

DATA SCIENCE

Business Administration, Analytics and Information Systems

Στόχοι Μαθήματος

Κατανόηση βασικών εννοιών:

1. μηχανικής μάθησης (είδη μηχανικής μάθησης, μέθοδοι εκπαίδευσης, μέτρηση ακρίβειας),
2. παλινδρόμησης, δέντρων αποφάσεων και μηχανών διανυσμάτων υποστήριξης,
3. αλγορίθμων ομαδοποίησης,
4. μεθόδων επιλογής χαρακτηριστικών και μείωσης διάστασης των δεδομένων,
5. εξοικείωση και χρήση R
6. ικανότητα ανάλυσης προβλημάτων και επιλογής του καταλληλότερου αλγορίθμου για την επίλυση του εκάστοτε προβλήματος
7. επίλυση συχνών προβλημάτων και λήψη μέτρων για την αποφυγή και επίλυσή τους

Προαπαιτούμενα Μαθήματος

- Δεν υπάρχουν αυστηρά προαπαιτούμενα
- Οι σημαντικότερες έννοιες παρουσιάζονται σε κάθε διάλεξη

Αξιολόγηση

Η τελική βαθμολογία προκύπτει:

- ✓ 100% από υποχρεωτικές εργασίες

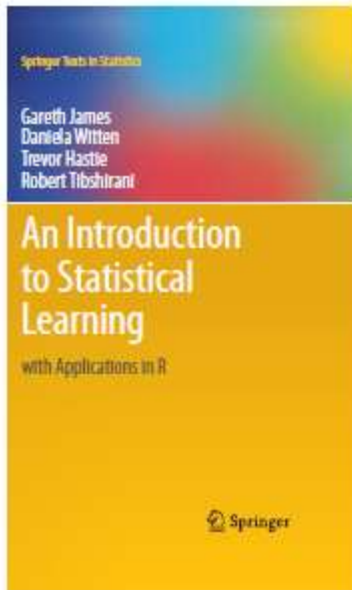
Υποχρεωτικές εργασίες:

- ✓ 3-4 υποχρεωτικές εργασίες
- ✓ Πρόγραμμα υλοποίησης: R
- ✓ Θεματολογία: Εφαρμογή αλγορίθμων και μεθοδολογίας ανάλυσης δεδομένων σε πραγματικά προβλήματα
- ✓ Παραδοτέα: Η λύση της εργασίας σε μορφή .docx και οι κώδικες R που αναπτύσσονται για την υλοποίηση της εργασίας (5-λεπτη παρουσίαση εργασιών)
- ✓ Τι βαθμολογείται: ορθότητα της λύσης | μεθοδολογική προσέγγιση | λεπτομέρεια ανάπτυξης επιχειρημάτων | δομή εργασίας | μορφή εργασίας | αποτελεσματική συγγραφή
- ✓ Σημείο Παράδοσης: eClass μαθήματος | ενότητα εργασίες

Διαδικαστικά

- Το υλικό του μαθήματος θα αναρτάται στο eclass
- Οι διαλέξεις θα πραγματοποιούνται δια ζώσης κάθε εβδομάδα
- Απορίες:
 - ✓ κατά τη διάλεξη (διακόπτετε όποτε θέλετε)
 - ✓ με email: e.vassiliou@aegean.gr

Course Text



Οι διαλέξεις του μαθήματος θα καλύψουν μεγάλο μέρος αυτού του συγγράμματος (2021). Στο τέλος κάθε κεφαλαίου, περιλαμβάνονται εργαστηριακές ενότητες όπου αναπτύσσονται πραγματικά παραδείγματα με τη χρήση της γλώσσας R

WHAT IS STATISTICAL LEARNING?

Chapter 02 – Part I

Outline

➤ What Is Statistical Learning?

- ✓ Why estimate f ?
- ✓ How do we estimate f ?
- ✓ The trade-off between prediction accuracy and model interpretability
- ✓ Supervised vs. unsupervised learning
- ✓ Regression vs. classification problems

What is Statistical Learning?

- Suppose we observe Y_i and $X_i = (X_{i1}, \dots, X_{ip})$ for $i = 1, \dots, n$ (supervised learning)
- We believe that there is a relationship between Y and at least one of the X 's.



- We can model the relationship as

$$Y_i = f(\mathbf{X}_i) + \varepsilon_i \quad (1)$$

- Where f is an unknown function and ε is a random error with mean zero.

What is Statistical Learning?

The approach formalized by equation (1) is general in statistics. That is, when there is variability on y , then we can try to split the total variability in *explained* or *systematic* component and *unexplained* (or *unsystematic*, or *random noise*) component, i.e.,

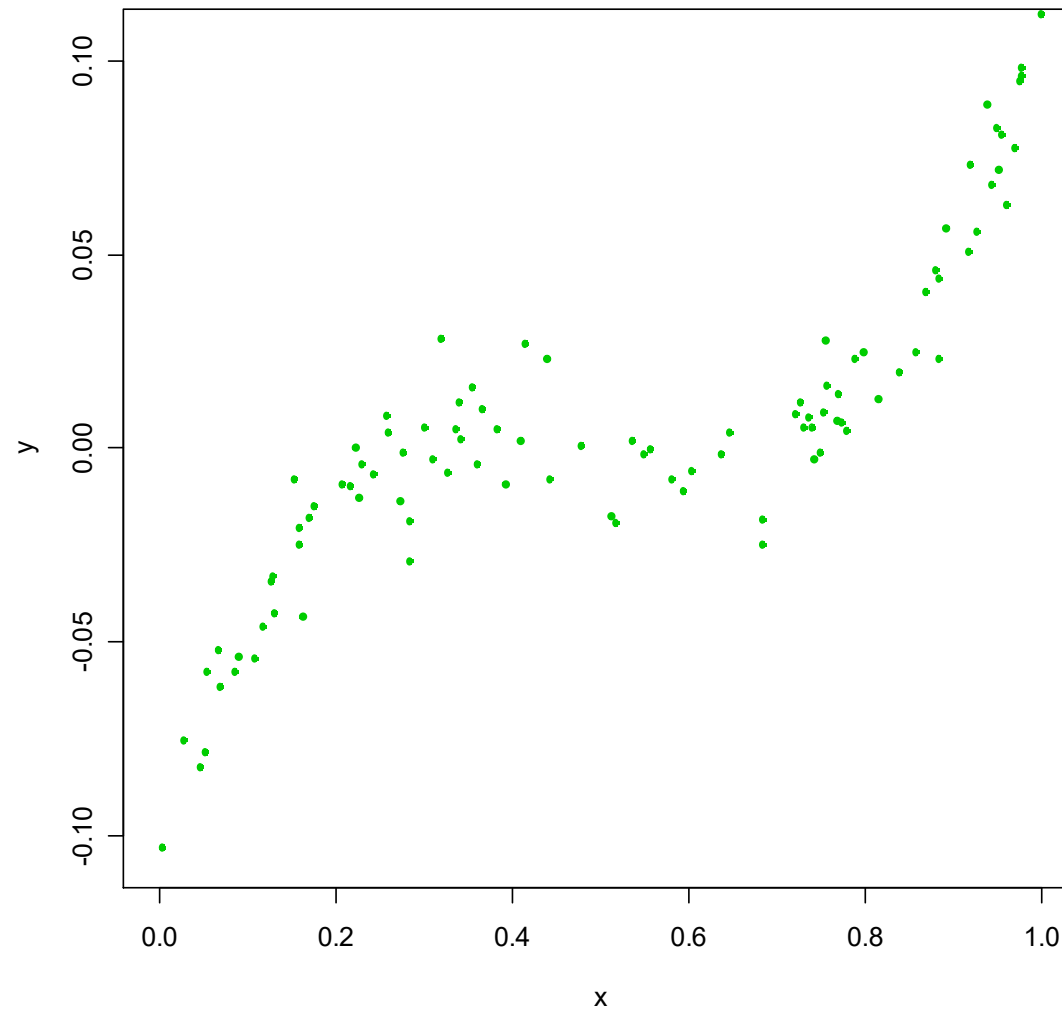
$$y = \text{systematic} + \text{unsystematic}$$

In equation (1) $f(x)$ is the systematic part and ε is the unsystematic part. The goal is to estimate f from available data.

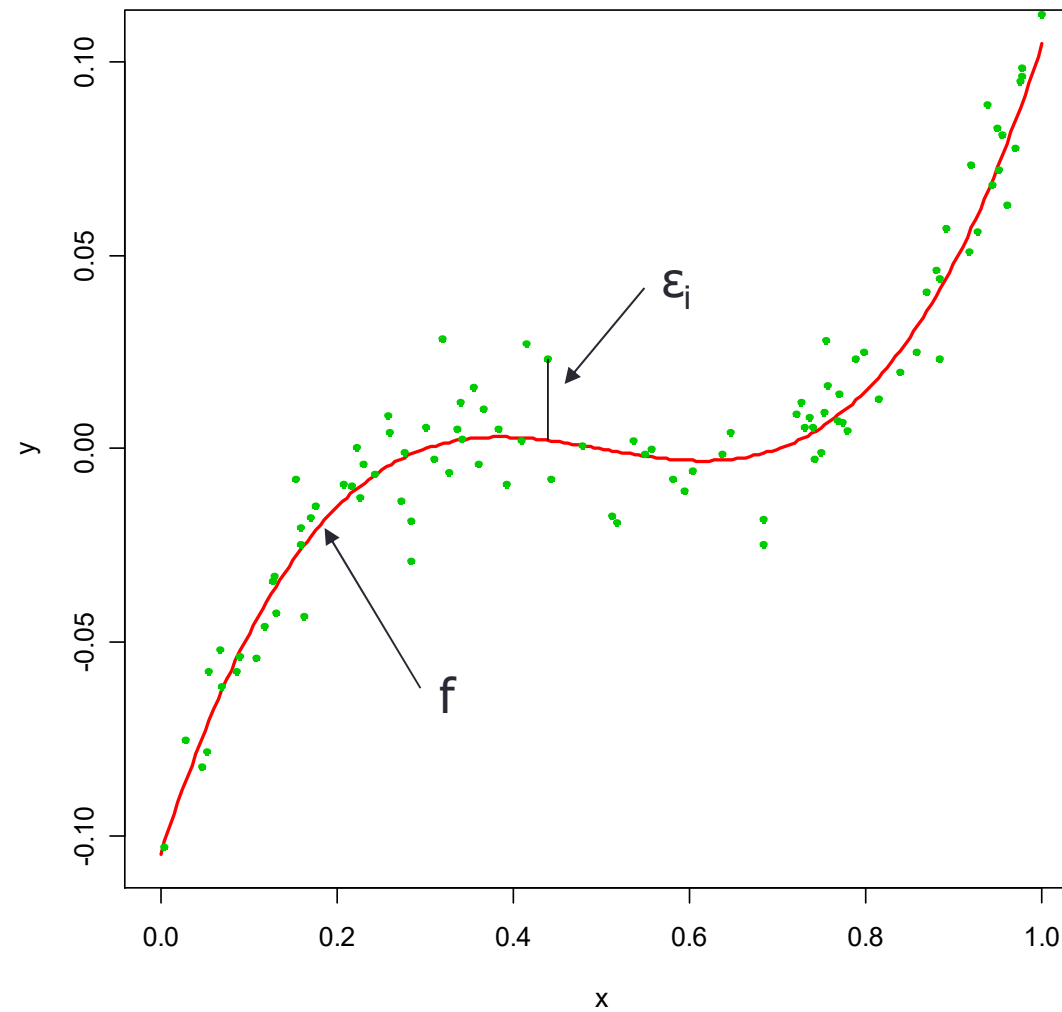
The book by James et al. actually defines statistical learning to a set of approaches for estimating f .

Two main reasons for estimating f is prediction and inference.

A Simple Example

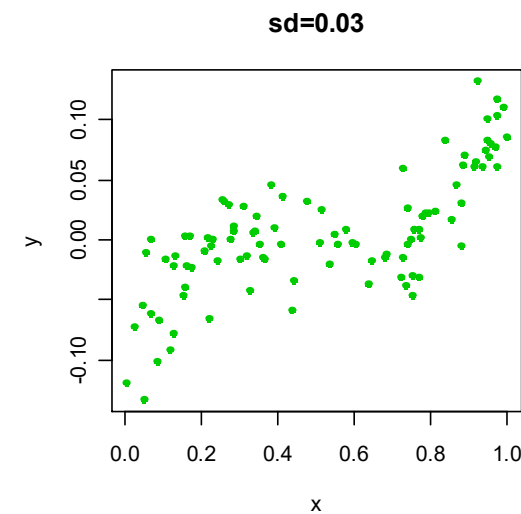
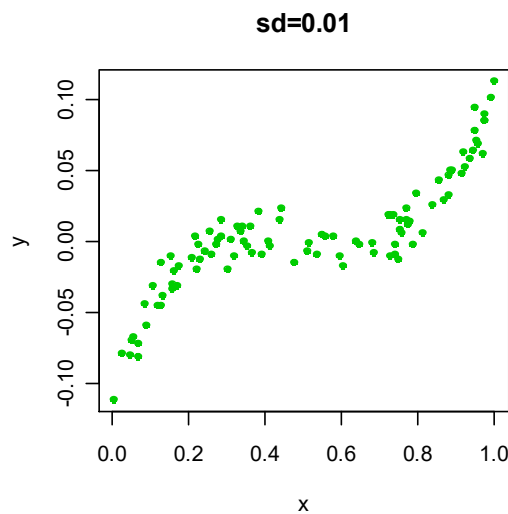
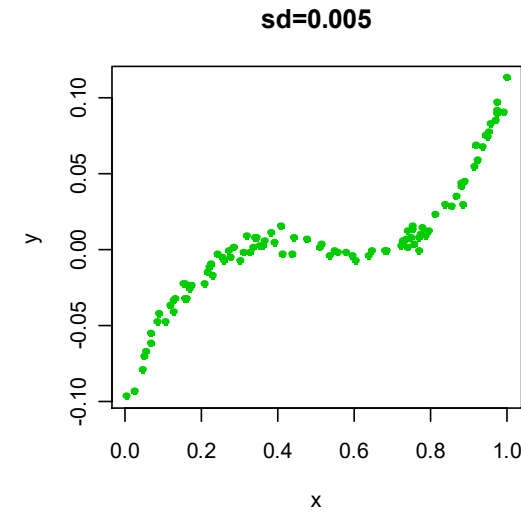
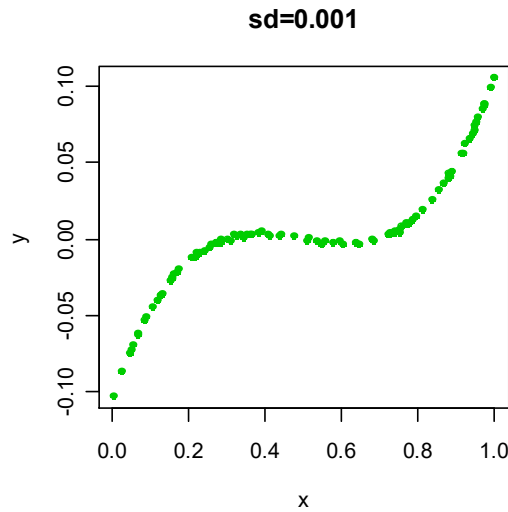


A Simple Example



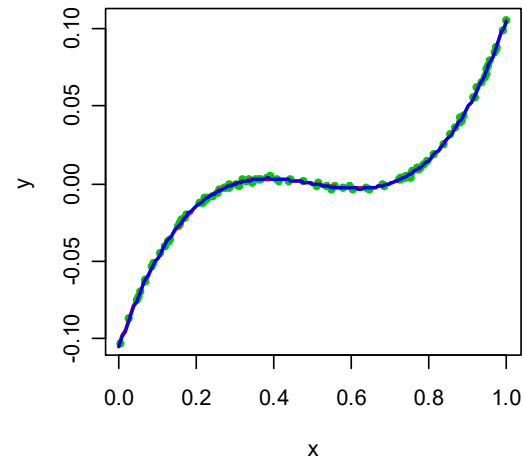
Different Standard Deviations

- The difficulty of estimating f will depend on the standard deviation of the ε 's.

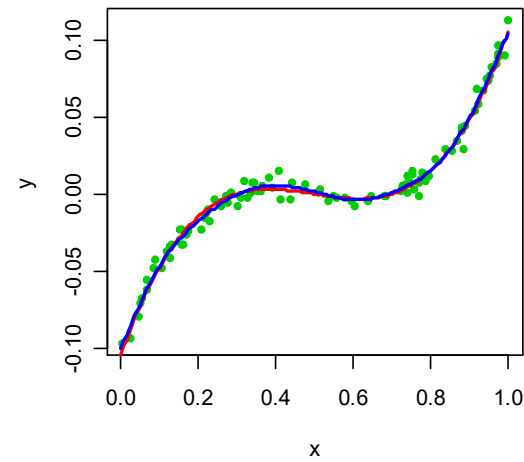


Different Estimates for f

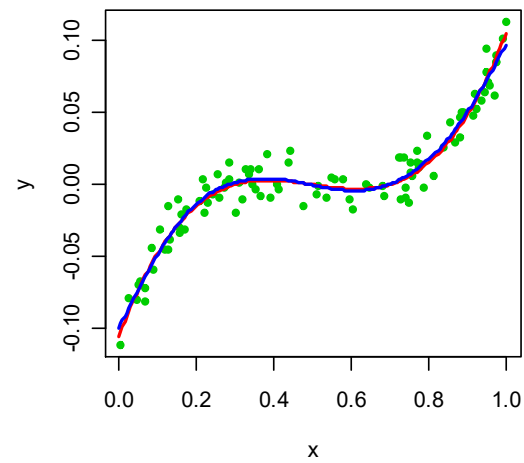
sd=0.001



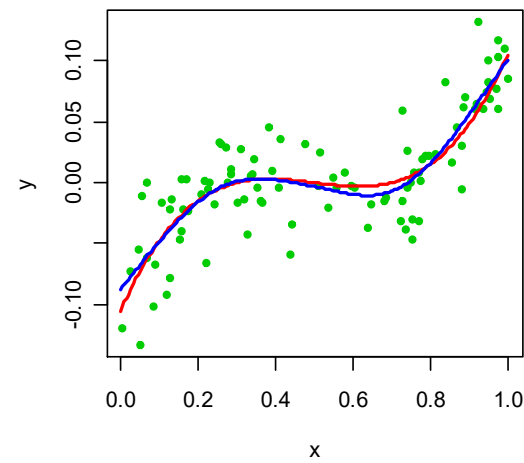
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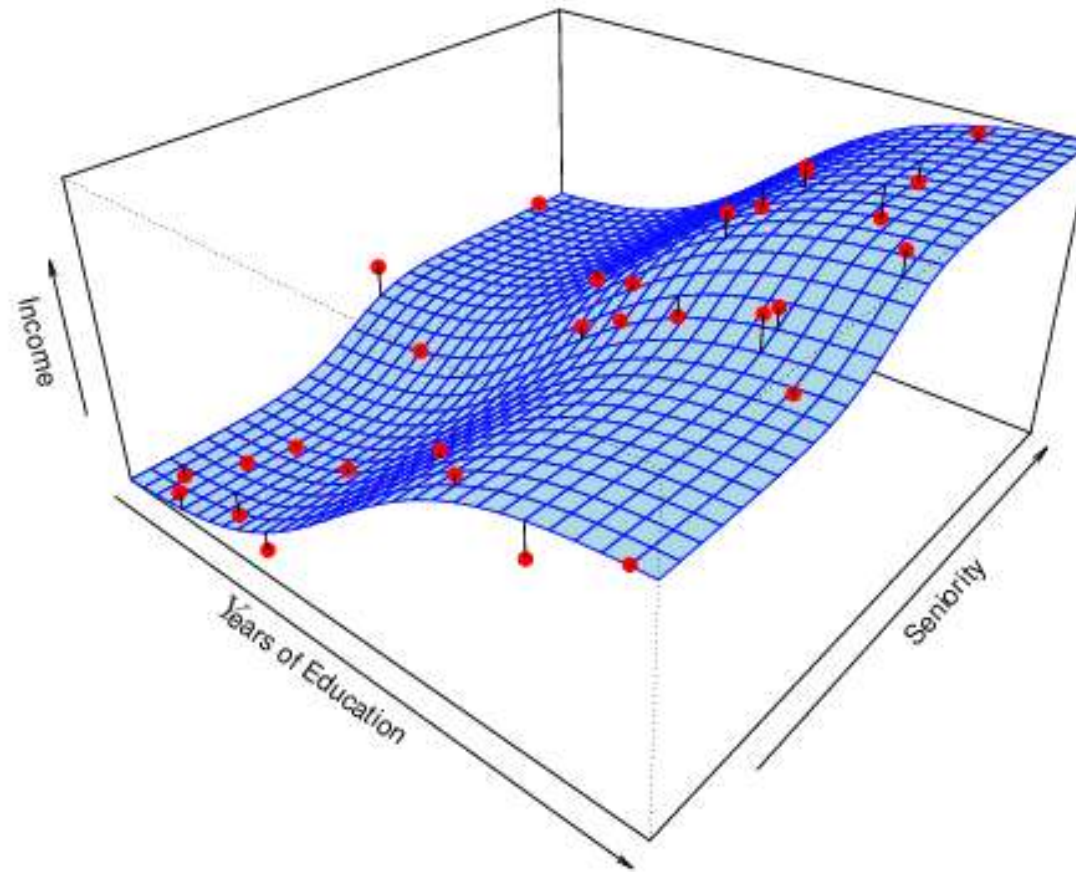
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sd=0.03



Income vs. Education Seniority



Why Do We Estimate f ?

- Statistical Learning, and this course, are all about how to estimate f .
- The term statistical learning refers to using the data to “learn” f .
- Why do we care about estimating f ?
- There are 2 reasons for estimating f ,
 - ✓ **Prediction** and
 - ✓ **Inference.**

1. Prediction

- If we can produce a good estimate for f (and the variance of ε is not too large) we can make accurate predictions for the response, Y , based on a new value of X .
- Given an estimate \hat{f} of f and inputs X , because the error term ε averages to zero, we can predict y as

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

In prediction context \hat{f} is often treated as a black box, i.e., the exact form of \hat{f} is not of concern, provided it yields accurate predictions for the outcome y ,

input \rightarrow black box \rightarrow prediction.

1. Prediction

Given an estimate \hat{f} of f , we can decompose the prediction error $y - \hat{y}$ as

$$y - \hat{y} = (f(\mathbf{X}) - \hat{f}(\mathbf{X})) + \varepsilon$$

in which the first component is due to the estimation and the second term due to the random error that by definition cannot be predicted by \mathbf{X} .

The estimation error $f(\mathbf{X}) - \hat{f}(\mathbf{X})$ can be potentially reduced by using the most appropriate statistical technique to estimate f .

Therefore, this error is called **reducible** error.

Even with a perfect estimate $f = \hat{f}$, \hat{y} deviates from y because of ε . Therefore, this error is called **irreducible** error.

1. Prediction

Assuming for a moment that both \hat{f} and \mathbf{X} are fixed, then

$$\begin{aligned} E(y - \hat{y})^2 &= E(f(\mathbf{X}) + \varepsilon - \hat{f}(\mathbf{X}))^2 \\ &= \underbrace{[f(\mathbf{X}) - \hat{f}(\mathbf{X})]^2}_{\text{Reducible}} - \underbrace{\text{var}(\varepsilon)}_{\text{Irreducible}} \end{aligned}$$

where $E(y - \hat{y})^2$ is the expected squared prediction error (difference of actual value and its prediction), and $\text{var}(\varepsilon)$ is the variance of the error term.

Example: Direct Mailing Prediction

- Interested in predicting how much money an individual will donate based on observations from 90,000 people on which we have recorded over 400 different characteristics.
- Don't care too much about each individual characteristic.
- Just want to know: For a given individual should I send out a mailing?

2. Inference

- Alternatively, we may also be interested in the type of relationship between Y and the X 's.
- For example,
 - ✓ Which particular predictors actually affect the response?
 - ✓ Is the relationship positive or negative?
 - ✓ Is the relationship a simple linear one or is it more complicated etc.?

2. Inference

Inference problems are related to understanding the way y changes as a function of $\mathbf{X} = (x_1, \dots, x_p)$, i.e., inference relies on model based approaches.

As a results, unlike in prediction, f cannot be considered any more as a black box.

Rather, the explicit form is of primary interest to find out

- predictors that are associated with the response,
- the particular relationship between the response with each predictor,
- the functional form of f (linear or more complicated).

Of course the interest can be a combination of these inferential an prediction purposes.

Example: Housing Inference

- Wish to predict median house price based on 14 variables.
- Probably want to understand which factors have the biggest effect on the response and how big the effect is.
- For example, how much impact does a river view have on the house value etc.

How Do We Estimate f ?

- We will assume we have observed a set of **training data**

$$\{(\mathbf{X}_1, Y_1), (\mathbf{X}_2, Y_2), \dots, (\mathbf{X}_n, Y_n)\}$$

- We must then use the training data and a statistical method to estimate f .
- Statistical Learning Methods:
 - ✓ Parametric Methods
 - ✓ Non-parametric Methods

Parametric Methods

- It reduces the problem of estimating f down to one of estimating a set of parameters.
- They involve a two-step model based approach

STEP 1:

Make some assumption about the functional form of f , i.e. come up with a model. The most common example is a linear model i.e.

$$f(\mathbf{X}_i) = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_p X_{ip}$$

However, in this course we will examine far more complicated, and flexible, models for f . In a sense the more flexible the model the more realistic it is.

Parametric Methods (cont.)

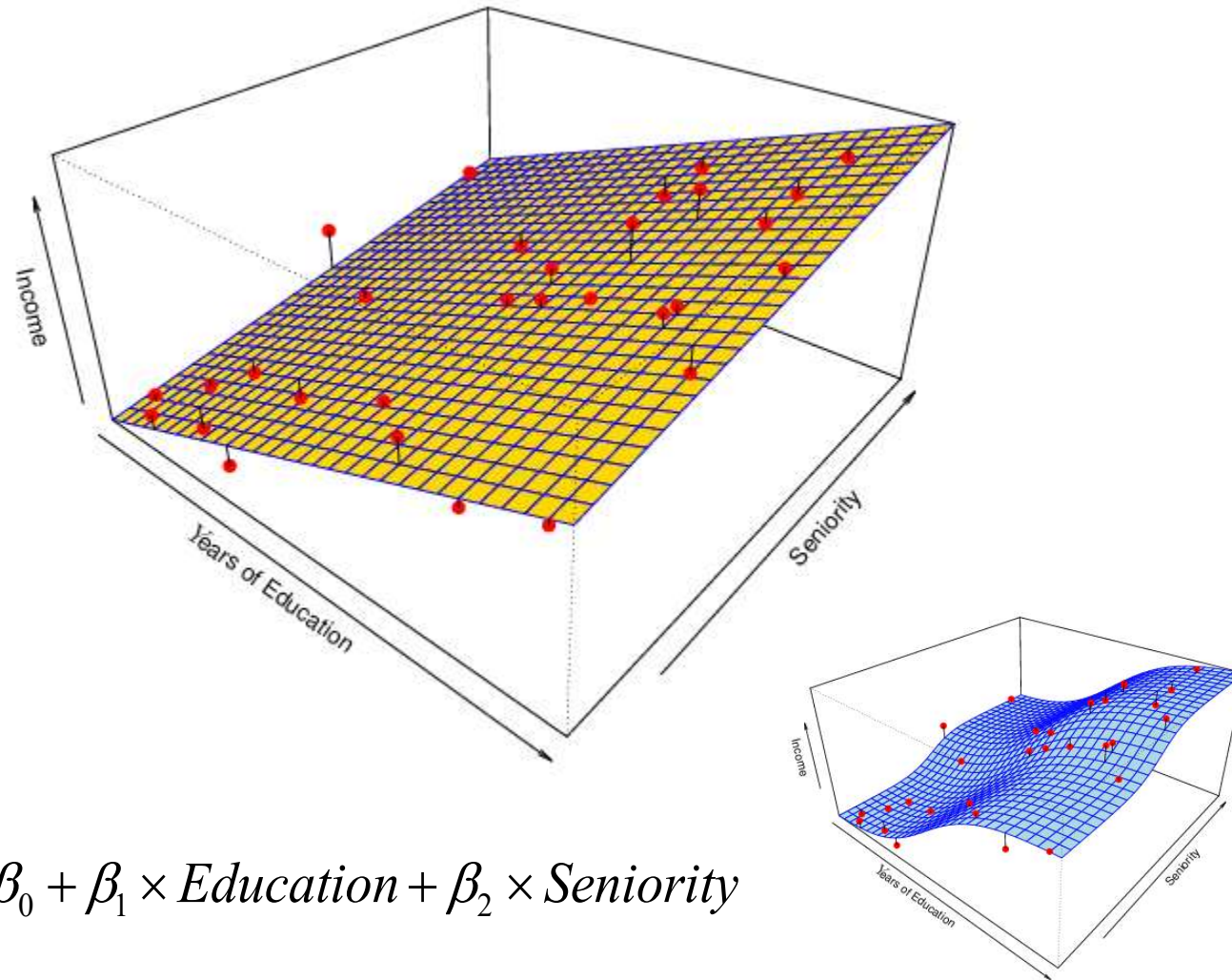
STEP 2:

Use the training data to fit the model i.e. estimate f or equivalently the unknown parameters such as $\beta_0, \beta_1, \beta_2, \dots, \beta_p$.

- The most common approach for estimating the parameters in a linear model is ordinary least squares (OLS).
- However, this is only one way.
- We will see in the course that there are often superior approaches.

Example: A Linear Regression Estimate

- Even if the standard deviation is low, we will still get a bad answer if we use the wrong model.



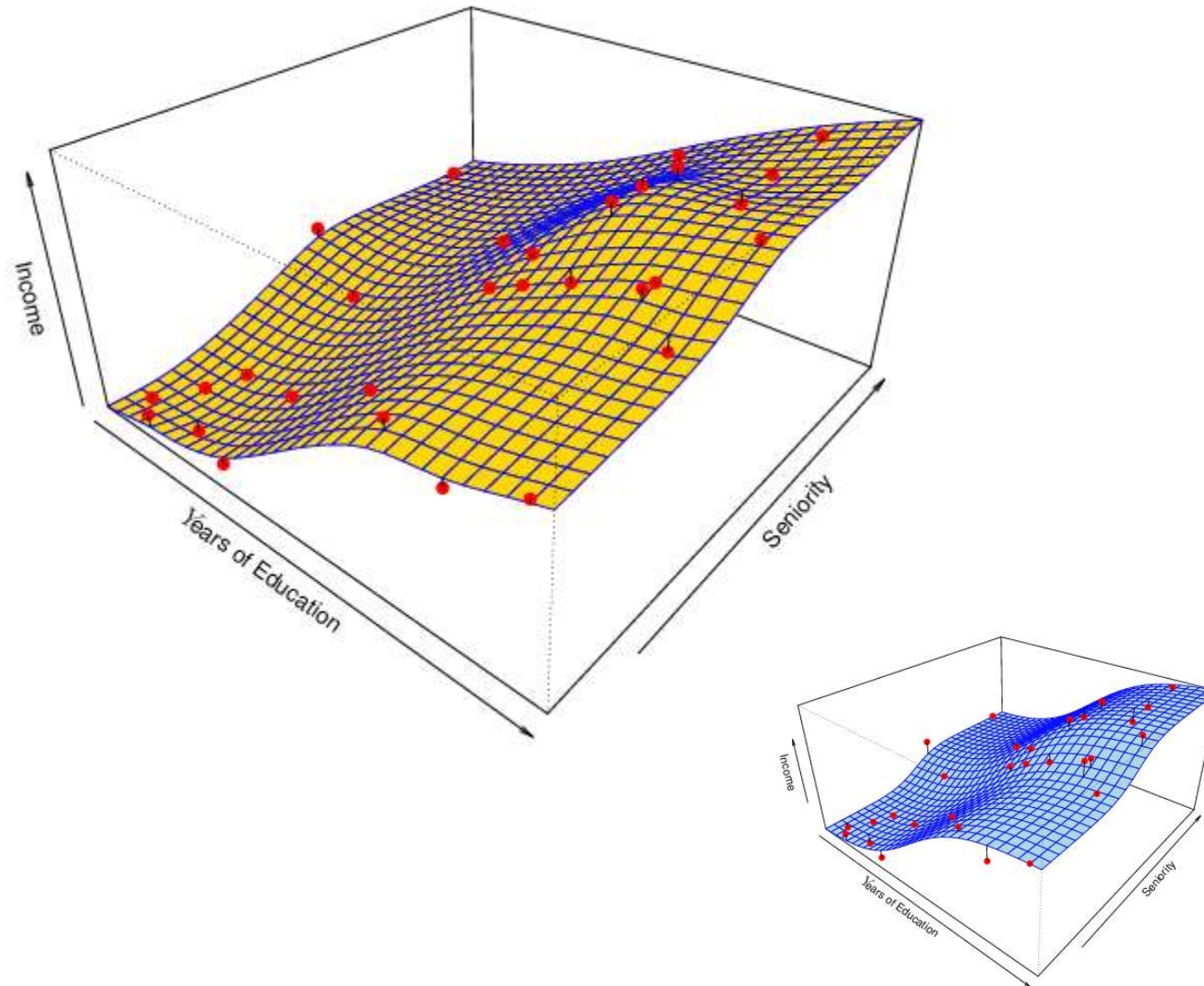
$$f = \beta_0 + \beta_1 \times Education + \beta_2 \times Seniority$$

Non-parametric Methods

- They do not make explicit assumptions about the functional form of f .
- Advantages: They accurately fit a wider range of possible shapes of f .
- Disadvantages: A very large number of observations is required to obtain an accurate estimate of f

Example: A Thin-Plate Spline Estimate

- Non-linear regression methods are more flexible and can potentially provide more accurate estimates.



Tradeoff Between Prediction Accuracy and Model Interpretability

- Why not just use a more flexible method if it is more realistic?
- There are two reasons

Reason 1:

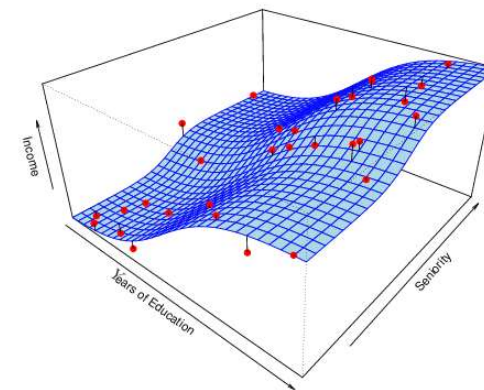
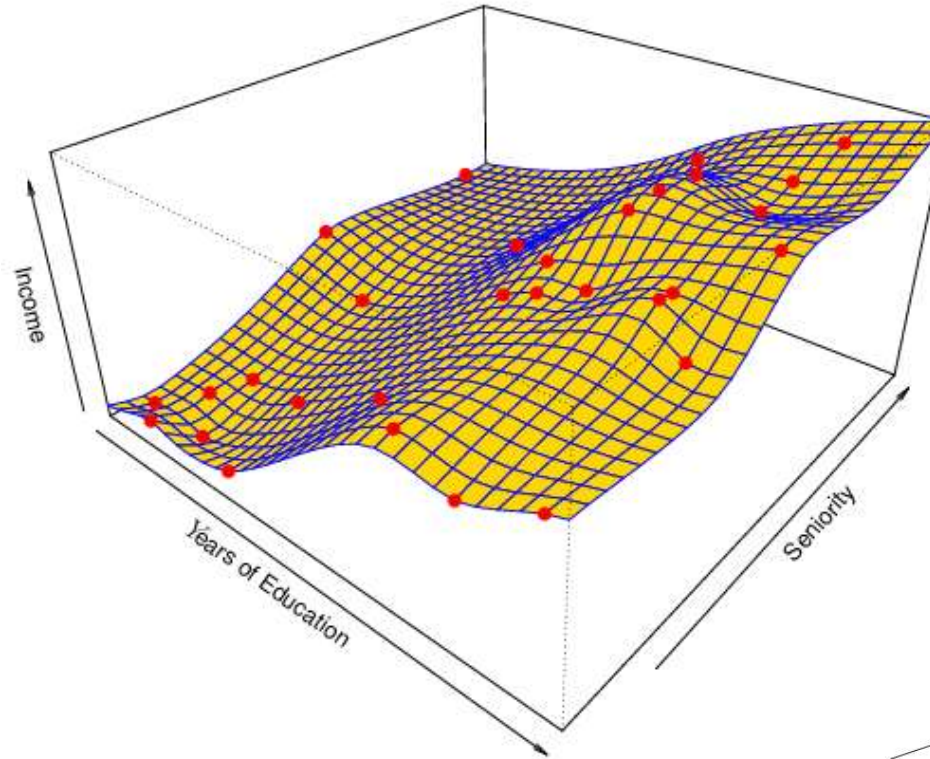
A simple method such as linear regression produces a model which is much easier to interpret (the Inference part is better). For example, in a linear model, β_j is the average increase in Y for a one unit increase in X_j holding all other variables constant.

Reason 2:

Even if you are only interested in prediction, so the first reason is not relevant, it is often possible to get more accurate predictions with a simple, instead of a complicated, model. This seems counter intuitive but has to do with the fact that it is harder to fit a more flexible model.

A Poor Estimate

- Non-linear regression methods can also be too flexible and produce poor estimates for f .



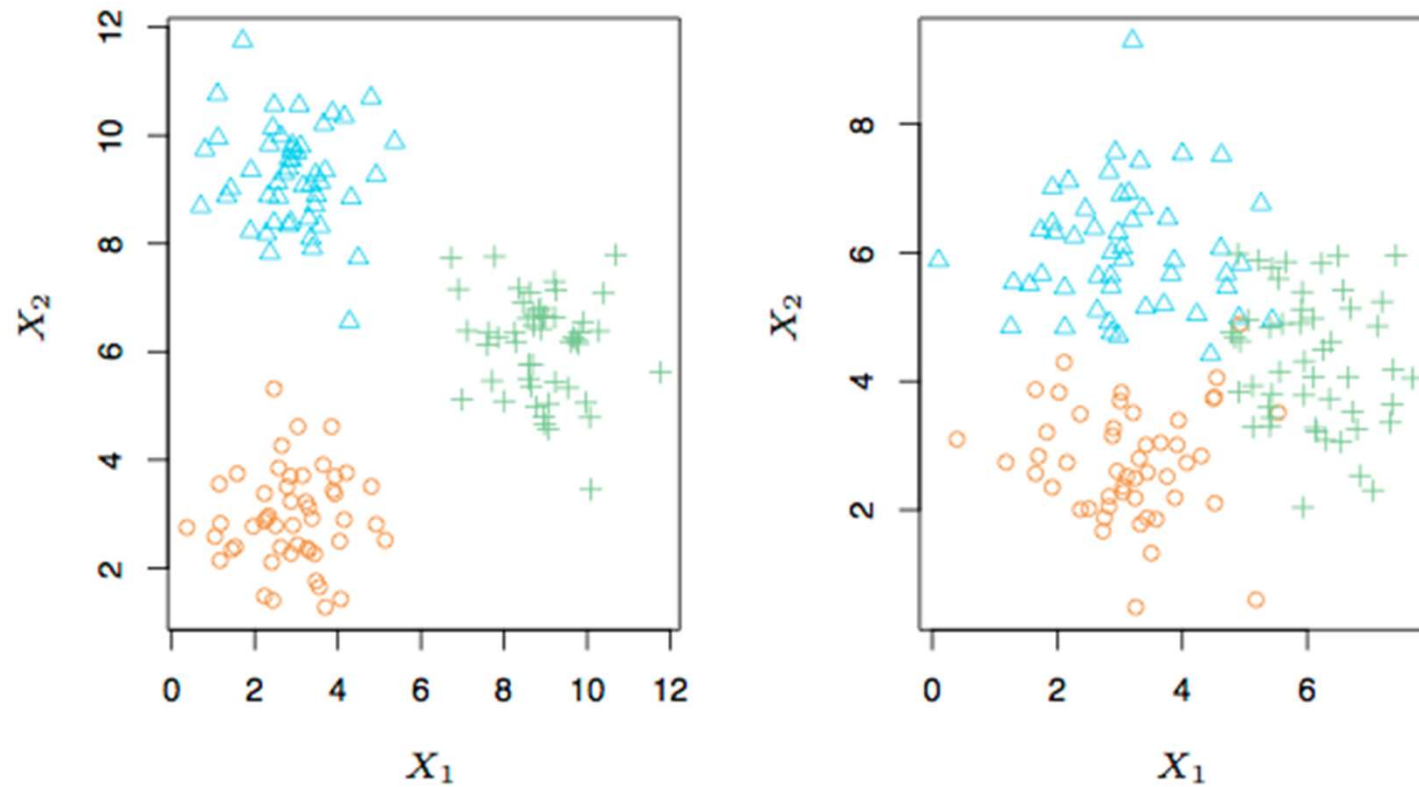
Supervised vs. Unsupervised Learning

- We can divide all learning problems into Supervised and Unsupervised situations
- Supervised Learning:
 - ✓ Supervised Learning is where both the predictors, X_i , and the response, Y_i , are observed.
 - ✓ This is the situation you deal with in Linear Regression classes.
 - ✓ Most of this course will also deal with supervised learning.

➤ Unsupervised Learning:

- ✓ In this situation only the X_i 's are observed.
- ✓ We need to use the X_i 's to guess what Y would have been and build a model from there.
- ✓ A common example is market segmentation where we try to divide potential customers into groups based on their characteristics.
- ✓ A common approach is clustering.
- ✓ We will consider unsupervised learning at the end of this course.

A Simple Clustering Example



Regression vs. Classification

- Supervised learning problems can be further divided into regression and classification problems.
- Regression covers situations where Y is continuous/numerical. e.g.
 - ✓ Predicting the value of the Dow in 6 months.
 - ✓ Predicting the value of a given house based on various inputs.
- Classification covers situations where Y is categorical e.g.
 - ✓ Will the Dow be up (U) or down (D) in 6 months?
 - ✓ Is this email a SPAM or not?

Different Approaches

- We will deal with both types of problems in this course.
- Some methods work well on both types of problem e.g. Neural Networks
- Other methods work best on Regression, e.g. Linear Regression, or on Classification, e.g. k-Nearest Neighbors.