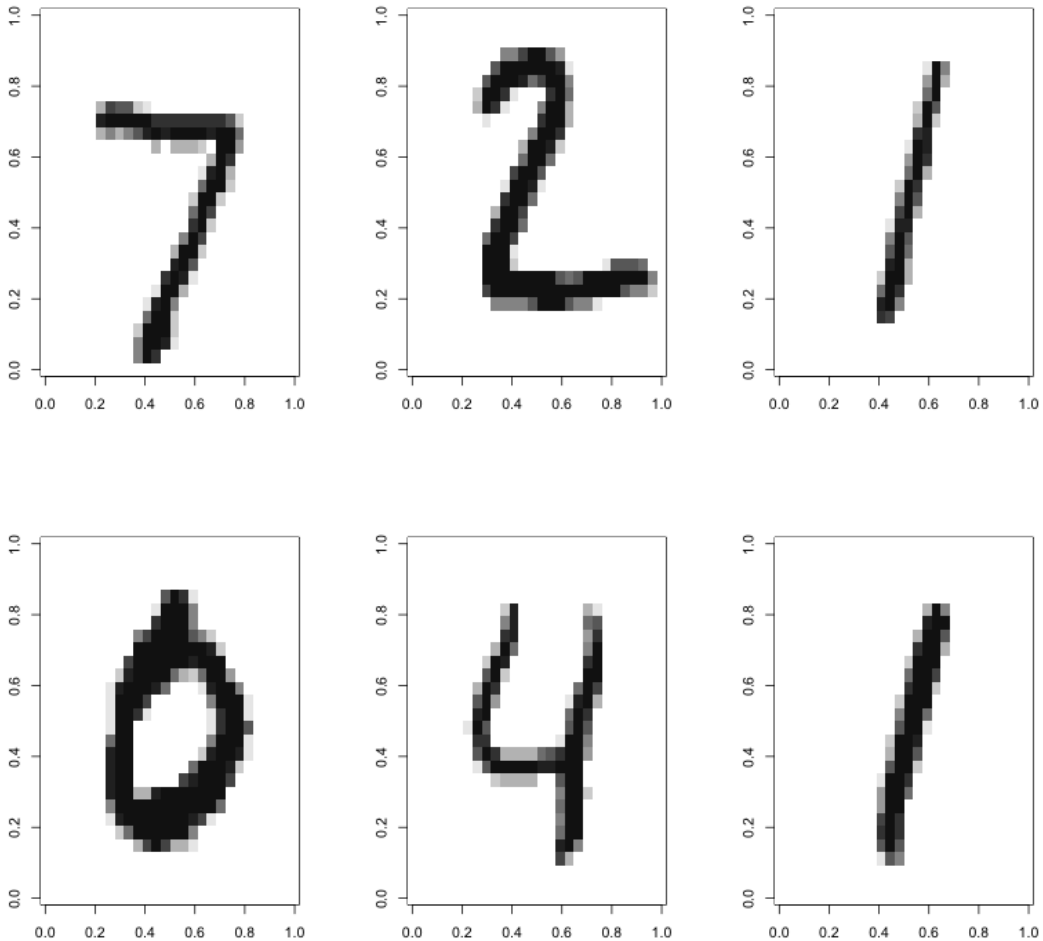
But why probability models?

- Probability models and statistical inference provide a **framework**.
- A principled **way to think** about any problem in machine learning.
- Probabilistic models can be **evaluated** in detail. Locate and understand the deficiencies in the model. Improve.
- Probabilistic models **quantify uncertainties**. Needed for data-driven decision making.

As robotics is now moving into the open world, the issue of ***uncertainty*** *has become a major stumbling block for the design of capable robot systems. Managing uncertainty is possibly the most important step towards robust real-world robot systems.*

from the book Probabilistic Robotics by Thrun et al.

CLASSIFYING HANDWRITTEN DIGITS



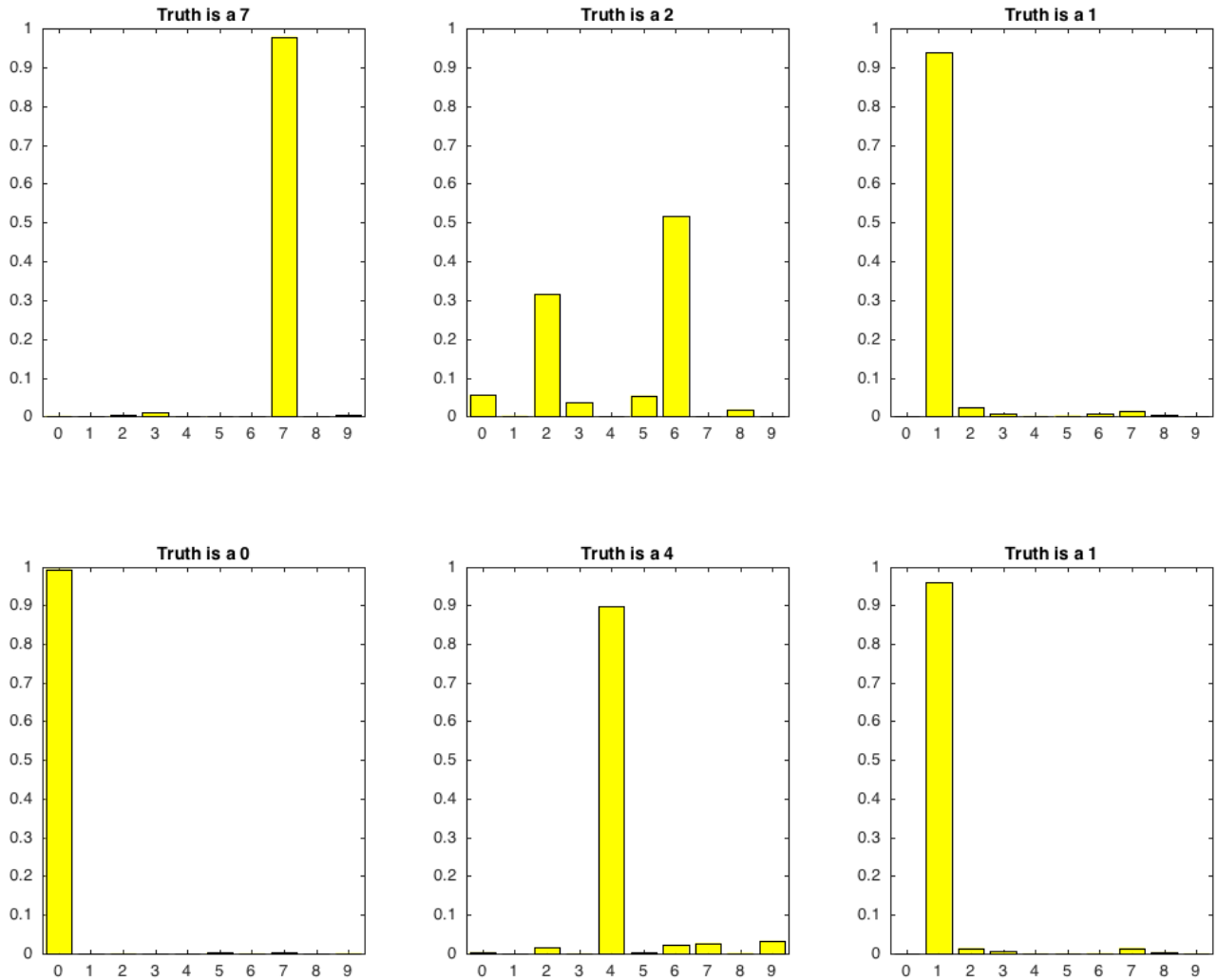
Classifying handwritten digits

- **Training** data: 60000 images.
- **Test** data: 10000 images.
- **Features**: use the intensities (0-255, but scaled to 0-1) in the $28 \times 28 = 784$ pixels as explanatory variables.
- **Multinomial regression**

$$Pr(\text{Digit} = i|\text{features}) = \frac{\exp\left(w_{0,i} + w_{1,i}x_1 + ... + w_{784,i}x_{784}\right)}{\sum_{j=0}^{9} \exp\left(w_{0,j} + w_{1,j}x_1 + ... + w_{784,j}x_{784}\right)}$$

- MANY parameters to estimate. **Overfitting** is a major concern.
- **Lasso** (**elastic net**) **penalty** on model complexity. The weights $w_{k,i}$ are shrunk toward zero, sometimes exactly to zero.
- **Support vector machine** (**SVM**).

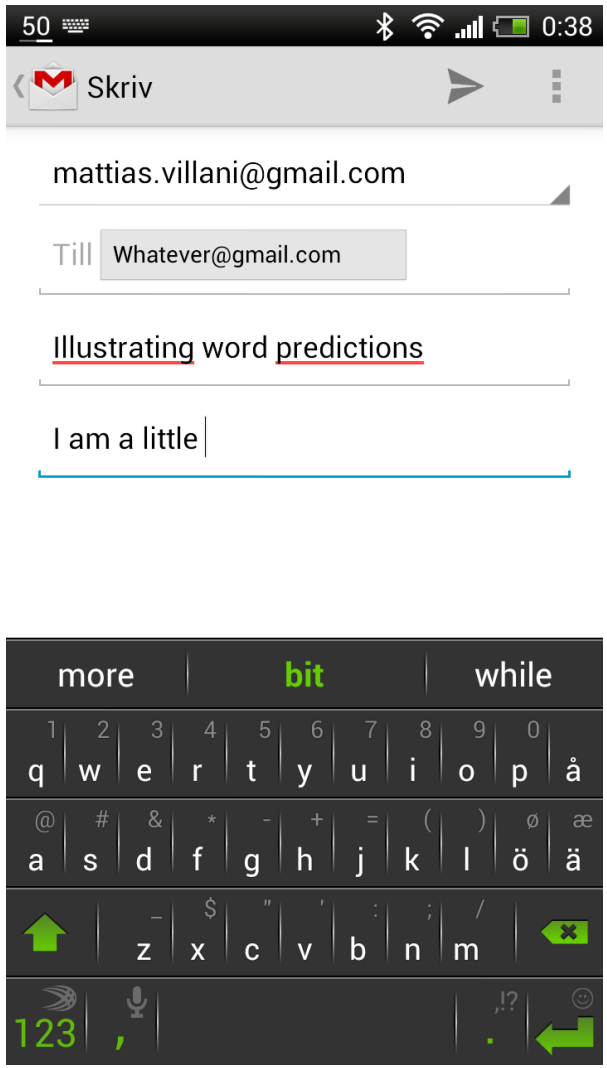
CLASSIFYING HANDWRITTEN DIGITS



HANDWRITTEN DIGITS - CONFUSION MATRIX

	0	1	2	3	4	5	6	7	8	9
0	966	0	8	1	1	7	9	2	4	6
1	0	1121	1	1	0	2	3	13	7	7
2	2	2	957	13	5	4	4	21	7	0
3	0	2	9	947	0	29	1	3	12	10
4	0	0	12	1	940	5	5	9	8	32
5	6	1	3	19	1	816	9	1	24	9
6	4	4	13	1	7	12	926	0	10	1
7	1	0	9	10	2	2	0	954	5	13
8	1	4	17	11	2	10	1	3	892	4
9	0	1	3	6	24	5	0	22	5	927

SMARTPHONE TYPING PREDICTIONS



SMARTPHONE TYPING PREDICTIONS

- Assume the following Markov model for a sentence

$$p(w_1 w_2 \cdots w_k) = p(w_1 | < s >) \cdot p(w_2|w_1) p(w_3|w_2) \cdots p(w_n|w_{n-1})$$

- Need a model for

$$p(w_k|w_{k-1})$$

- Example:

$$p(\text{person}|\text{stupid}) = 0.2$$

$$p(\text{Mattias}|\text{stupid}) = 0.0001$$

- Maximum Likelihood (ML) estimate:

$$\hat{p}(w_k|w_{k-1}) = \frac{\text{Number of times word } w_k \text{ follows directly after } w_{k-1}}{\text{Number of times } w_{k-1} \text{ appears in the text}}$$

- **Decision** problem: which word to suggest?
- SwiftKey is now using Neural Networks: https://youtu.be/-vZL3e02SnE.

Detecting banknote fraud

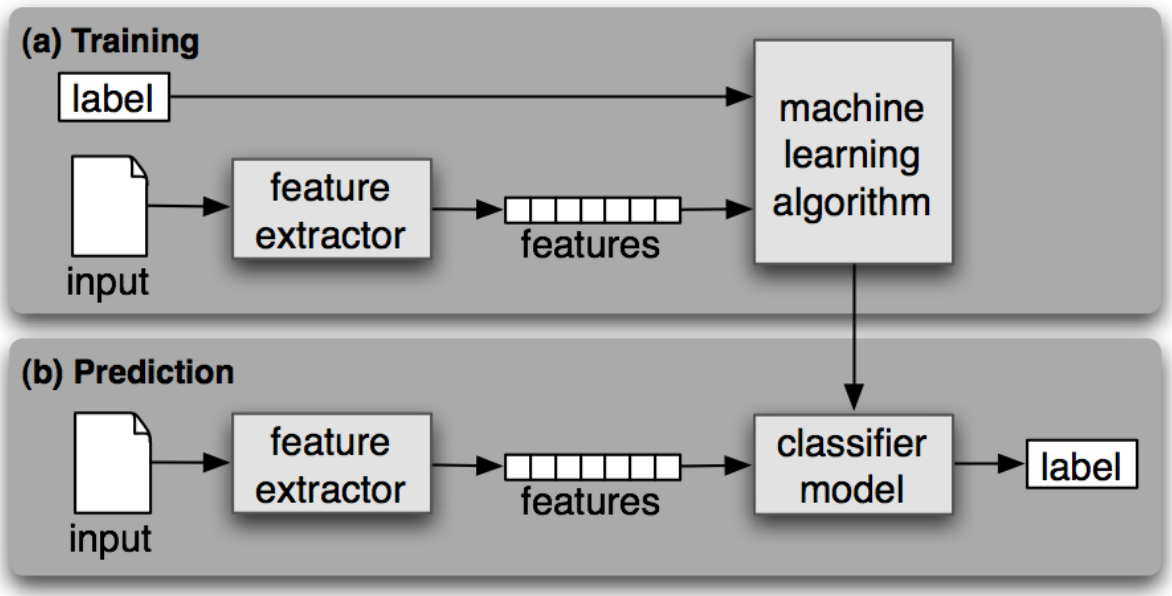
- Dataset with 1372 photographed banknotes. 610 of them are fraud.
- Raw data: $400 \times 400 = 160000$ gray-scale pixels.
- Often better performance if using a smaller set of summarizing variables, so called **features**, that capture the important aspects of the images.
- The 160000 pixel variables are condensed to four **features** using wavelets:
  - variance of Wavelet Transformed image
  - skewness of Wavelet Transformed image
  - curtosis of Wavelet Transformed image
  - entropy of image

Detecting banknote fraud

- 1000 images for training.
- Predictions on 372 test images.
- **Decision**: signal fraud if $P(\text{Fraud}|\mathbf{x}) > 0.5$.
- **Confusion matrix**

		Truth	
		No fraud	Fraud
Decision	No Fraud	208	1
	Fraud	3	160

THE MACHINE LEARNING WORK FLOW



Unsupervised vs Supervised learning

- **Unsupervised**: **target values** (responses/**labels**) are unknown. Goals:
  - to discover groups or patterns in the data.
  - which observations are similar?
  - to learn a compact representation of the inputs. PCA.
- Example models for unsupervised learning:
  - **Mixture models**
  - **Association learning**
- **Supervised**: targets are known. Goals:
  - Build a prediction machine: inputs $\rightarrow$targets.
- Example models for supervised learning:
  - **Regression**: Linear regression. Gaussian processes.
  - **Classification**: Logistic regression, Support vector machines etc.
- **Semi-supervised**: targets are known only for some observations.
- **Active learning**. Strategies for deciding which observations to label.

Histogram and kernel density estimation

- Histograms: Partition x-space into g bins of length Δ: $B_1, ..., B_g$. Let n_i denote the number of observations falling in bin i.
- **Histogram estimate of the density**: density is constant over each bin and the density over bin i is

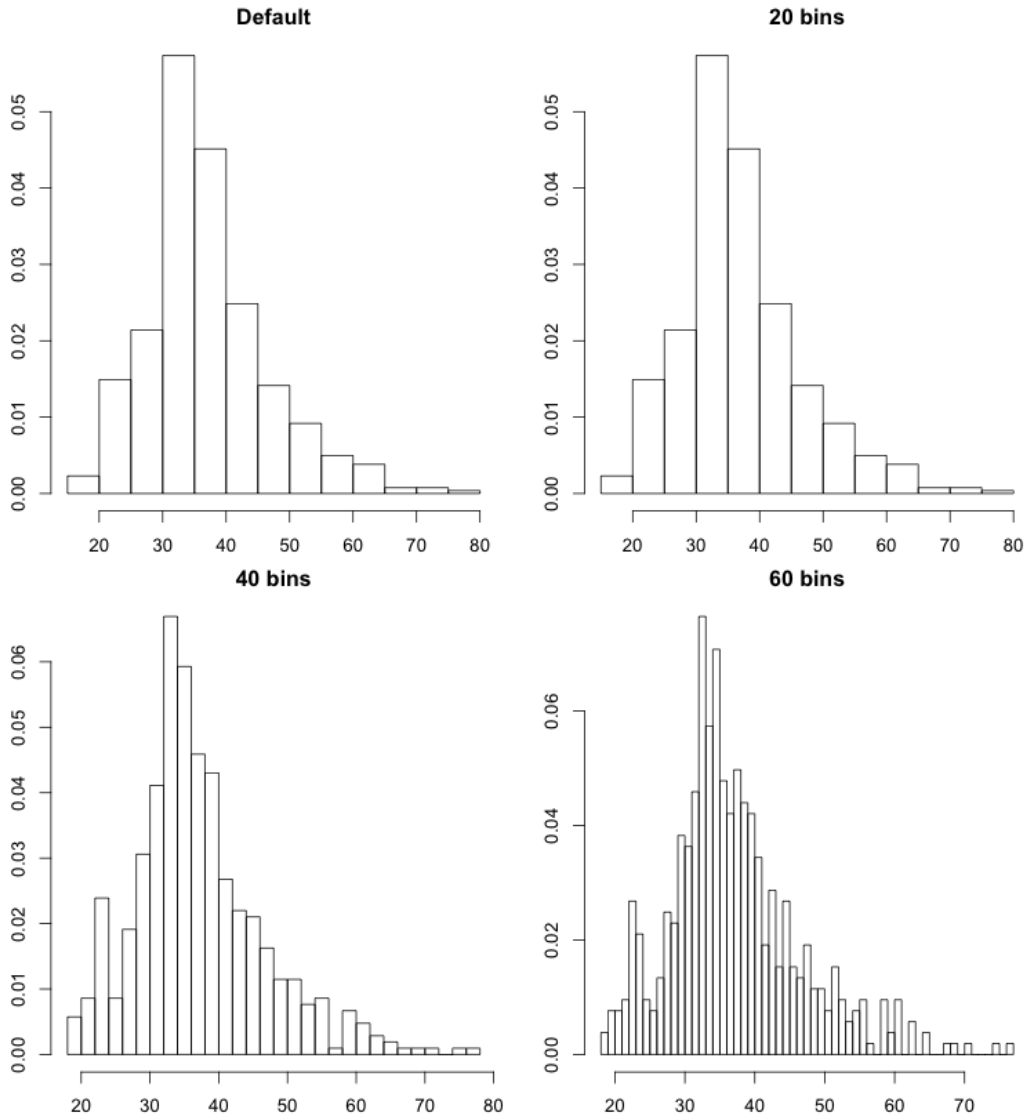
$$p(x) = \frac{n_i}{N\Delta} \text{ for } x \in B_i$$

- **Kernel density estimator**

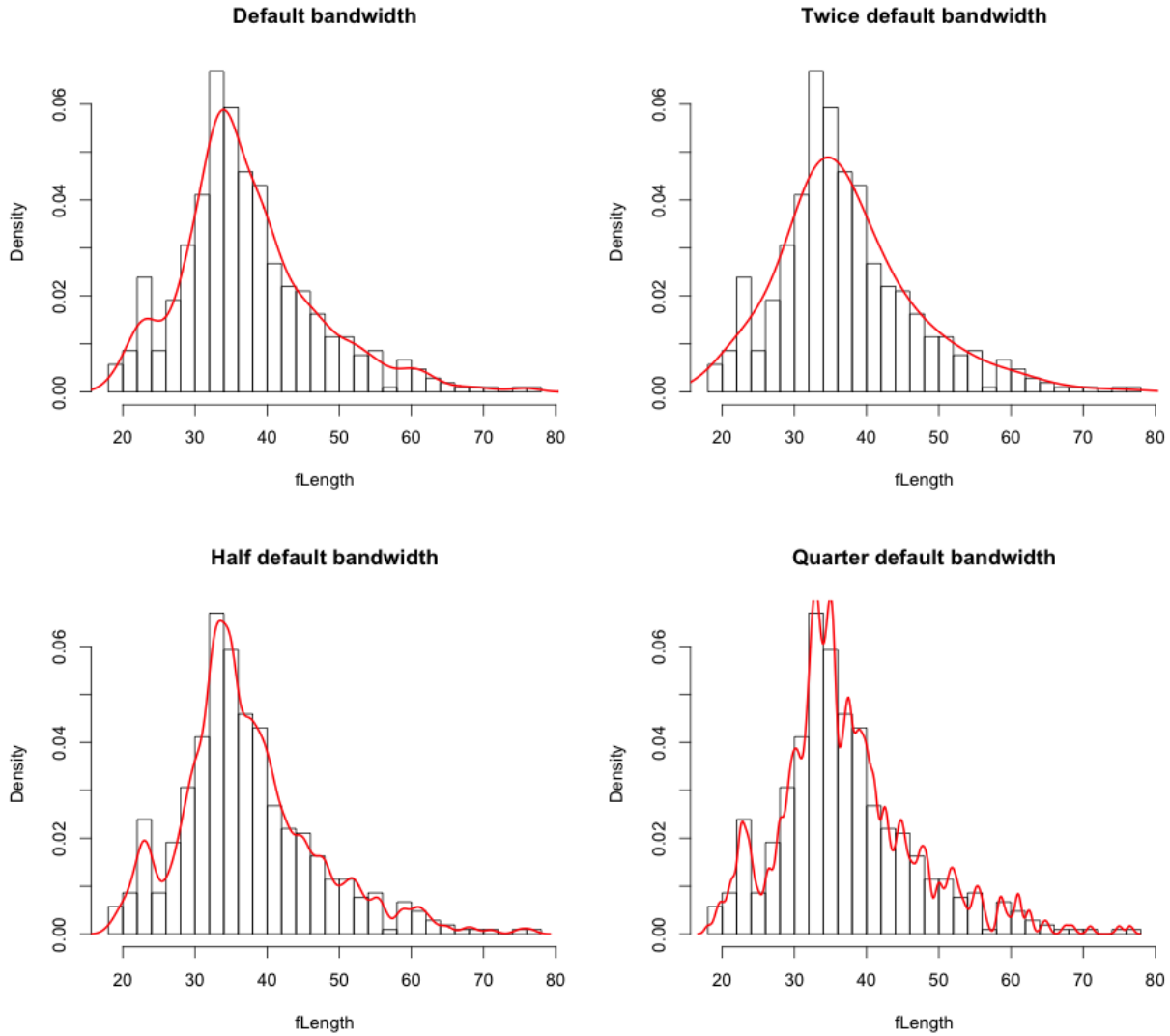
$$p(x) = \frac{1}{N} \sum_{i=1}^{n} \frac{1}{h} k\left(\frac{x - x_i}{h}\right)$$

where $k(\cdot)$ is a kernel function, e.g. the normal density. h is a bandwidth parameter, e.g. the standard deviation σ in a normal density.

FISH LENGTH - HISTOGRAM DENSITY ESTIMATES



FISH LENGTH - KERNEL DENSITY ESTIMATES



K-NEAREST NEIGHBOURS DENSITY ESTIMATION

- *k*-**nearest neighbours** (**kNN**):

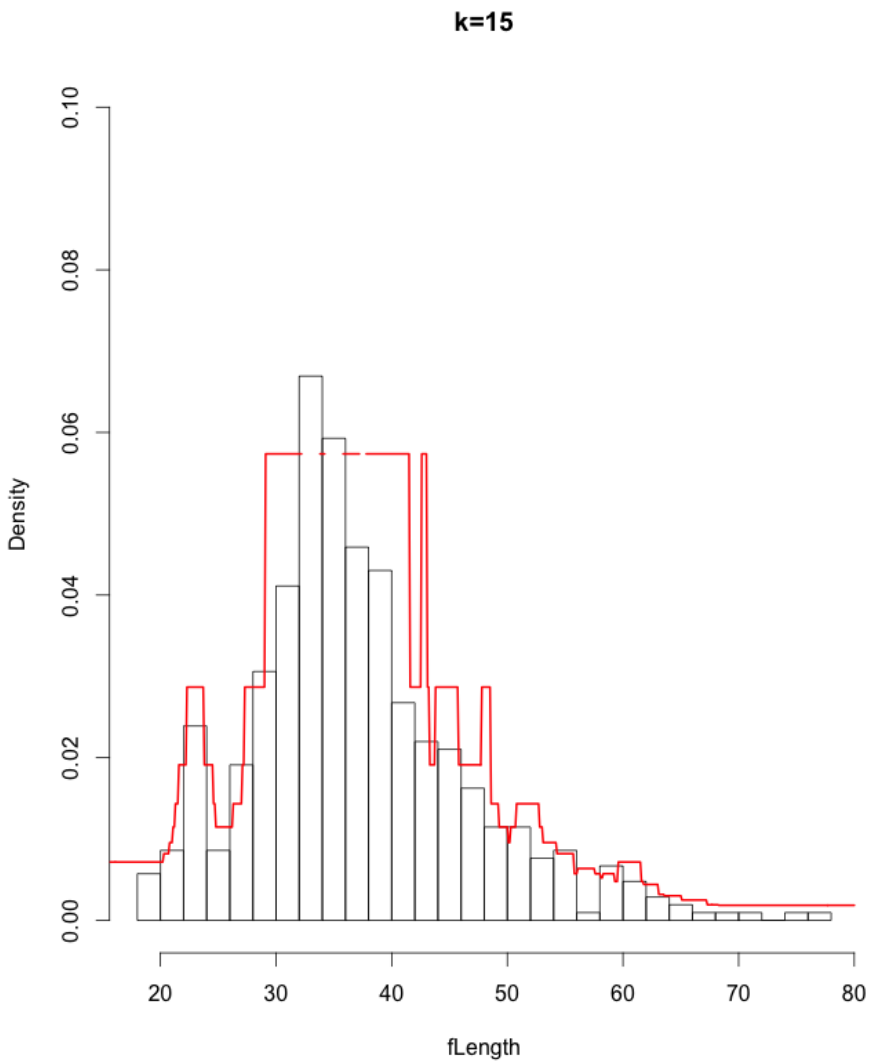
$$p(x) = \frac{K}{NV}$$

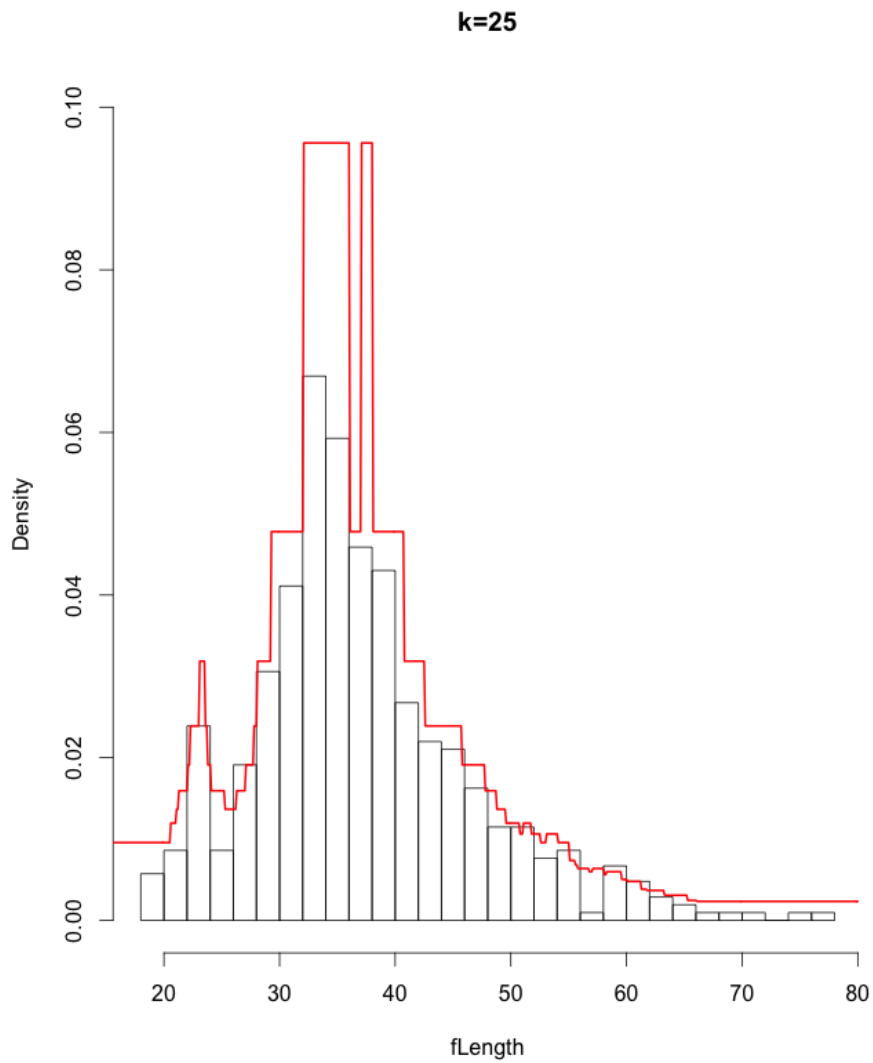
where

  - N is the number of data observations
  - K is the number of neighbours
  - V is the width of the smallest bin that contains exactly the K neighbours of $\mathbf{x}$.

- Histograms: fix Δ and count the number of observations in a bin
- k-nearest neighbours: fix the number of observations K in a bin, and make sure that the bin width V is large enough.

FISH LENGTH - KNN DENSITY ESTIMATES





Mixture of normals density estimation

- Two-component **mixture of normals**

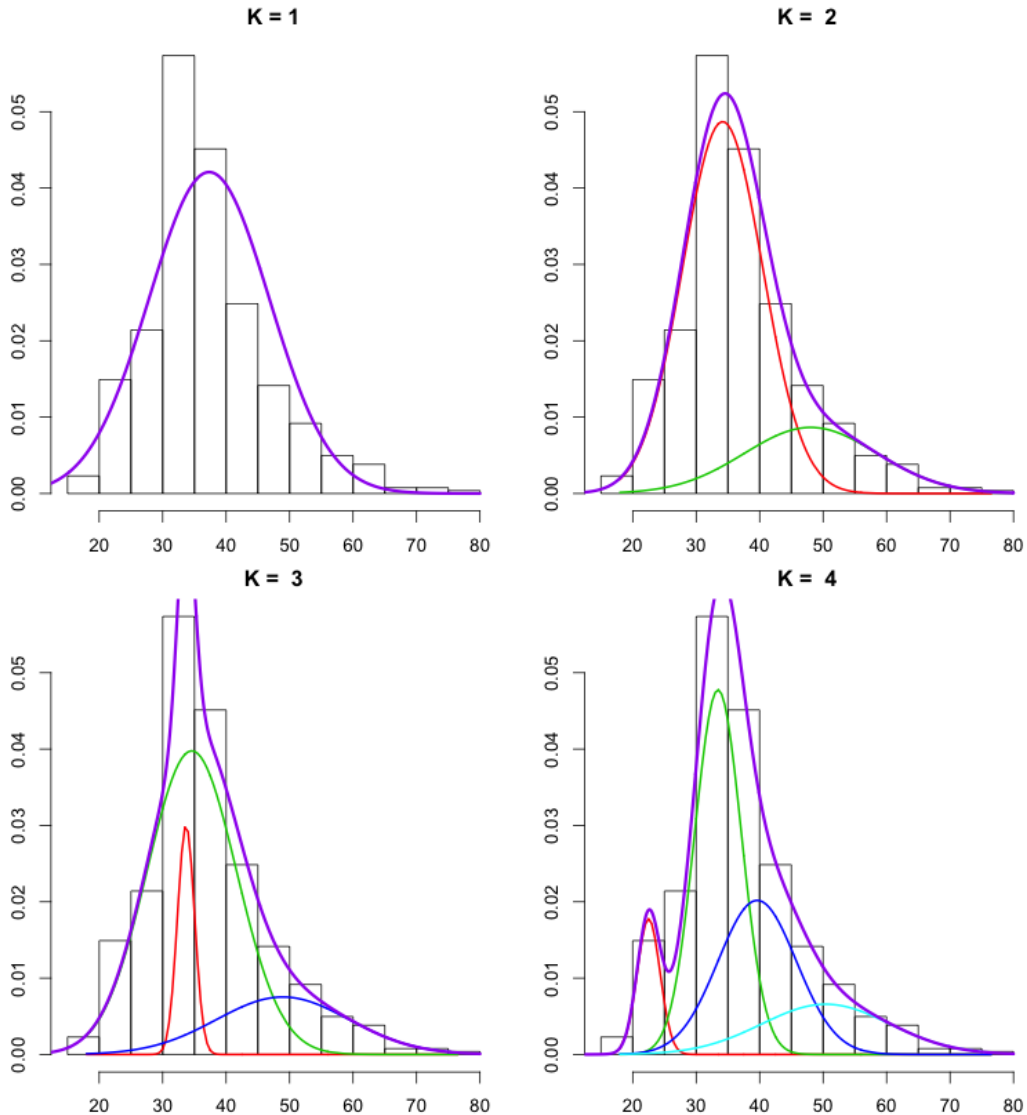
$$p(y) = \pi_1 \cdot \phi(y|\mu_1, \sigma_1^2) + \pi_2 \cdot \phi(y|\mu_2, \sigma_2^2)$$

- Mixture of normals with K components

$$p(y) = \sum_{k=1}^{K} \pi_k \cdot \phi(y|\mu_k, \sigma_k^2)$$

- Maximum likelihood or Bayesian methods to estimate the model parameters: $\pi_1, ..., \pi_K$, $\mu_1, ..., \mu_K$ and $\sigma_1, ..., \sigma_K$.
- It is possible to use other distrbutions than the normal in the mixture. Example: mixture of Poissons for count data.

FISH LENGTH - MIXTURE OF NORMALS



THREE TYPES OF SUPERVISED MODELS

- **Generative models**: models inputs and targets jointly:
  - $p(\mathbf{Y}, \mathbf{X})$ when the target Y is continuous
  - $p(\mathcal{C}_k, \mathbf{X})$ when the target is a class $\mathcal{C}_k$.
- **Discriminative models**: Models $p(\mathcal{C}_k|\mathbf{x})$ directly.
- **Discriminant function models**: uses a function $f(\mathbf{x})$ that maps any $\mathbf{x}$ to a class label $\mathcal{C}_k$. No probabilities are involved.

- Generative models can be used to generate synthetic data.
- Discriminative models typically have fewer parameters than generative models.
- Discriminative models tend to give better predictions, especially when the generative model for $\mathbf{x}$ is bad.

Generative models - Bayesian classification

- **Bayesian classification** among K classes

$$\underset{k \in \{1,\ldots,K\}}{\operatorname{argmax}} \; p(\mathcal{C}_k|\mathbf{x})$$

  where $\mathbf{x} = (x_1, \ldots, x_n)$ is a feature vector.
- By **Bayes' theorem**

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\mathbf{x})} \propto p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)$$

- Bayesian classification

$$\underset{k \in \{1,\ldots,K\}}{\operatorname{argmax}} \; p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)$$

- $p(\mathcal{C}_k)$ can easily be estimated by the proportion of observations from class k.
- But how do we compute $p(\mathbf{x}|\mathcal{C}_k)$?

k-NEAREST NEIGHBOURS CLASSIFICATION

- **kNN** models the class-conditional distributions by

$$p(\mathbf{x}|\mathcal{C}_k) = \frac{K_k}{N_k \cdot V},$$

where

  - V is the volume of the smallest sphere centered on $\mathbf{x}$ that contains exactly K neighbours.
  - K_k is number observations from class k in that sphere.
  - N_k is the total number of observations in class k.

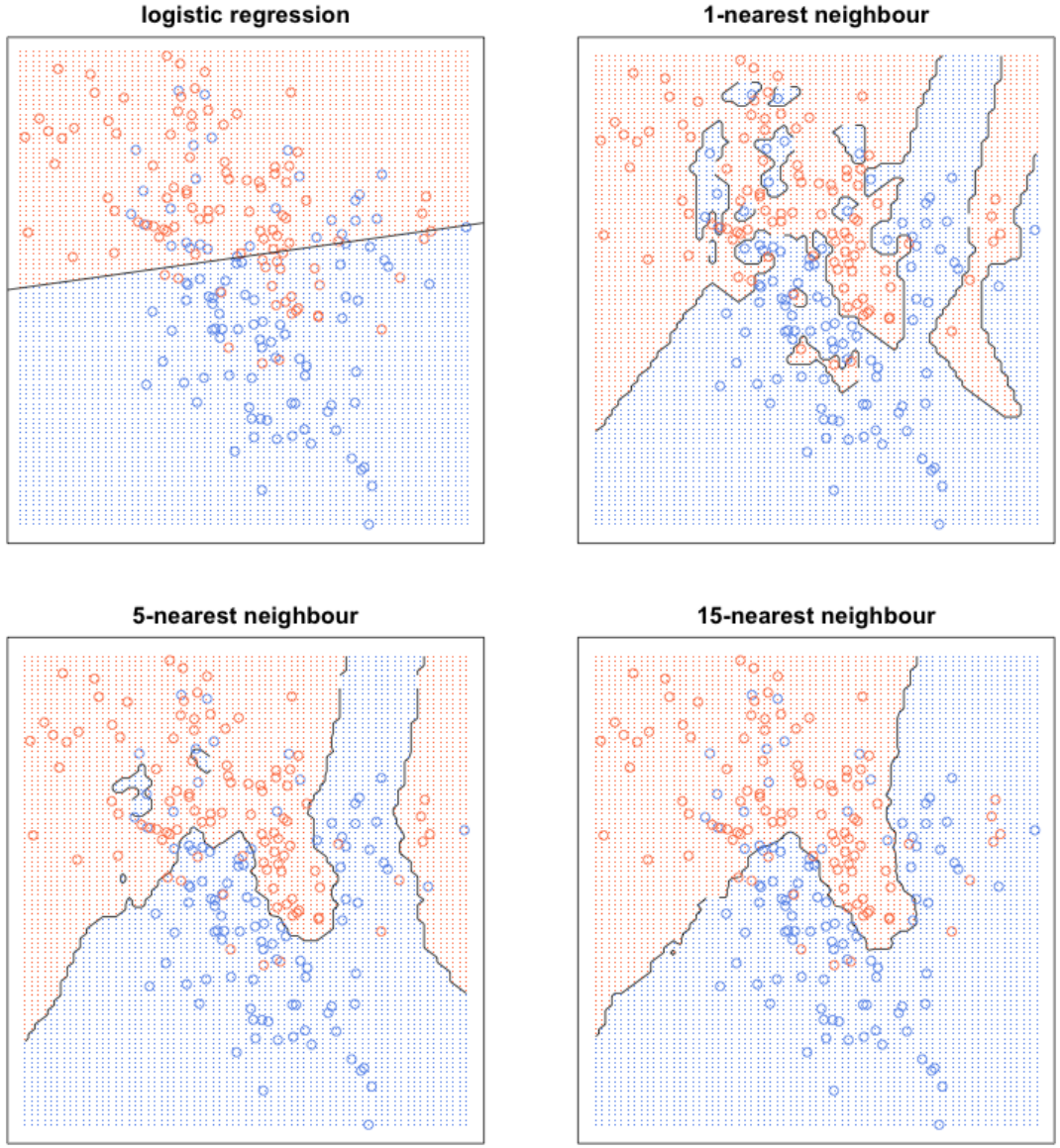
- kNN model of $p(\mathbf{x})$ and $p(\mathcal{C}_k)$

$$p(\mathbf{x}) = \frac{K}{N \cdot V} \qquad p(\mathcal{C}_k) = \frac{N_k}{N}$$

- kNN classification probabilities:

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\mathbf{x})} = \frac{K_k}{K}.$$

CLASSIFICATION



Generative models - naive Bayes

- **Naive Bayes**: **features** are assumed **independent**

$$p(\mathbf{x}|\mathcal{C}_k) = \prod_{j=1}^{n} p(x_j|\mathcal{C}_k)$$

- Naive Bayes solution

$$\underset{k\in\{1,\ldots,K\}}{\operatorname{argmax}} \left[\prod_{j=1}^{n} p(x_j|\mathcal{C}_k)\right] p(\mathcal{C}_k)$$

- Example: $K = 2$. $\mathcal{C}_1$ =positive movie review and $\mathcal{C}_2$ =negative movie review
- Binary word features: x_j = has('fantastic')

$$\hat{p}\left(\text{has('fantastic')}|\text{positive}\right) = \frac{\#\text{ positive reviews with the word 'fantastic'}}{\#\text{ of positive reviews}}$$

- For **continuous features** we can use a normal distribution for each class:

$$x_j|\mathcal{C}_k \sim N(\mu_{jk}, \sigma_{jk}^2)$$

Discriminative models

- Direct modeling of $p(\mathcal{C}_k|\mathbf{x})$. No need to model $p(\mathbf{x}|\mathcal{C}_k)$.
- **Logistic regression**

$$Pr(\textbf{positive review}|\mathbf{x}) = \frac{\exp(w_0 + w_1 \cdot x_1 + ... + w_p x_p)}{1 + \exp(w_0 + w_1 \cdot x_1 + ... + w_p x_p)}$$

- When the response is continuous: direct models of $p(Y|\mathbf{x})$.
- **Linear regression**:

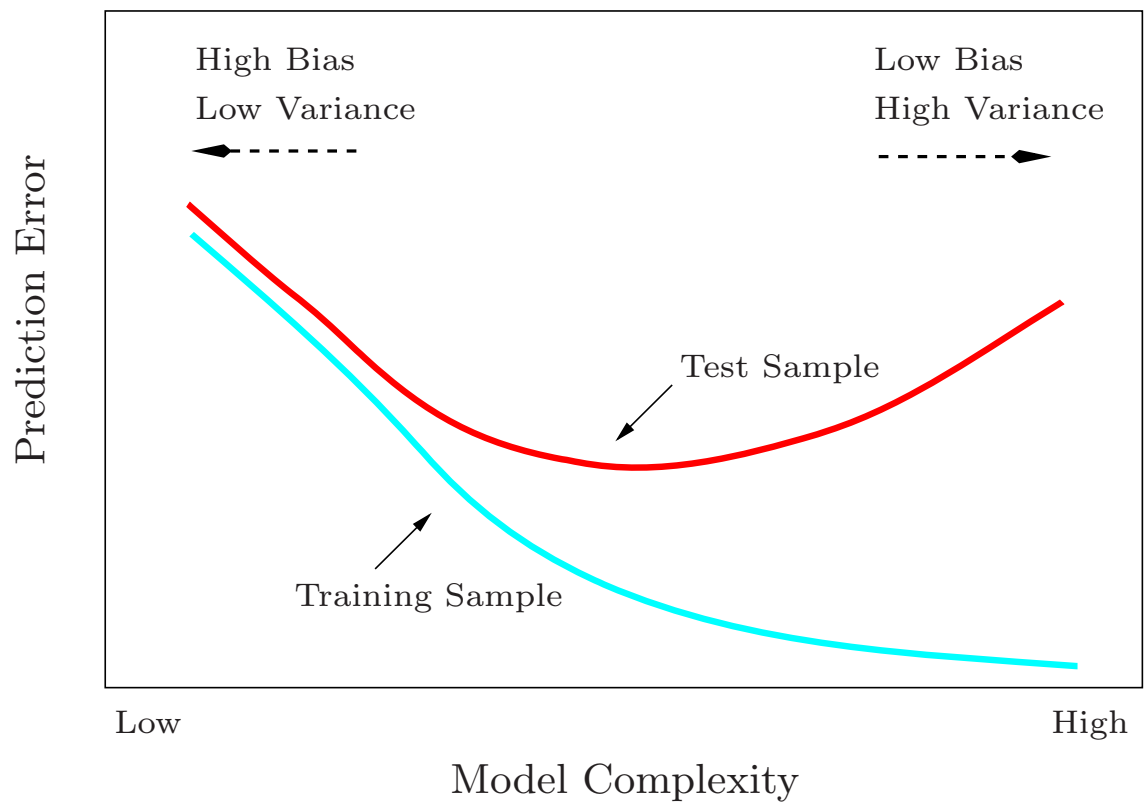
$$Y = w_0 + w_1 \cdot x_1 + ... + w_p x_p + \varepsilon, \quad \varepsilon \overset{indep}{\sim} N(0, \sigma^2)$$

- **Poisson regression** for counts ($Y \in \{0, 1, 2, ...\}$):

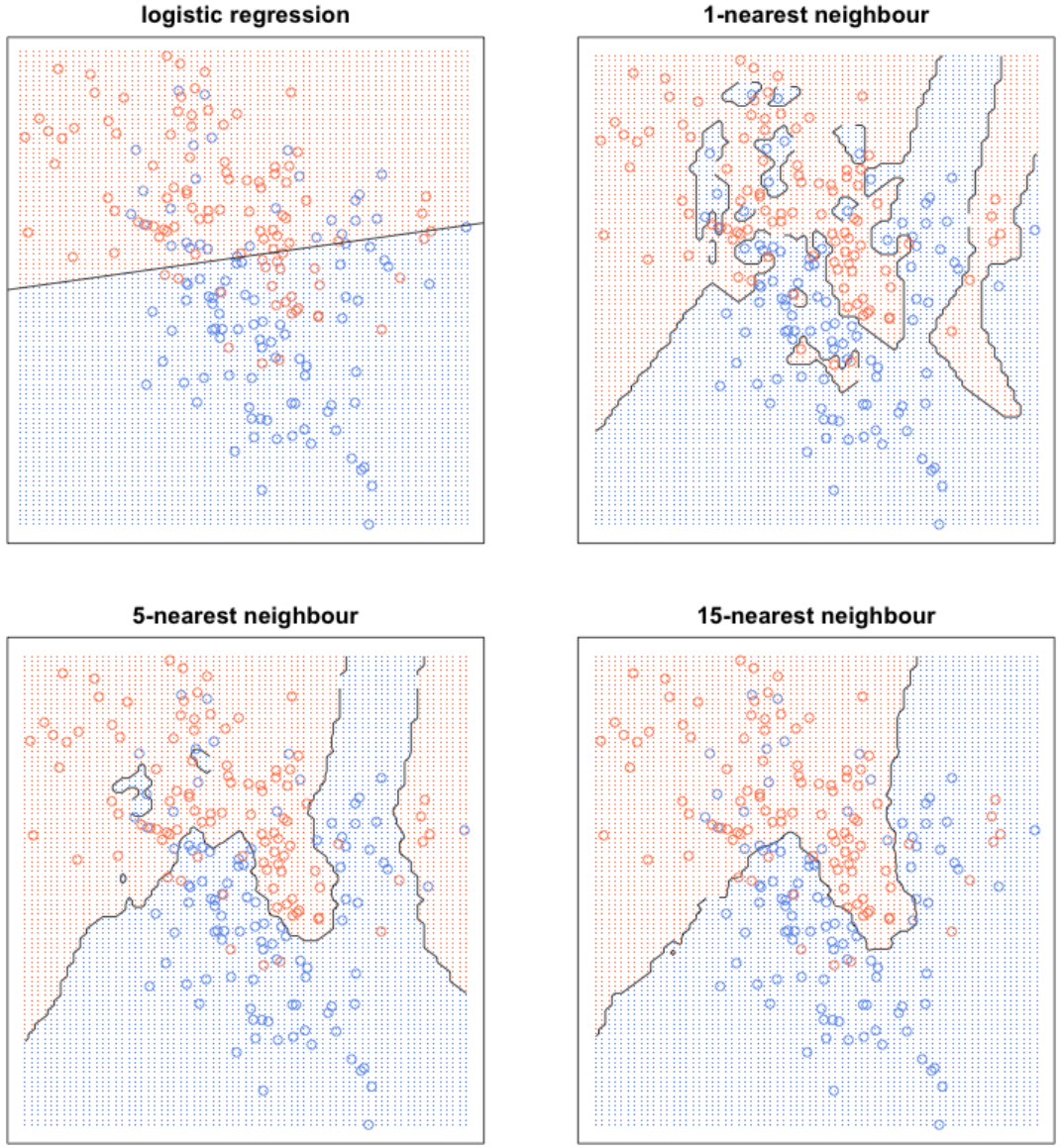
$$Y|\mathbf{x} \overset{iid}{\sim} Poisson\left[\lambda = \exp\left(w_0 + w_1 \cdot x_1 + ... + w_p x_p\right)\right]$$

The Bias-Variance trade-off

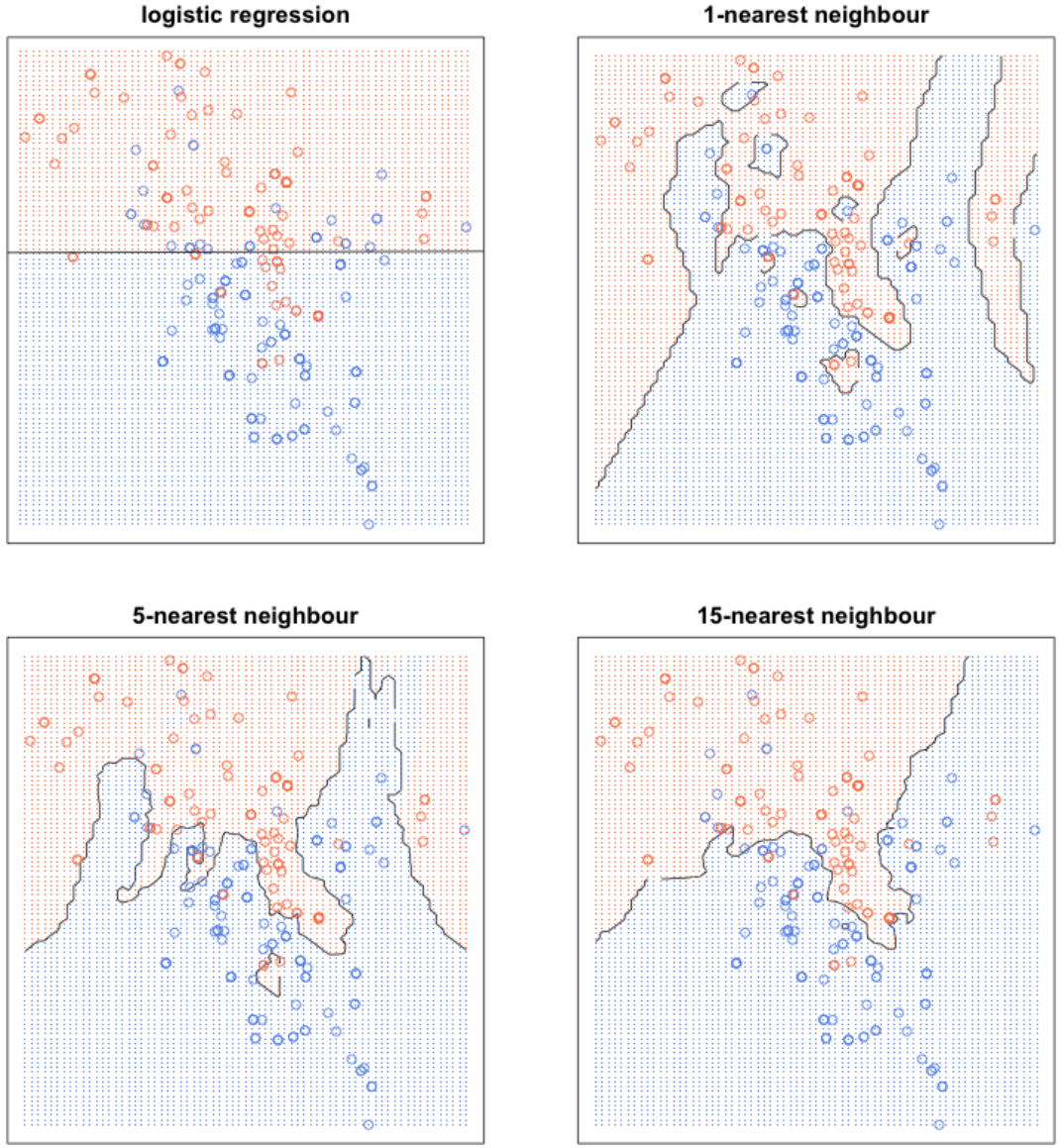
- Logistic regression has low variance, but may have large bias if truth is non-linear.
- kNN can have large variance, but low bias since it can adapt to non-linearities.
- Bias variance trade-off



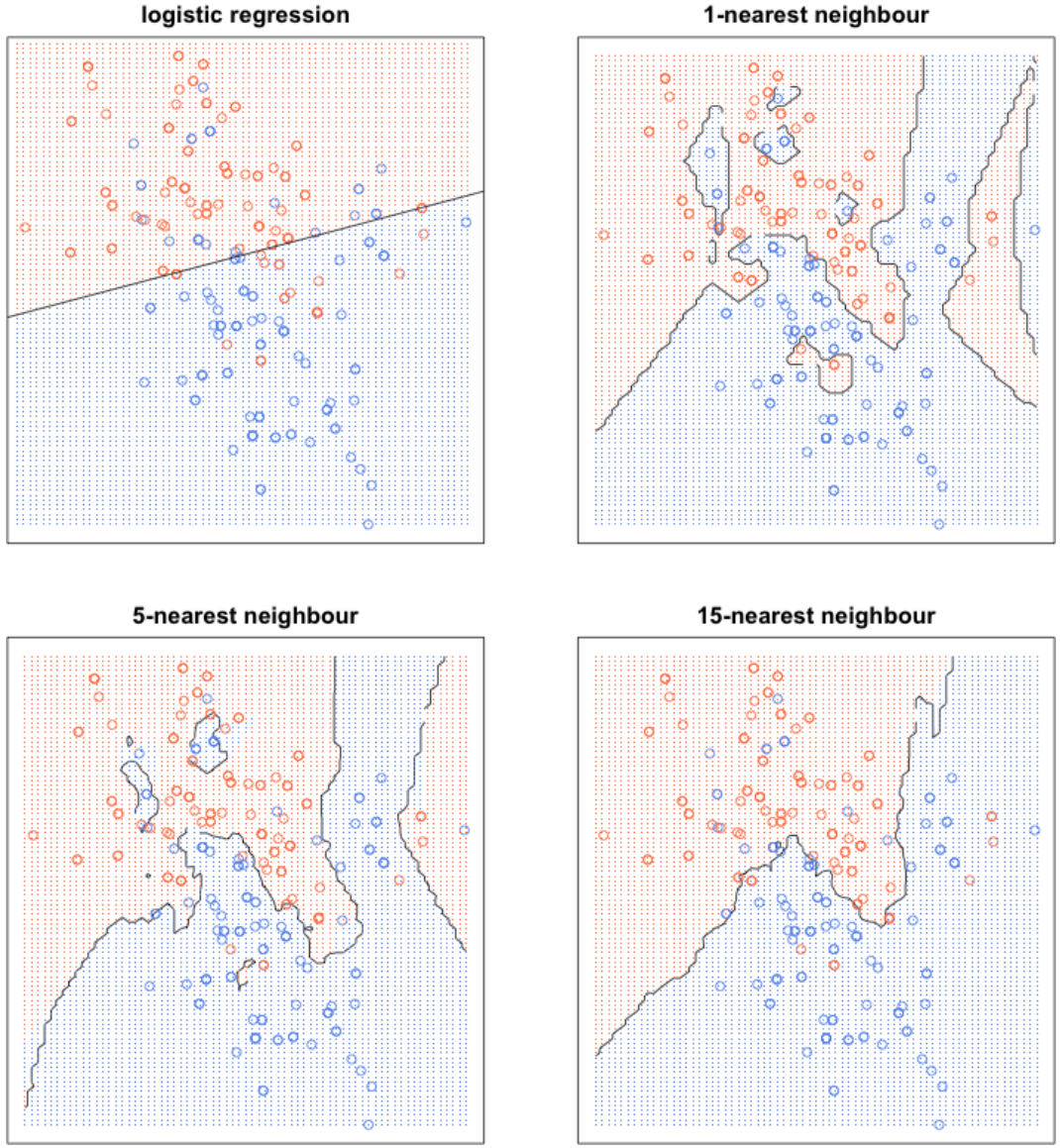
CLASSIFICATION



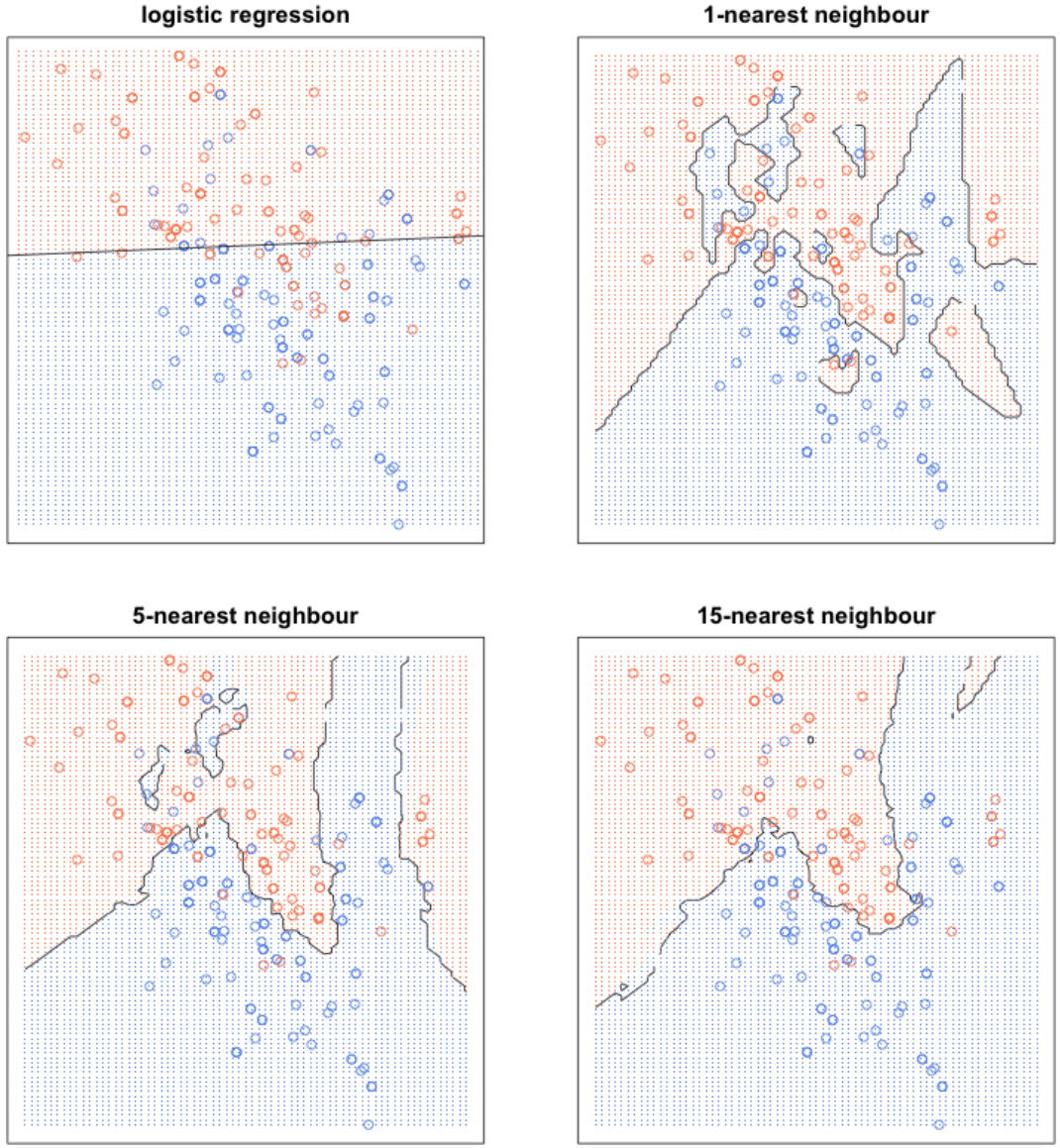
CLASSIFICATION - BOOTSTRAP SAMPLE 1



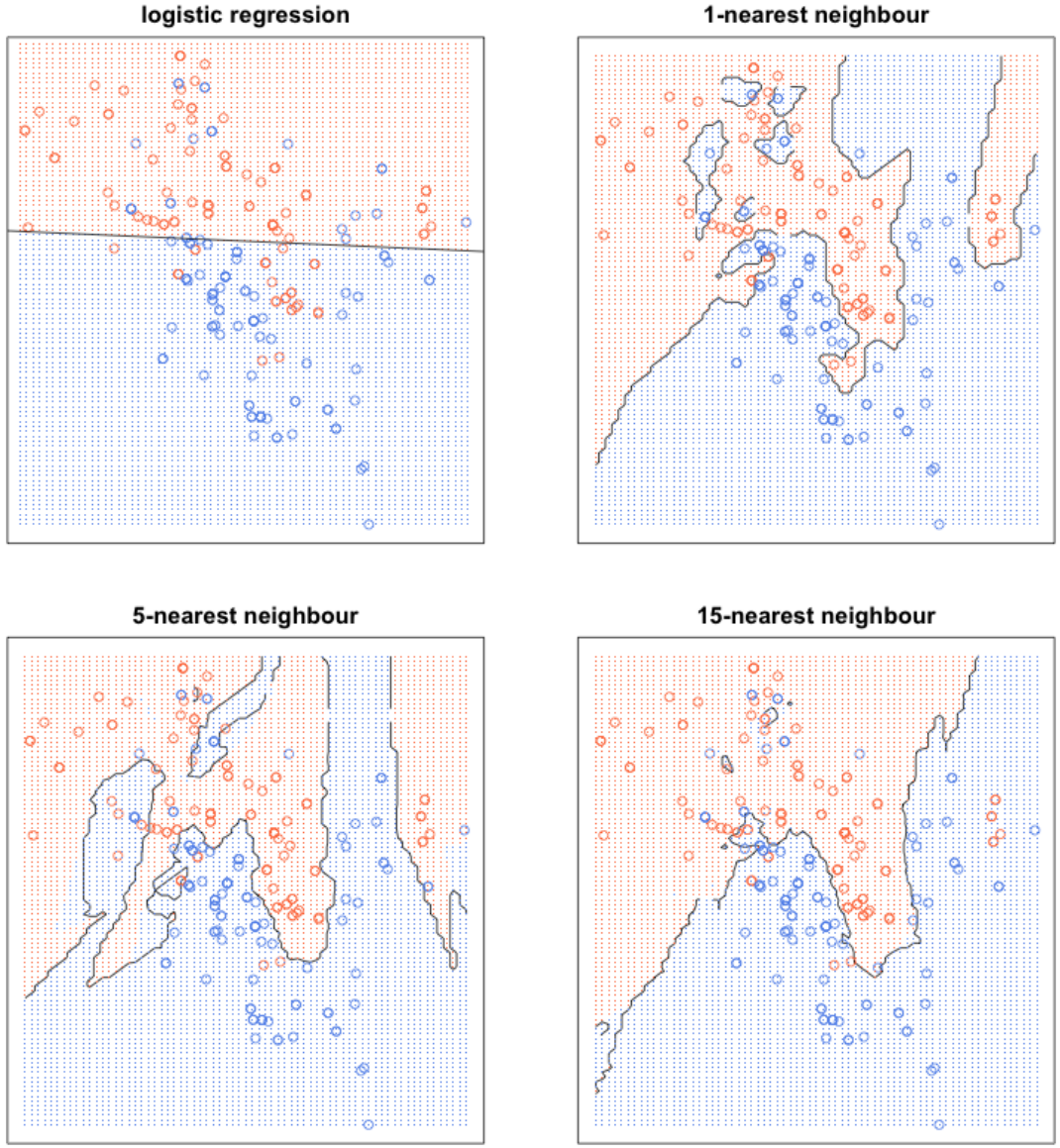
CLASSIFICATION - BOOTSTRAP SAMPLE 2



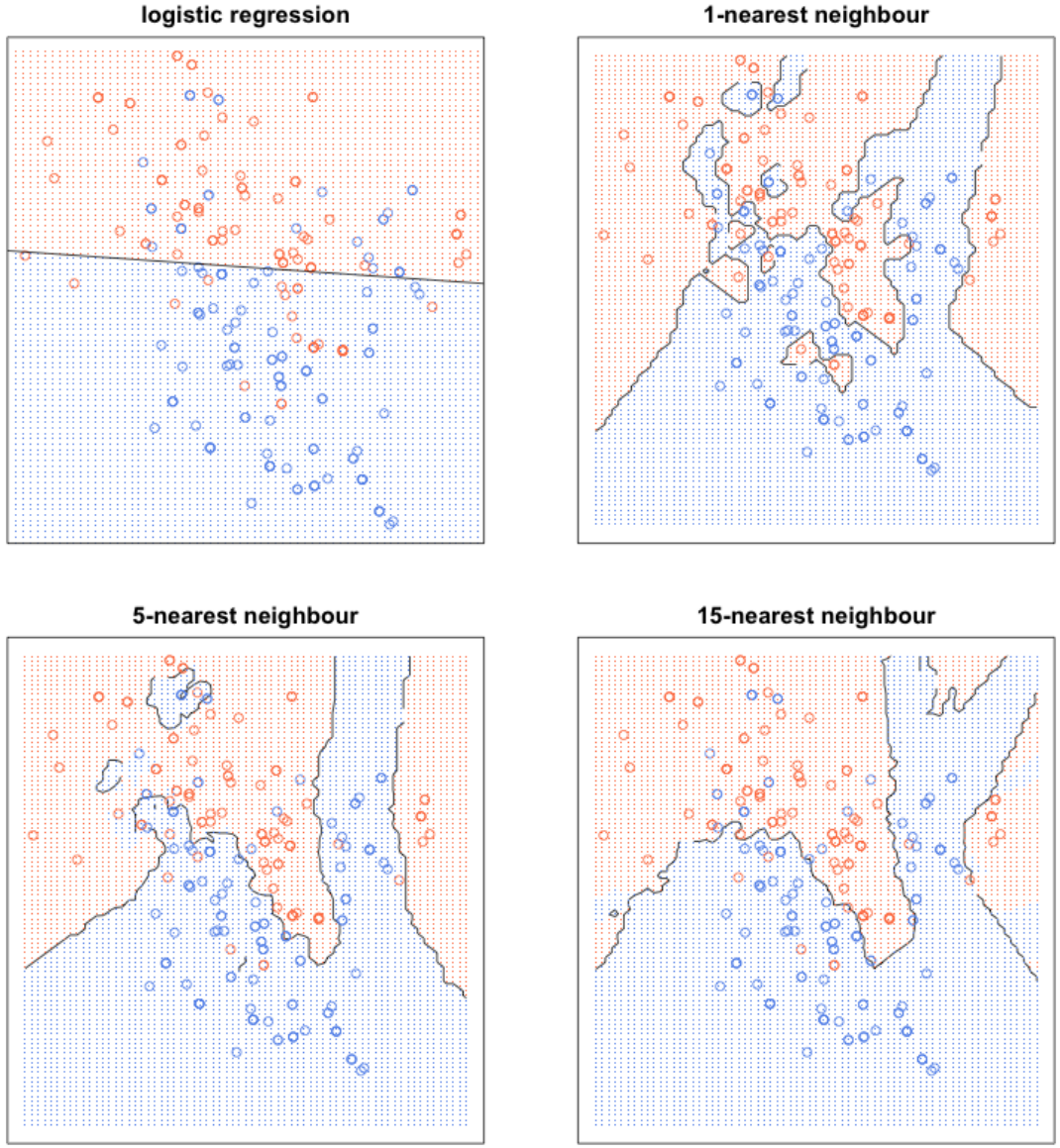
CLASSIFICATION - BOOTSTRAP SAMPLE 3



CLASSIFICATION - BOOTSTRAP SAMPLE 4



CLASSIFICATION - BOOTSTRAP SAMPLE 5



Overfitting

- Many problems in machine learning need **flexible models**:
  - Flexible mean (non-linear)
  - Flexible decision boundary in classification
  - Flexible distributions (heavy tails for outliers)
- But allowing for too much flexibility leads to **overfitting**.
- Overfitting leads to poor **generalization performance** on **new** data.

Regularization

- The solution to the flexible-without-overfitting dilemma is **regularization**.
- Example: polynomial regression

$$y = w_0 + w_1 x + w_2 x^2 + ... + w_p x^p + \varepsilon \qquad \varepsilon \overset{iid}{\sim} N(0, \sigma^2)$$

- Two sides of the same (regularization) coin:
  - **Complexity penalty**

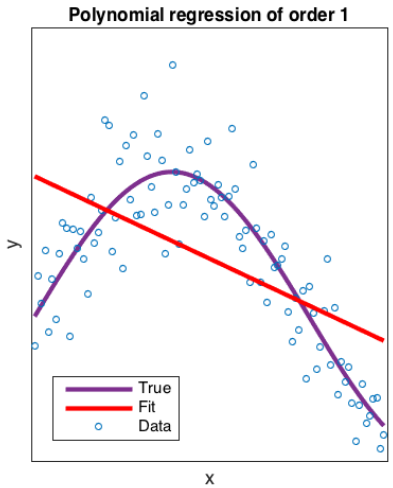
$$\log p(y_1, ..., y_n | \mathbf{w}) - \lambda \sum_{j=1}^{p} w_j^2$$

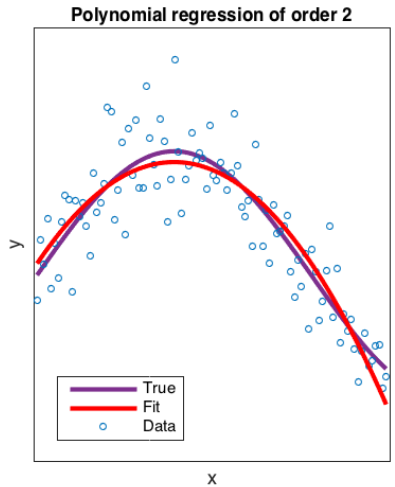
  - **Bayesian prior**

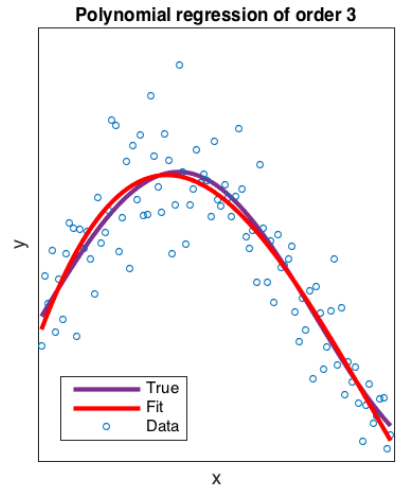
$$w_j \overset{iid}{\sim} N\left(0, \lambda^{-1}\right)$$

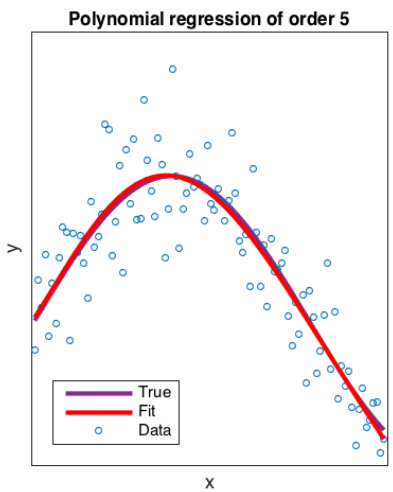
- Regularization or **Shrinkage parameter** λ.

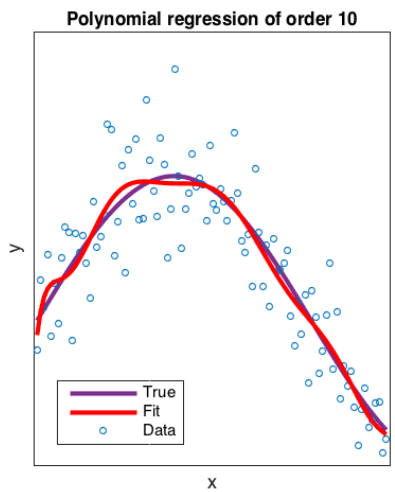
Overfitting - Polynomials

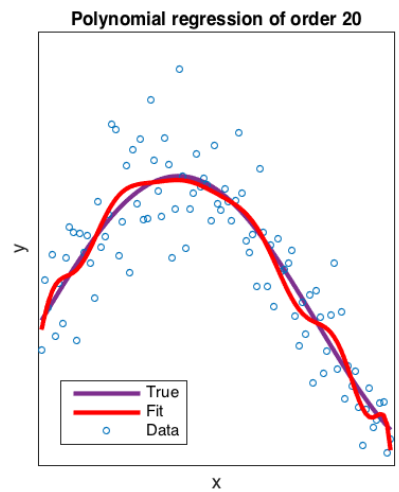




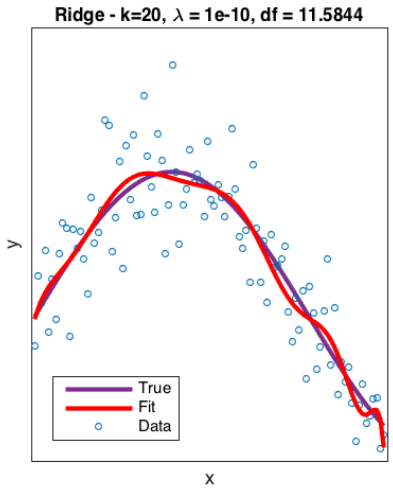


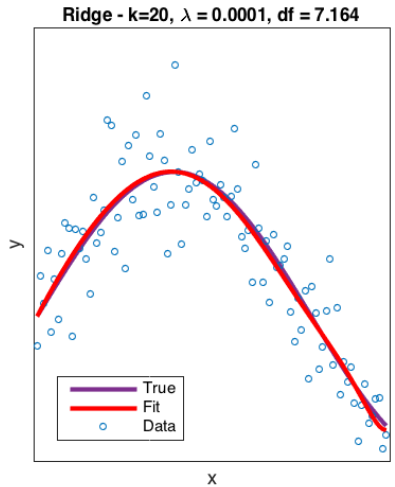


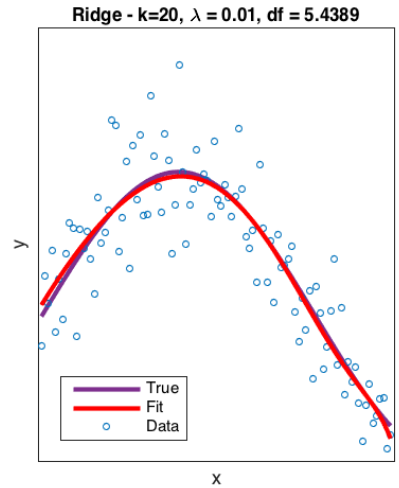


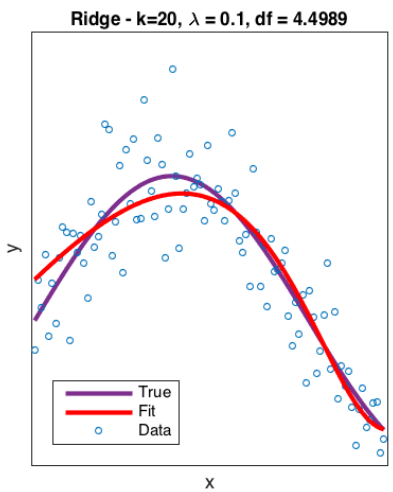


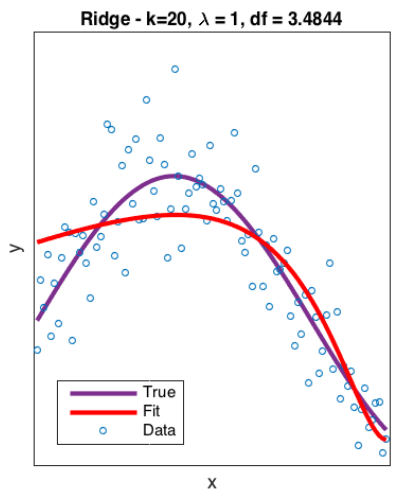
OVERFITTING - SMOOTHNESS PRIOR

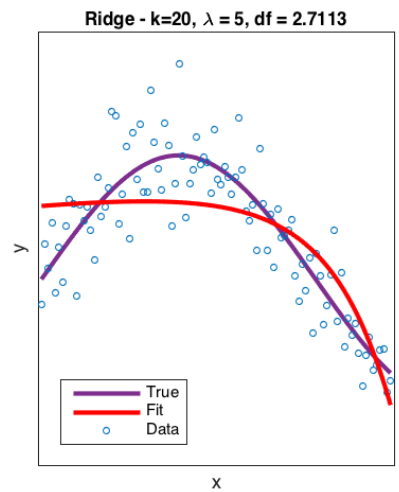












Prediction and Model evaluation

- The ultimate test of a model: does it **predict new data** well?
- Split the data into **Training** and **Test** sets.
- Sometimes split into Training, Validation and Testing.
- The test set is sometime called **hold-out sample**.
- K**-fold cross-validation**:
  - Partition the data into K sets (folds).
  - Use $K-1$ folds for training and then predict the remaining fold.
  - Repeat K times, each time with a new fold as test.

Evaluating a regression model

- Point predictions based on features $\mathbf{x}_i$: $\hat{y}_i = f(\mathbf{x}_i)$.
- **Mean Squared Prediction Errors** (MSPE)

$$MSPE = \frac{1}{n_{test}} \sum_{i \in Test} (y_i - f(\mathbf{x}_i))^2$$

- $RMSPE = \sqrt{MSPE}$
- **Log Predictive Score** (LPS)

$$LPS = \frac{1}{n_{test}} \sum_{i \in Test} \log p(y_i | \mathbf{x}_i, \hat{\mathbf{w}})$$

- Om $p(y_i|\mathbf{x}_i, \hat{\mathbf{w}})$ is Gaussian, then $LPS \propto -MSPE$.

Evaluating a classifier: confusion matrix

- **Confusion** matrix:

		Truth	
		Positive	Negative
Decision	Positive	tp	fp
	Negative	fn	tn

- tp = true positive, fp = false positive, fn = false negative, tn = true negative.
- Example: **spam/ham**

		Truth	
		Spam	Ham
Decision	Spam	tp	fp
	Ham	fn	tn

Evaluating a classifier: Accuracy

- **Accuracy** is the proportion of correctly classified items

$$\text{Accuracy} = \frac{tp + tn}{tp + tn + fn + fp}$$

		Truth	
		Positive	Negative
Decision	Positive	**tp**	fp
	Negative	fn	**tn**

Evaluating a classifier: Precision

- **Precision** is the proportion of truly positive items among those signaled as positive:

$$\text{Precision} = \frac{tp}{tp + fp}$$

		Truth	
		Positive	Negative
Decision	Positive	**tp**	fp
	Negative	fn	tn

- High precision: when you say positive we can trust you to be right. People pointed out as fraudulent are almost always frauds.

Evaluating a classifier: Recall

- **Recall** is the proportion of signaled positive items among those that are truly positive:

$$\text{Recall} = \frac{tp}{tp + fn}$$

		Truth	
		Positive	Negative
Decision	Positive	**tp**	fp
	Negative	fn	tn

- High recall: you will find the positive items. Don't be fraudulent, you will be caught.
- Recall is also called the **True Positive Rate** (**TPR**)
- There is a trade-off between Precision and Recall.

Evaluating a classifier: False Positive Rate

- False Positive Rate (FPR) is the proportion of signaled positive items among those that are truly negative:

$$\text{FPR} = \frac{fp}{fp + tn}$$

		Truth	
		Positive	Negative
Decision	Positive	tp	**fp**
	Negative	fn	tn

- Low FPR: you will very rarely signal a positive for negative items. People will not be falsely accused of fraud.

Evaluating a classifier: ROC curve

- Precision and recall depends on the **decision threshold.**
- $Pr(\text{Spam}|\text{text in an email}) = 0.9$. Do we send it to the spam-box?
- Is $Pr(\text{Spam}|\text{text in an email}) > 0.5$ a good threshold?
- **Optimal decisions** depend on the consequences.
- **ROC-curve**: Receiver Operating Characteristic.
- ROC: Plots the true positive rate (TPR) against the false positive rate (FPR) at various thresholds.
- **AUC** = Area Under Curve. Area under the ROC curve.

Evaluating a classifier: ROC curve