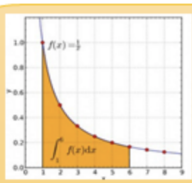
# What is Statistical Learning?

*"Statistical learning refers to a vast set of tools for understanding data."*

*— ISL*

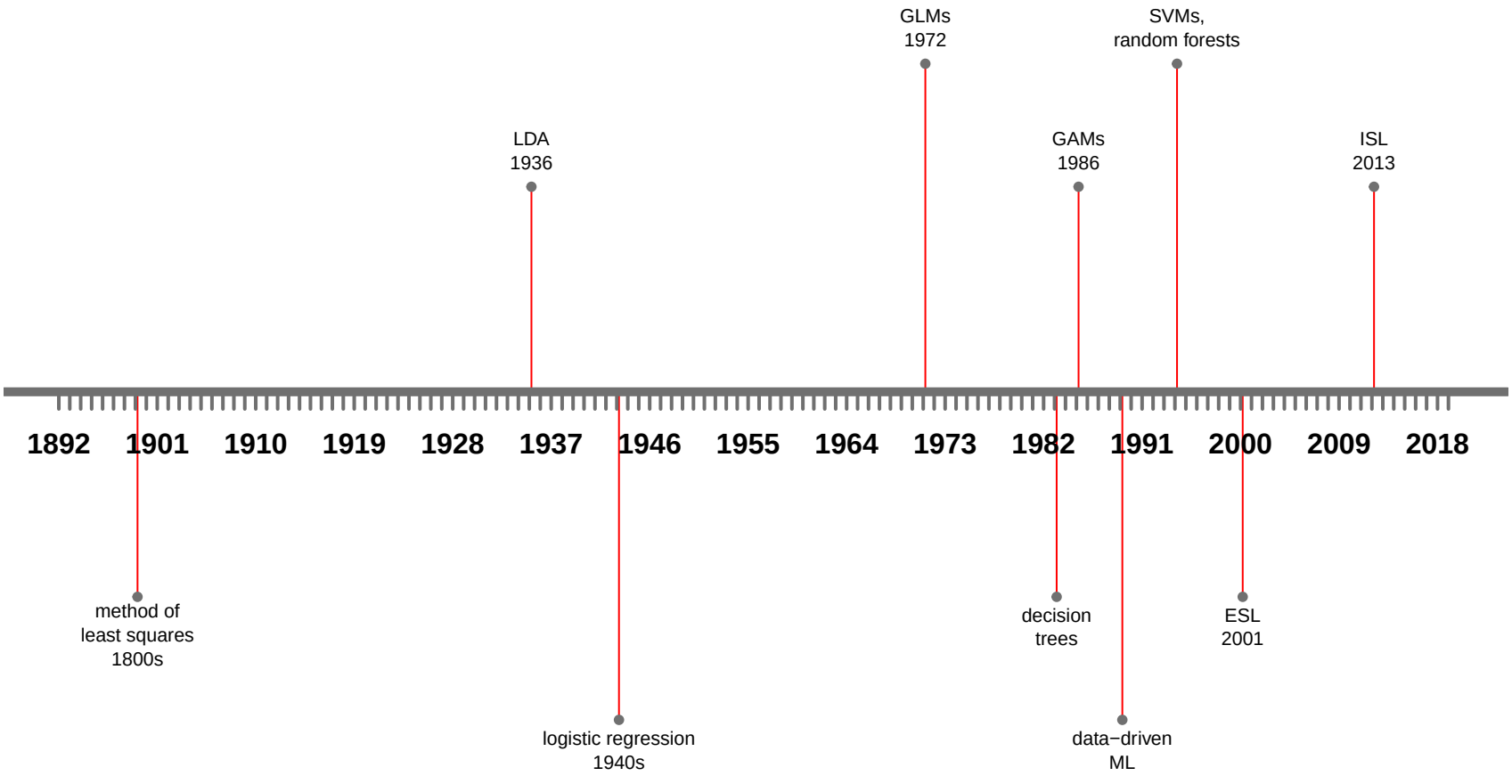
# Statistical vs. Machine Learning?



**Statistics** +  **Machine Learning** = $\sum_{i=1}^{n}(y_i - \sum_j x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j|$ **Statistical Learning**

| | Statistics | Machine Learning | Statistical Learning |
|---|---|---|---|
| Subfield of... | Mathematics | Computer Science (AI) | Statistics & Machine Learning |
| Focus on... | Building models with explicitly programmed instructions | Creating systems that learn from data | Sets of tools for modeling and understanding complex data |
| Purpose | Inferences; Relationships between variables | Optimization; Prediction accuracy | Building statistical models for prediction; understanding data |
| Prior assumptions about data | Some knowledge about population usually required | None | Some knowledge about population may be required |
| Dimensionality of data | Usually applied to low-dimensional data | Usually applied to high dimensional data; ML learns from data | Usually applied to high dimensional data |
| Knowledge overlap | No ML knowledge required | Some stats knowledge usually needed: stats is basis for algorithms | Knowledge of statistics and ML required |

# Timeline of Statistical Learning



# Elements of Statistical Learning (2001)

- One of the first reference textbooks on fundamentals of statistical machine learning
- More comprehensive than ISL in terms of number of approaches and depth
- More technical details & in-depth mathematical treatment

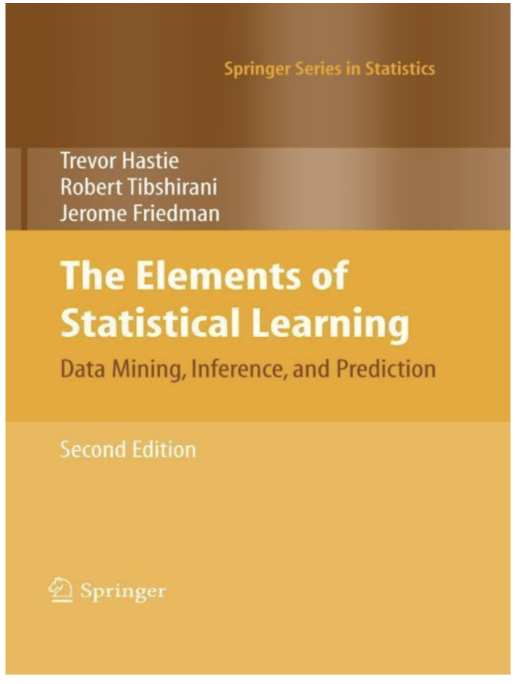



Figure 1: Elements of Statistical Learning

# Introduction to Statistical Learning (2013)

- More of a hands-on introduction to computational aspects of statistical learning with real-world data.
- Uses R as 'the language of choice for academic statisticians' (also a bridge across disciplines!)

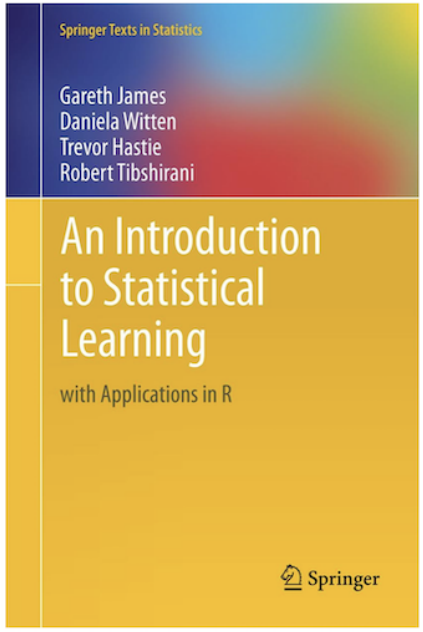



Figure 2: Introduction to Statistical Learning

# Statistical Learning Approaches

**Supervised methods**

- Regression (observe input & quantitative output)
- Classification (observe input & categorical output)

**Unsupervised methods**

- Data are not labeled (observe only input)
- Goal may be learning relationships among variables and data structure (e.g. how many population clusters are there?)

# Supervised Learning: Regression or Classification?

- Predicting whether or not a patient has cancer based on expression patterns of 5,000 genes?
- Predicting quantity of a certain protein, given expression patterns of 5,000 genes?
- Estimating plant height according to variation at 5,000 positions in the genome?
- Determine whether pixels in a satellite image indicate an agricultural field, river, or forest?
- Determine how many different types of bacterial communities have been sampled using microbiome sequence data from 10 tissues?

# Another definition...

Consider a quantitative response, $Y$, and $p$ different predictors, $X_1, X_2, ..., X_p$.

We assume some relationship between $Y$ and $X = (X_1, X_2, ..., X_p)$, which can be written in the general form:

$$Y = f(X) + \epsilon$$

where $f$ is a fixed but unknown function of $X_1, X_2, ..., X_p$ and $\epsilon$ is a random error term which is independent of $X$ and has mean zero.

# What is Statistical Learning?

*"Statistical learning is a set of tools for estimating $f(X)$."*
*— ISL*

How should we choose what tool to use to estimate $f(X)$?

# Why estimate $f$?

1. Prediction

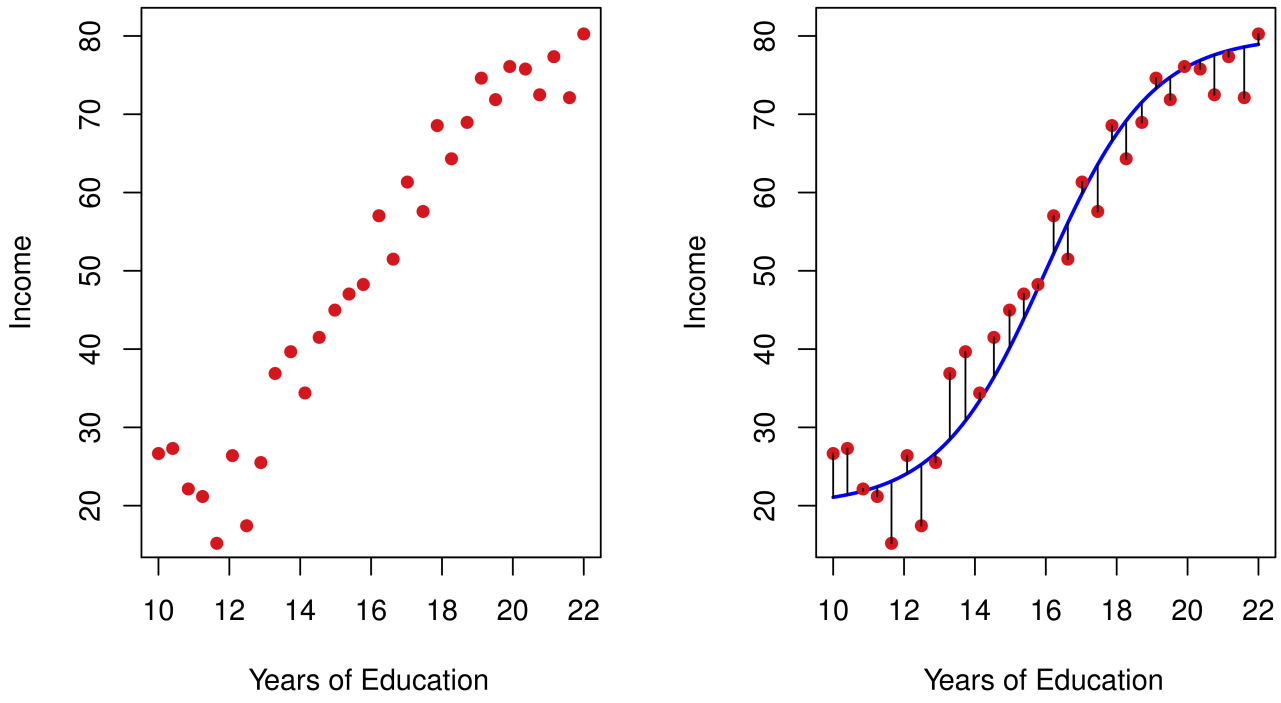



Figure 3: ISL Fig. 2.2

# Linear model fit to Income data

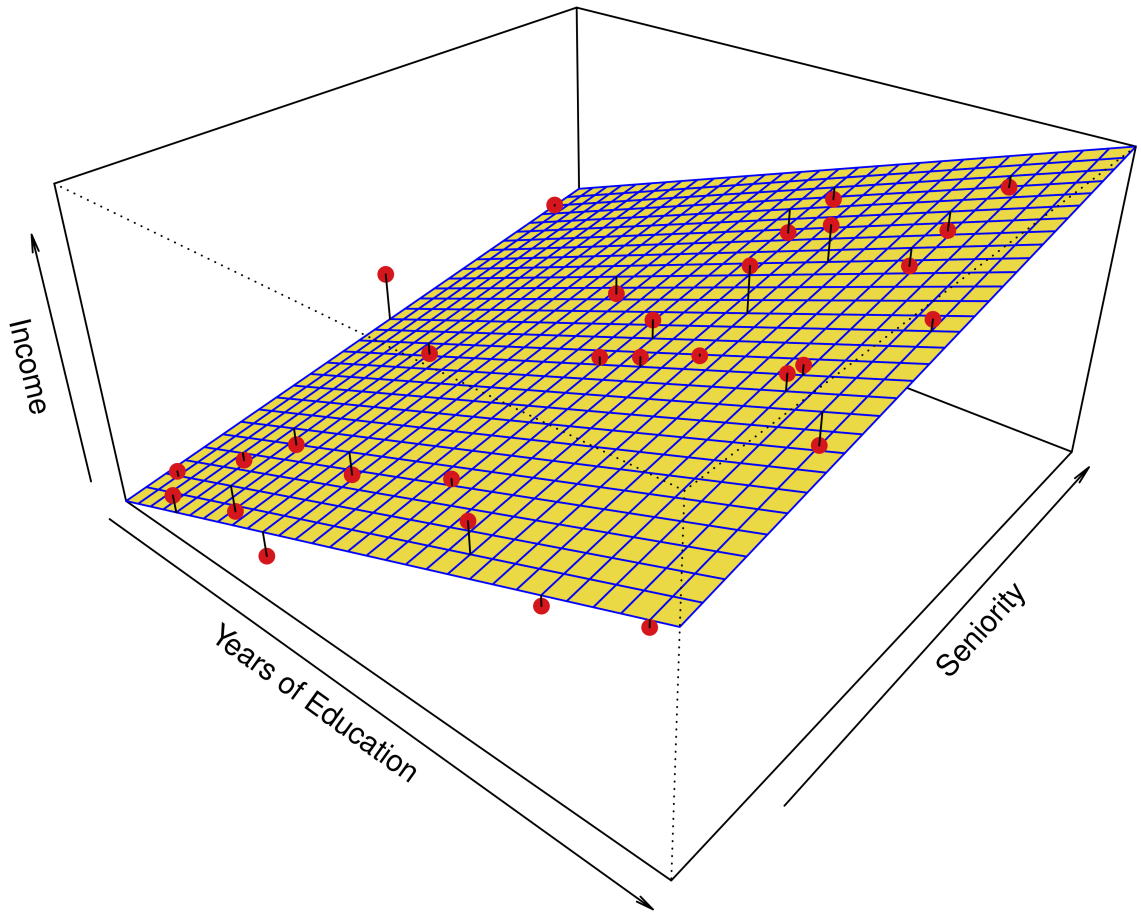



Figure 4: Fig 2.4

linear model fit by least squares

# Non-parametric model fit to data

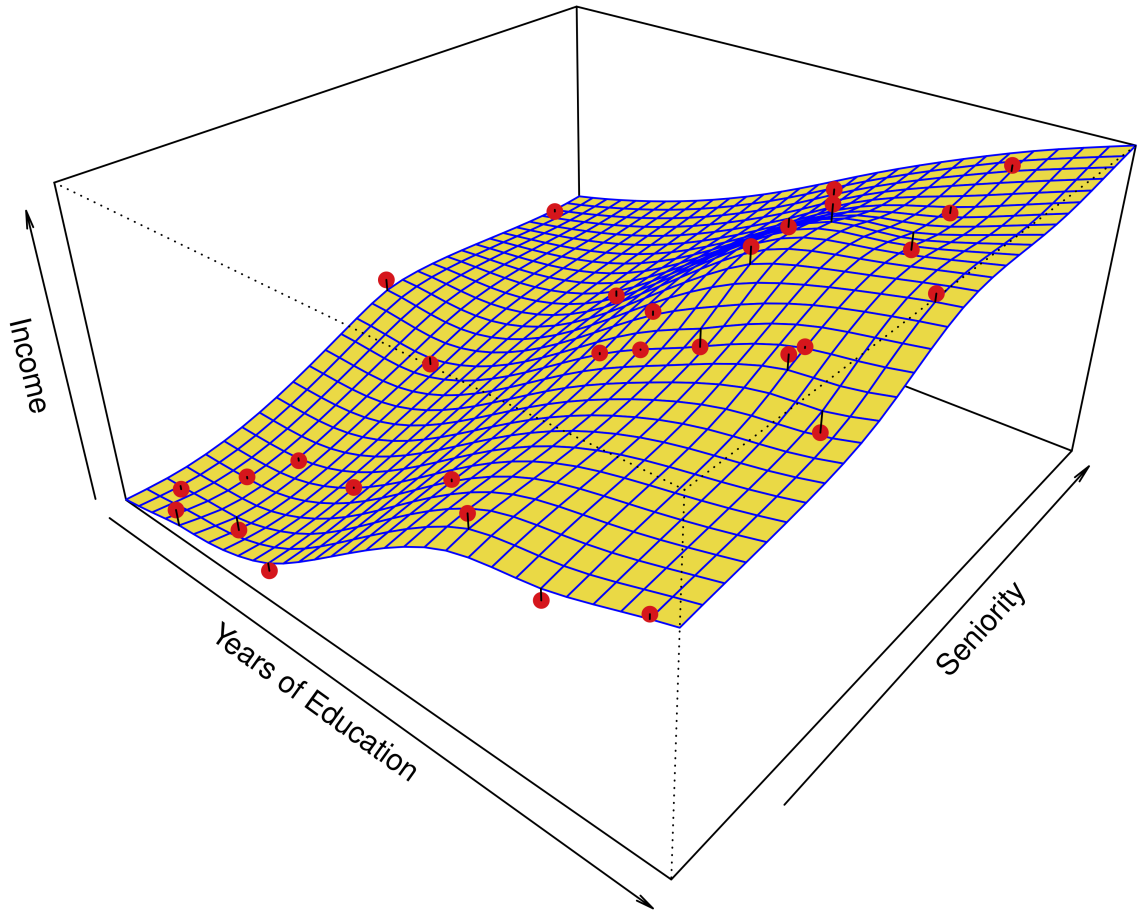



Figure 5: Fig 2.5

fit w/thin-plate spline

Considering our prediction of $Y$:

$$\hat{Y} = \hat{f}(X)$$

The expected value of the squared error is then:

$$E(Y - \hat{Y})^2 = [f(X) - \hat{f}(X)]^2 + \text{Var}(\epsilon)$$

**We can choose different modeling techniques to improve our estimate of $f$, and minimize the reducible error.**

# Why estimate $f$?

2. Inference

- Which predictors are associated with the response?
- What is the relationship between the response and each predictor?
- Can the relationship between $Y$ and each predictor be adequately summarized using a linear equation, or is it more complicated?

# Trade-offs: Flexibility vs. interpretability

- Whether we are interested in inference vs. prediction influences how we choose to estimate $f$.
- It determines whether we might choose a **parametric** vs. **non-parametric** approach.


Figure 6: Fig. 2.7

# Parametric methods

- Assume a specific form for $f$.
  - e.g. the linear model is an example of a parametric model.

$$f(X) = \beta_0 + \beta_1 X_1 + \beta_1 X_2 + ... + \beta_p X_p$$

- Fit/train the model
  - e.g. using ordinary least squares (Chp. 3) or other methods (Chp. 6).
- Instead of having to estimate an arbitrary $p$-dimensional function, we only need to estimate $p + 1$ coefficients $\beta_0, \beta_1, ..., \beta_p$.

# Non-parametric methods

- Do not make explicit assumptions about the form of $f$.
- More flexible, can provide a better fit to $f$.

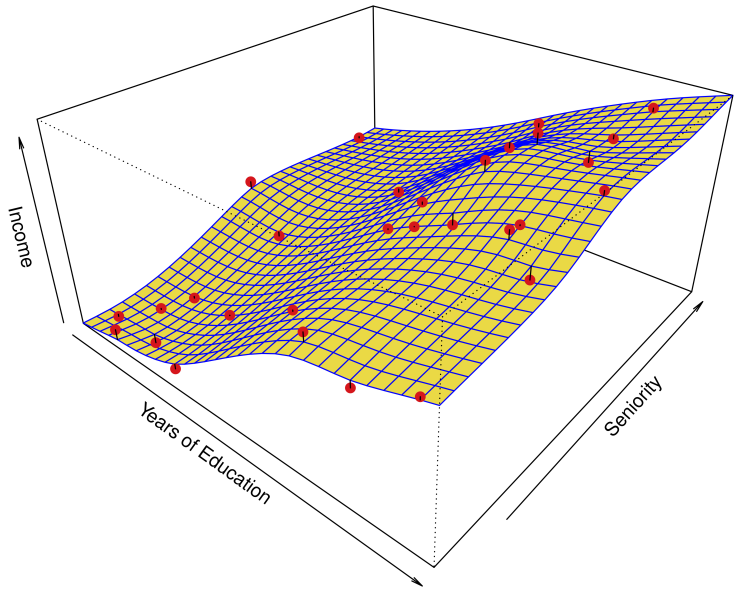



Figure 7: Fig 2.5

fit w/thin-plate spline

# Non-parametric methods

- Typically need larger sample size compared to parametric approach to get accurate estimate of $f$.
- Can suffer from overfitting (model learns 'noise' in the training data & performs well on training data but poorly on test data)
- More difficult to interpret

# Parametric vs. non-parametric methods

**Linear methods (Part I)**
Chp. 3: Linear methods for regression
Chp. 4: Linear methods for classification
Chp. 5: Resampling
Chp. 6*: Alternatives to fitting with least squares

**Non-linear methods (Part II)**
Chp. 7: Non-linear methods w/single & multiple input variables
Chp. 8: Tree-based methods
Chp. 12: Unsupervised methods
Chp. 9: Support vector machines
Ch. 10*: Deep Learning

*Lectures optional for MBS students, see schedule

# Measuring the Quality of Fit

- In regression, one commonly used measure is the mean squared error (MSE).
- The MSE is a measure of how close the predicted response is to the true response for an observation.

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{f}(x_i))^2$$

- We want to choose the method that gives the lowest MSE on a *testing* dataset, not the lowest MSE on a *training* dataset

# Measuring the Quality of Fit

- No guarantee that the model with the lowest training MSE will also have the lowest test MSE.
- Note characteristic 'U-shape' of test MSE (red).

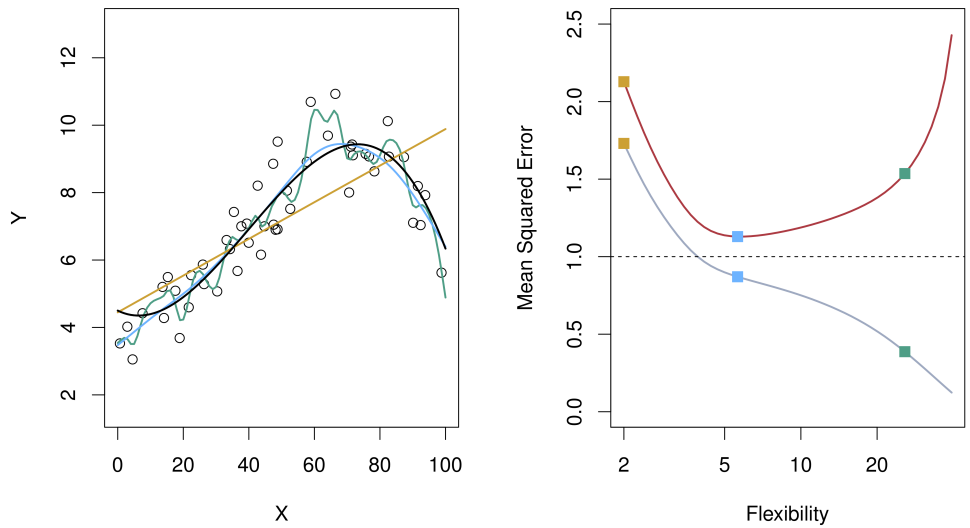



Figure 8: Fig 2.9

Left: Three estimates of $f$ based on simulated data (open circles); linear regression (orange line), and two different smoothing splines (blue and green curves) Right: Training MSE (grey curve) and

# Measuring the Quality of Fit

- Depending on the true shape of $f$, more interpretable methods like linear regression may provide a very good fit to the data.

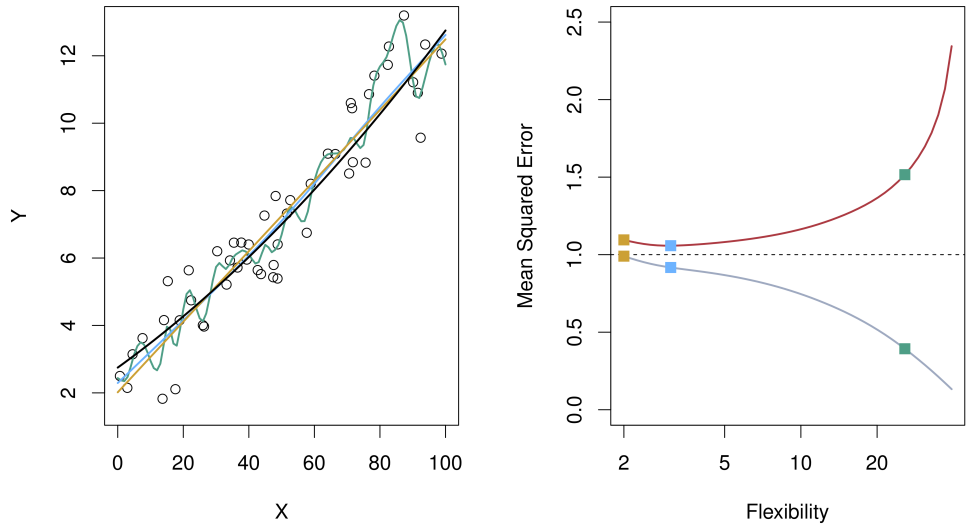



Figure 9: Fig 2.10

ISL Fig. 2.10

# How do we minimize the expected test MSE?

Imagine repeatedly estimating $f$ using a using a large number of training sets, and testing each of the $\widehat{f}$ at a given value, $x_0$.

**The expected test MSE at $x_0$ is given by:**

$$\mathbb{E}(y_0 - \widehat{f}(x_0))^2 = \text{Var}(\widehat{f}(x_0)) + [\text{Bias}(\widehat{f}(x_0))]^2 + \text{Var}(\epsilon)$$

Average across all $x_0$ in test set to get overall expected test MSE.

# Trade-off: Bias vs. Variance

To minimize the average test error, we need to select a statistical learning method that simultaneously has low variance and low bias.

# Trade-off: Bias vs. Variance

*Variance* is the amount by which $\widehat{f}$ changes from one training set to another. Ideally, $\widehat{f}$ does not change a lot between different training sets.

$$\text{Var}(\hat{f}(x)) = \mathbb{E}[(\hat{f}(x) - \mu)^2]$$

where $\mu = \mathbb{E}[\hat{f}(x)]$

More flexible methods generally have higher variance.

# Trade-off: Bias vs. Variance

*Bias* refers to the error introduced by approximating a complicated problem by a much simpler model.

$$\text{Bias}(\hat{f}(x)) = \mathbb{E}(\hat{f}(x)) - f(x)$$

More flexible methods generally have lower bias.

# Trade-off: Bias vs. Variance

The 'best' method (low variance AND low bias) depends on the true form of $f$.

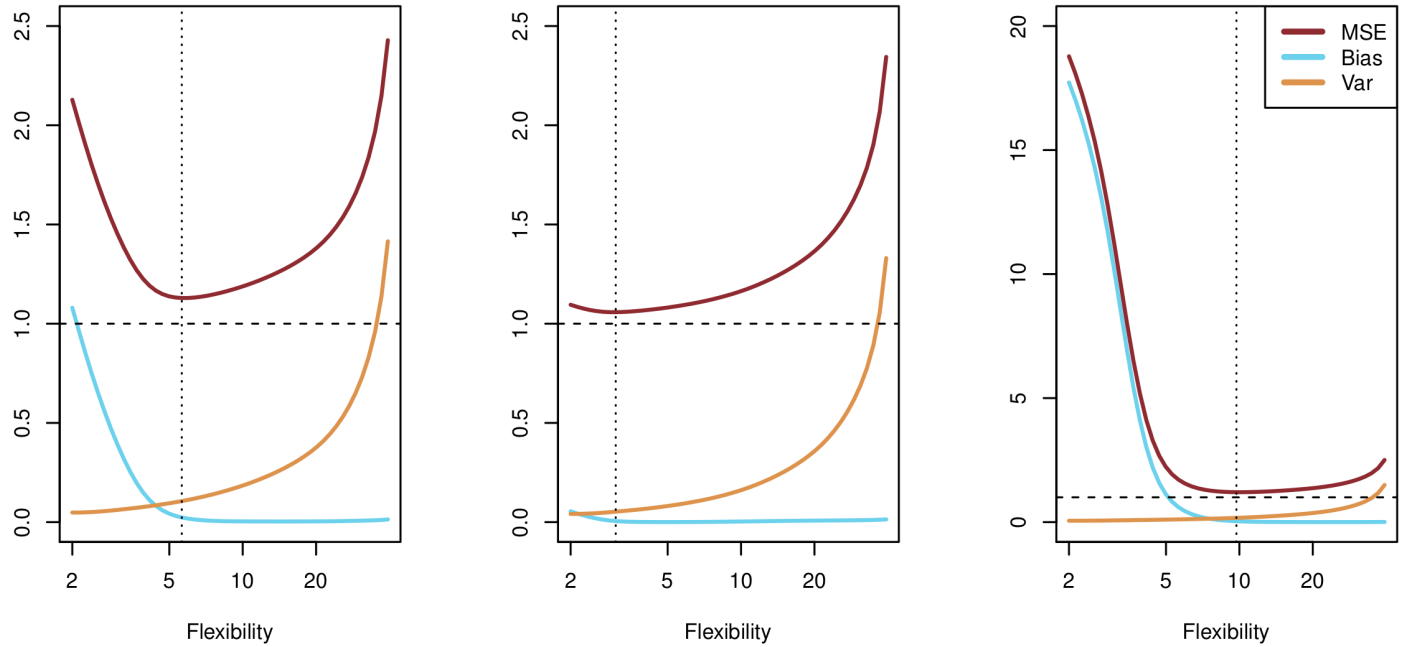



Figure 10: Fig 2.12

# Model Accuracy in Classification

- The test error rate is minimized on average by a simple classifier (the Bayes classifier) that *assigns each observation to the most likely class, given its predictor values.*
- Test error is given by

$$\text{Avg}(I(y_0 \neq \hat{y}_0))$$

where $I(y_0 \neq \hat{y}_0) = 1$ if $y_0 \neq \hat{y}_0$ but 0 otherwise.

# Model Accuracy in Classification

With 2 classes, Bayes decision boundary corresponds to predicting class one if $Pr(Y = 1|X = x_0) > 0.5$ and class two otherwise

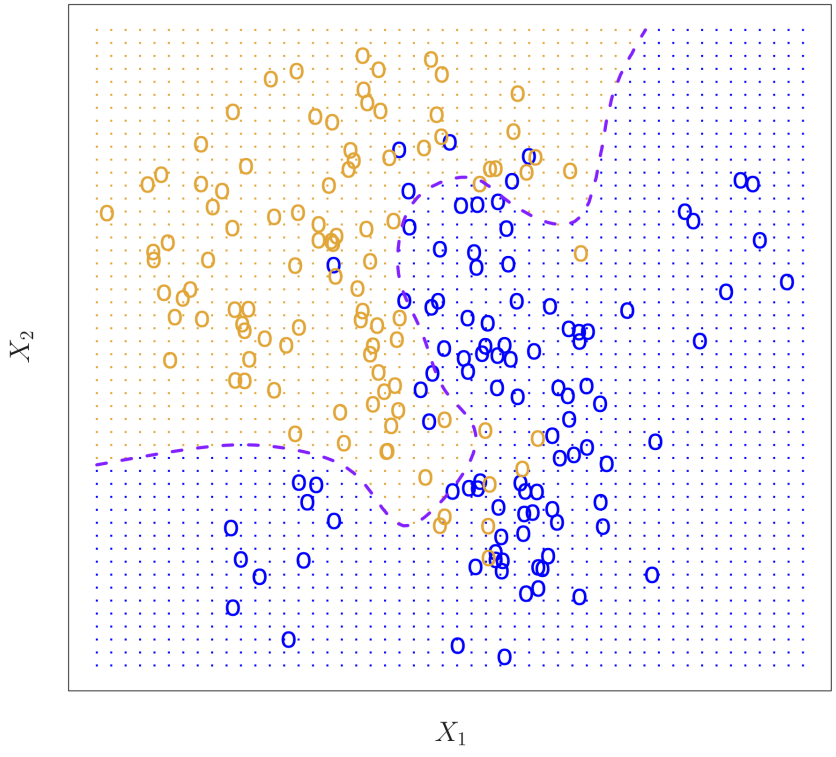



Figure 11: Fig 2.13

ISL Fig. 2.13; Purple dashed line: Bayes decision boundary

# Non-parametric classification: KNN

In reality, we never know the conditional probability of $Y$ given $X$! The Bayes Classifier boundary is therefore an unattainable 'gold standard'. But, we can estimate it using various methods (logistic regression, KNN classification, LDA, QDA).

$K$-Nearest Neighbors classification

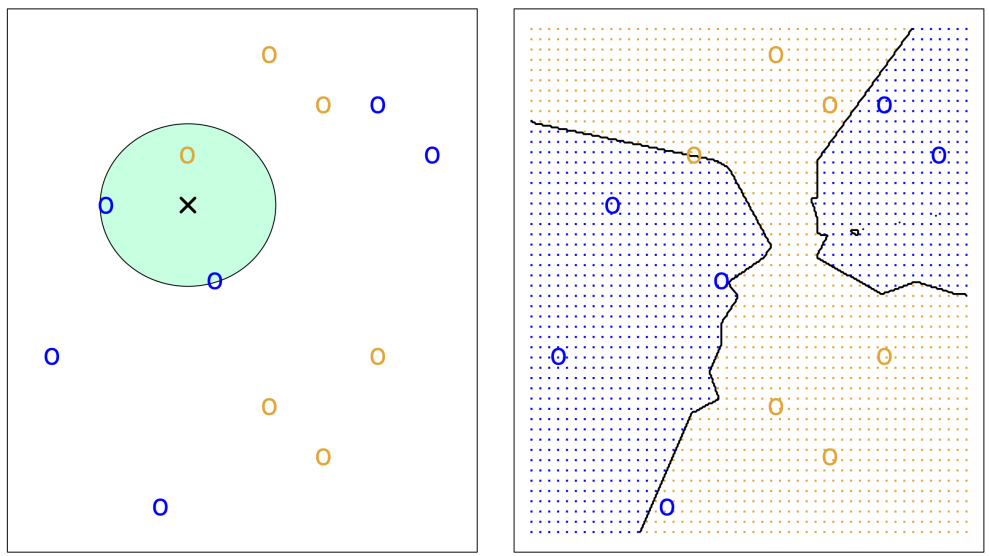


Figure 12: Fig 2.14

ISL Fig. 2.14. KNN decision boundary for $K$=3

# Non-parametric classification: KNN

Choosing appropriate level of flexibility

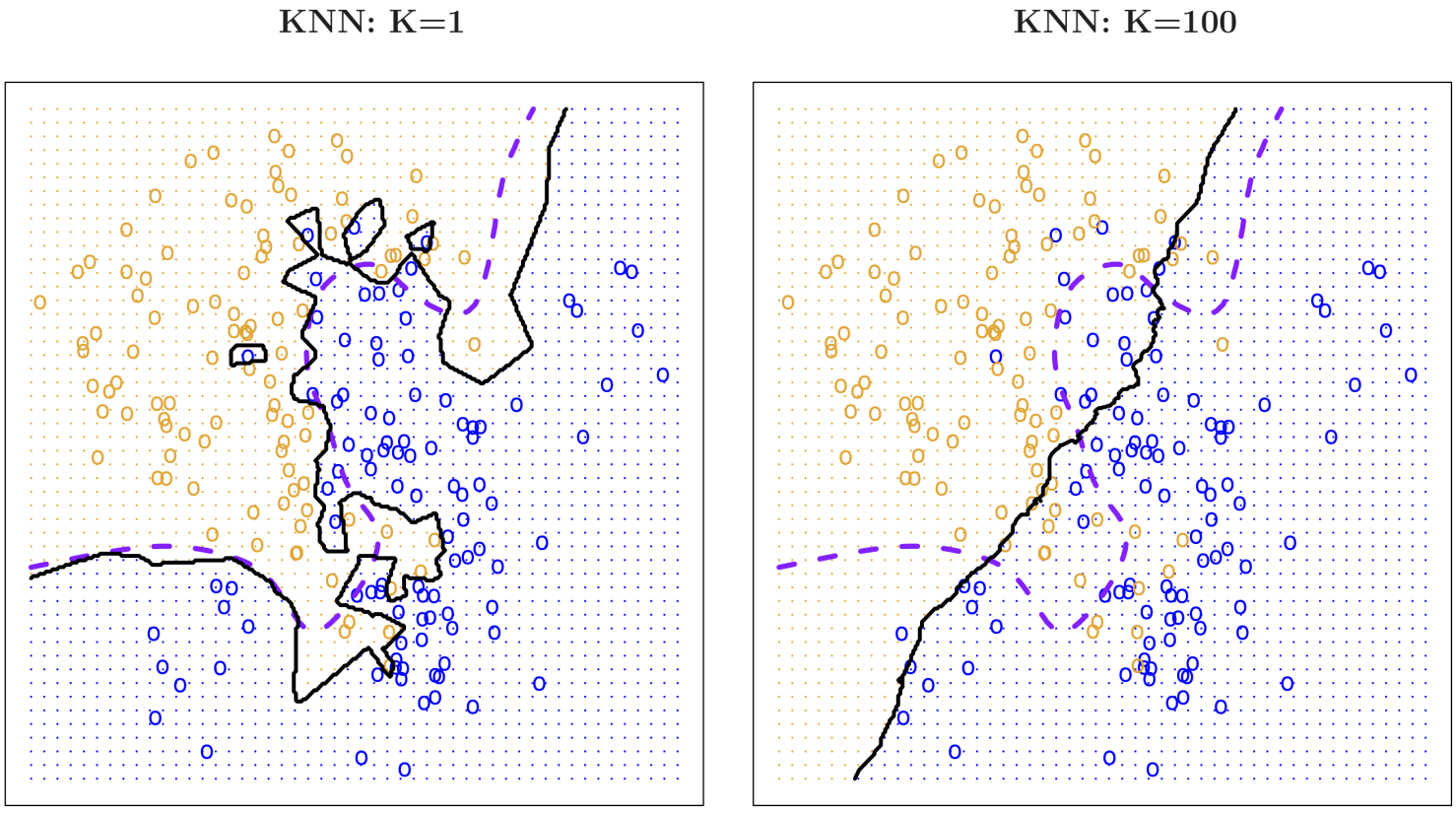



Figure 13: Fig 2.16

ISL Fig. 2.16

# Non-parametric classification: KNN

## Bias-variance trade-off

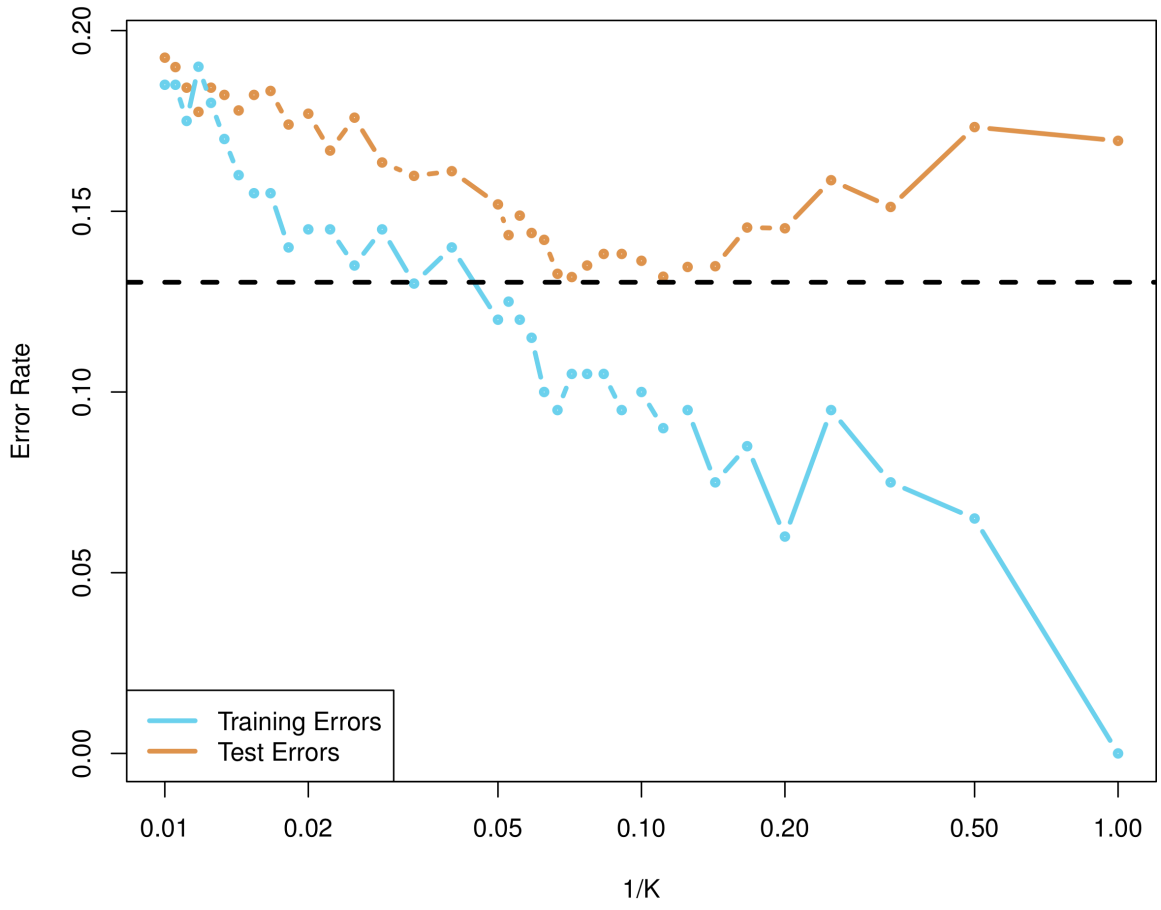



Figure 14: Fig 2.17

ISL Fig. 2.17

# In summary:

- Statistical learning refers to a vast set of tools for understanding data, and estimating $f(X)$.
- How we choose $f(x)$ is shaped by a trade-offs.
- Whether we are more interested in accuracy vs. interpretability determines whether we might choose a more flexible model and whether the model is characterized by relatively higher bias vs. variance.