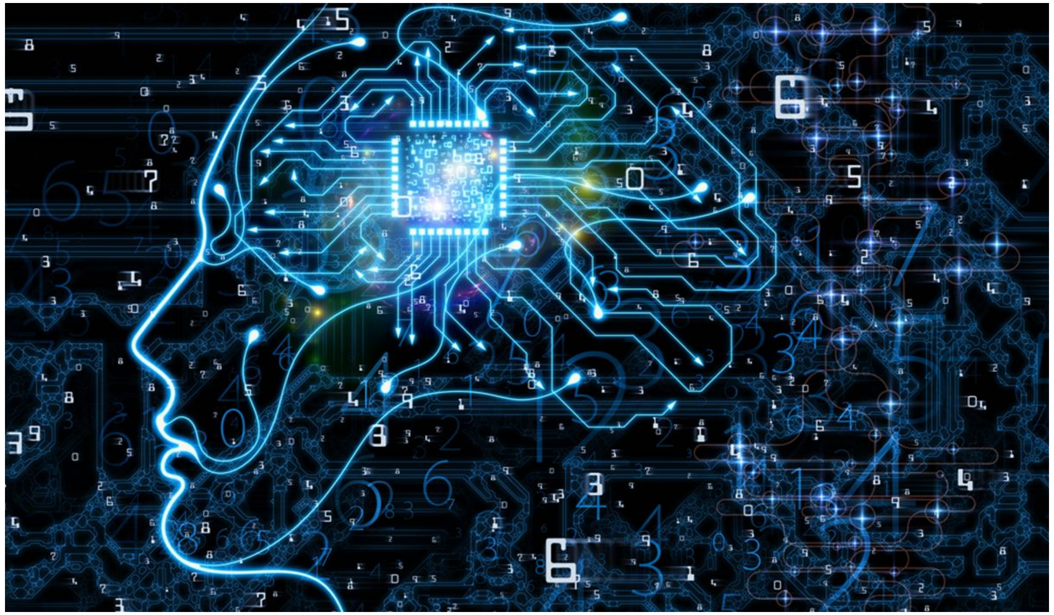
University of Ljubljana, Faculty of Computer and Information Science

Statistical Predictive Modeling



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Intelligent Systems
Edition 2025

Learning

- **Learning** is the act of acquiring new, or modifying and reinforcing existing, knowledge, behaviors, skills, values, or preferences and may involve synthesizing different types of information.

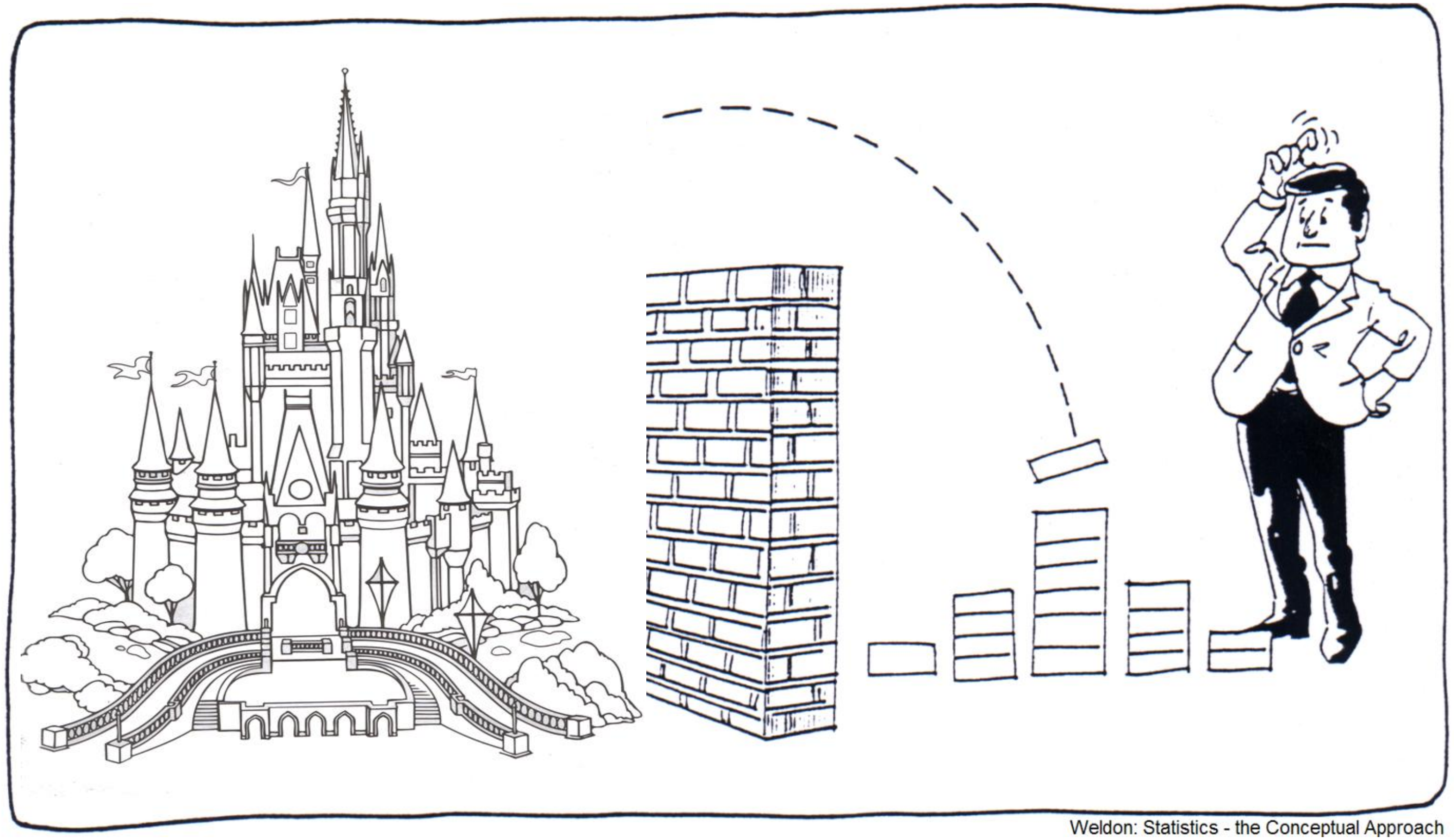
- **Statistical learning** deals with the problem of finding a predictive function based on data.

- The primary goals of statistical learning: prediction and understanding.

- Many different learning settings and data types, rapidly spreading in many areas of science, technology, and analytics, e.g., the Nobel prize in physics in 2024 to Hopfield and Hinton

Statistics and machine learning

- Definition from Wikipedia:
  ML algorithms operate by building a model from example inputs *i.e., samples.*



Weldon: Statistics - the Conceptual Approach

- ML can also be viewed as compression

The Data

Provided by the Institute of Oncology, Ljubljana

Post-surgery data for about 1000 breast cancer patients.

+

Recurrence and time of recurrence.

The Data

	class1	class2	menop	stage	grade	hType	PgR	inv	nLymph	cTh	hTh	famHist	LVI	ER	maxNode	posRatio	age
300	11.82	0	1	2	2	1	0	0	1	1	0	3	0	1	2	3	2
301	4.89	1	0	1	2	1	0	0	2	1	0	0	0	2	1	4	3
302	14.63	0	1	1	4	2	0	0	0	0	0	1	0	1	1	1	3
303	21.83	0	0	1	4	2	1	0	1	0	0	9	0	4	1	2	2
304	19.87	0	0	1	2	1	0	0	0	0	0	0	0	1	2	1	2
305	7.54	0	1	2	3	1	9	2	1	0	1	1	0	3	3	3	4
306	15.15	0	0	1	4	2	1	0	0	0	0	2	0	4	1	1	2
307	0.30	1	0	2	2	1	0	0	3	0	0	9	0	1	1	4	2
308	12.49	0	1	2	2	3	1	0	0	0	0	0	0	4	1	1	5
309	1.77	1	0	2	3	1	1	2	2	1	0	9	1	3	3	3	2

Each patient is described with 17 values:

- 15 patient's features
- 2 values, which describe the outcome

1 instance = 1 patient

	class1	class2	menop	stage	grade	hType	PgR	inv	nLymph	cTh	hTh	famHist	LVI	ER	maxNode	posRatio	age
300	11.82	0	1	2	2	1	0	0	1	1	0	3	0	1	2	3	2
301	4.89	1	0	1	2	1	0	0	2	1	0	0	0	2	1	4	3
302	14.63	0	1	1	4	2	0	0	0	0	0	1	0	1	1	1	3
303	21.83	0	0	1	4	2	1	0	1	0	0	9	0	4	1	2	2
304	19.87	0	0	1	2	1	0	0	0	0	0	0	0	1	2	1	2
305	7.54	0	1	2	3	1	9	2	1	0	1	1	0	3	3	3	4
306	15.15	0	0	1	4	2	1	0	0	0	0	2	0	4	1	1	2
307	0.30	1	0	2	2	1	0	0	3	0	0	9	0	1	1	4	2
308	12.49	0	1	2	2	3	1	0	0	0	0	0	0	4	1	1	5
309	1.77	1	0	2	3	1	1	2	2	1	0	9	1	3	3	3	2

- **Menopause?**
- **Tumor stage**
- **Tumor grade**
- **Histological type**
- **Progesterone receptor lvl.**
- **Invasive tumor type**
- **Number of positive lymph nodes**

- **Hormonal therapy?**
- **Chemotherapy?**
- **Family medical history**
- **Lymphovascular invasion?**
- **Estrogen receptor lvl.**
- **Size of max. removed node**
- **Ratio of positive lymph nodes**
- **Age group**

Prognostic Features

	class1	class2	menop	stage	grade	hType	PgR	inv	nLymph	cTh	hTh	famHist	LVI	ER	maxNode	posRatio	age
300	11.82	0	1	2	2	1	0	0	1	1	0	3	0	1	2	3	2
301	4.89	1	0	1	2	1	0	0	2	1	0	0	0	2	1	4	3
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307	0.30	1	0	2	2	1	0	0	3	0	0	9	0	1	1	4	2
308	12.49	0	1	2	2	3	1	0	0	0	0	0	0	4	1	1	5
309	1.77	1	0	2	3	1	1	2	2	1	0	9	1	3	3	3	2

- Menopause?
- Tumor stage
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- Histological type
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- Hormonal therapy?
- Chemotherapy?
- Family medical history
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- Estrogen receptor lvl.
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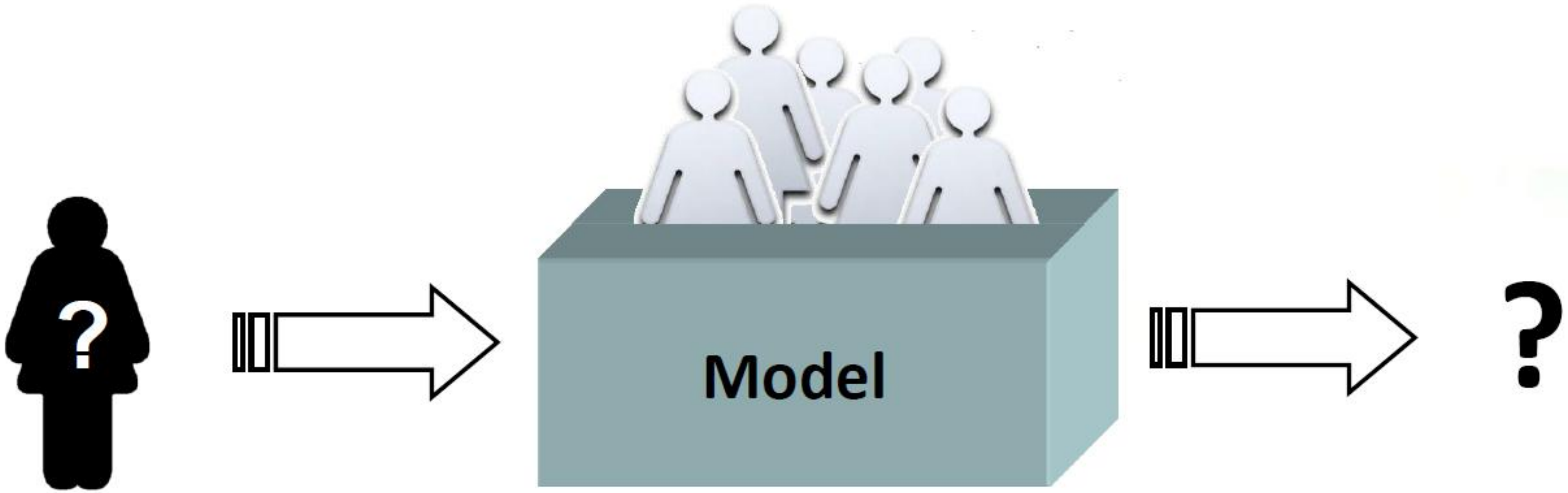
Oncologists use these attributes for prognosis in every-day medical practice.

Basic Task in ML

We want to learn from past examples,with known outcomes.



To predict the outcome for a new patient.

Basic notation of predictive modelling

- Cancer recurrence is a statistical variable named response or target or prediction variable that we wish to predict. We usually refer to the response as Y .
- Other input variables are called attributes, features, inputs, or predictors; we name them $X_{.j}$
- One observation, called also an instance or example is denoted as $X_{i,.}$
- The input vectors form a matrix **X**

$$\mathbf{X} = \begin{pmatrix} x_{11} & x_{12} & \ldots & x_{1p} \\ x_{21} & x_{22} & \ldots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \ldots & x_{np} \end{pmatrix}$$

- The model we write as

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

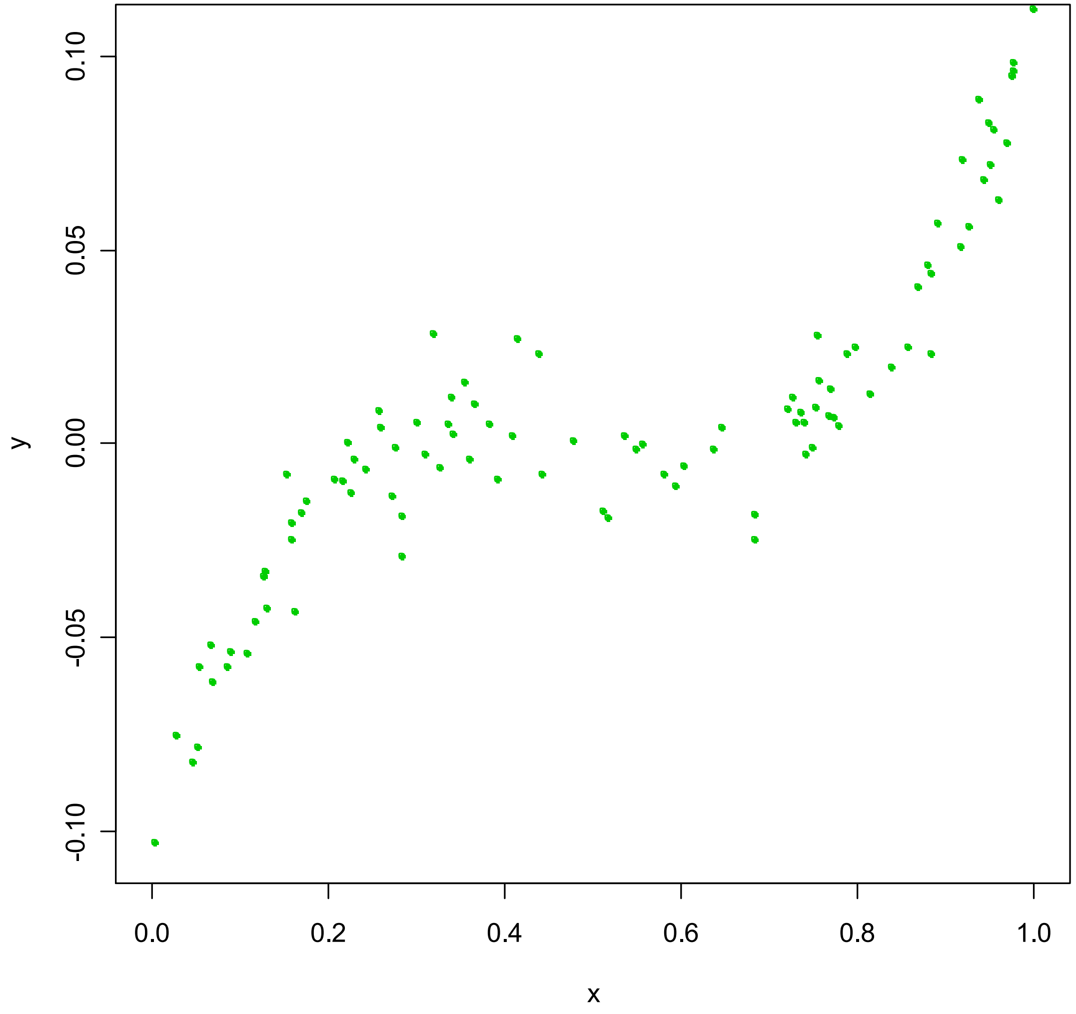
where ∈ is independent of X, has zero mean and represents measurement errors and other discrepancies.

Further notation for instances and attributes

- Suppose we observe Y_i and $X_i = \left(x_{i,1}, x_{i,2}, \ldots x_{i,p}\right)$for $i = 1,2, \ldots n$
- We believe that there is a relationship between Y and X.
- We can model the relationship as $$Y_i = f(\mathbf{X}_{i.}) + \varepsilon_i$$
- Where f is an unknown function and ε is a random error with mean zero.
- Take care, the notation may be confusing, we also use

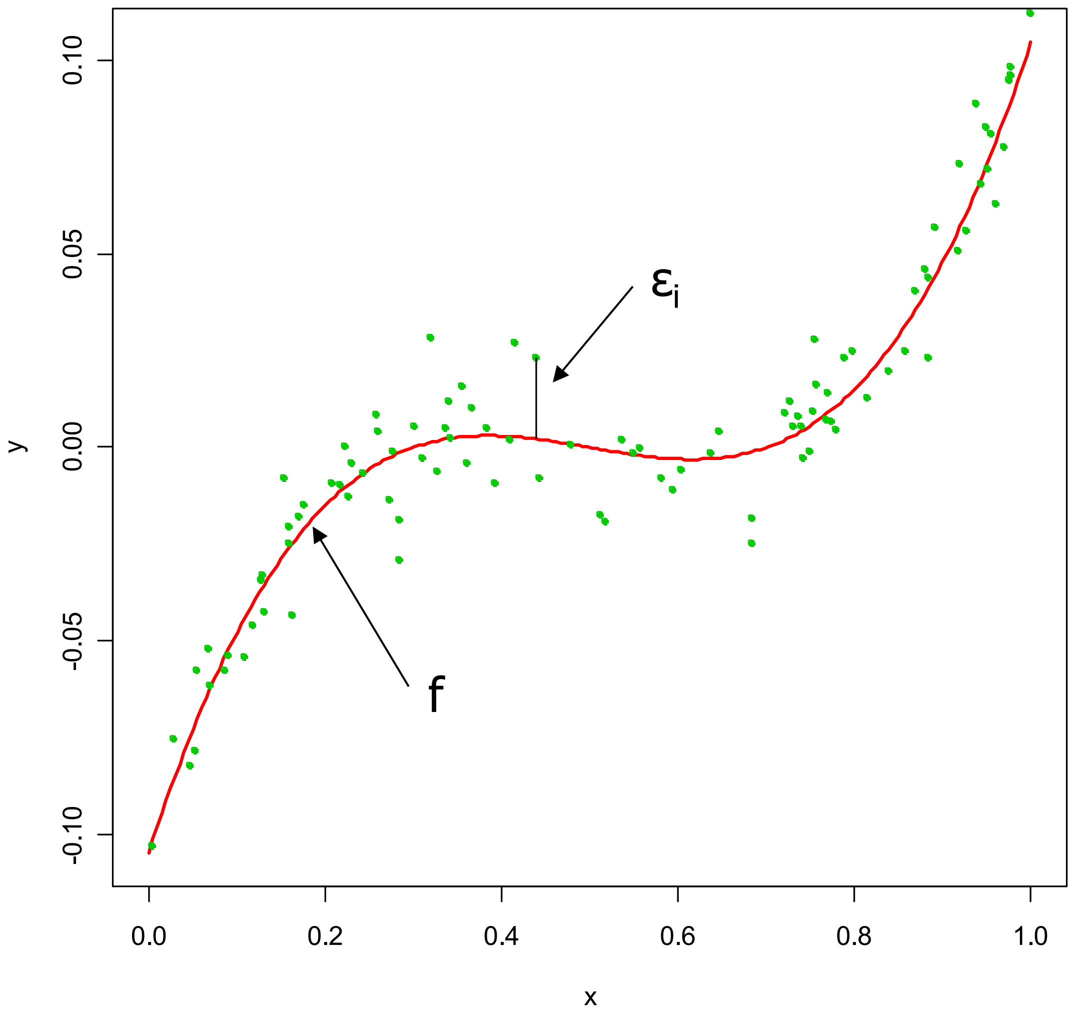
$$\mathbf{x}_j = \begin{pmatrix} x_{1j} \\ x_{2j} \\ \vdots \\ x_{nj} \end{pmatrix}$$

A simple example



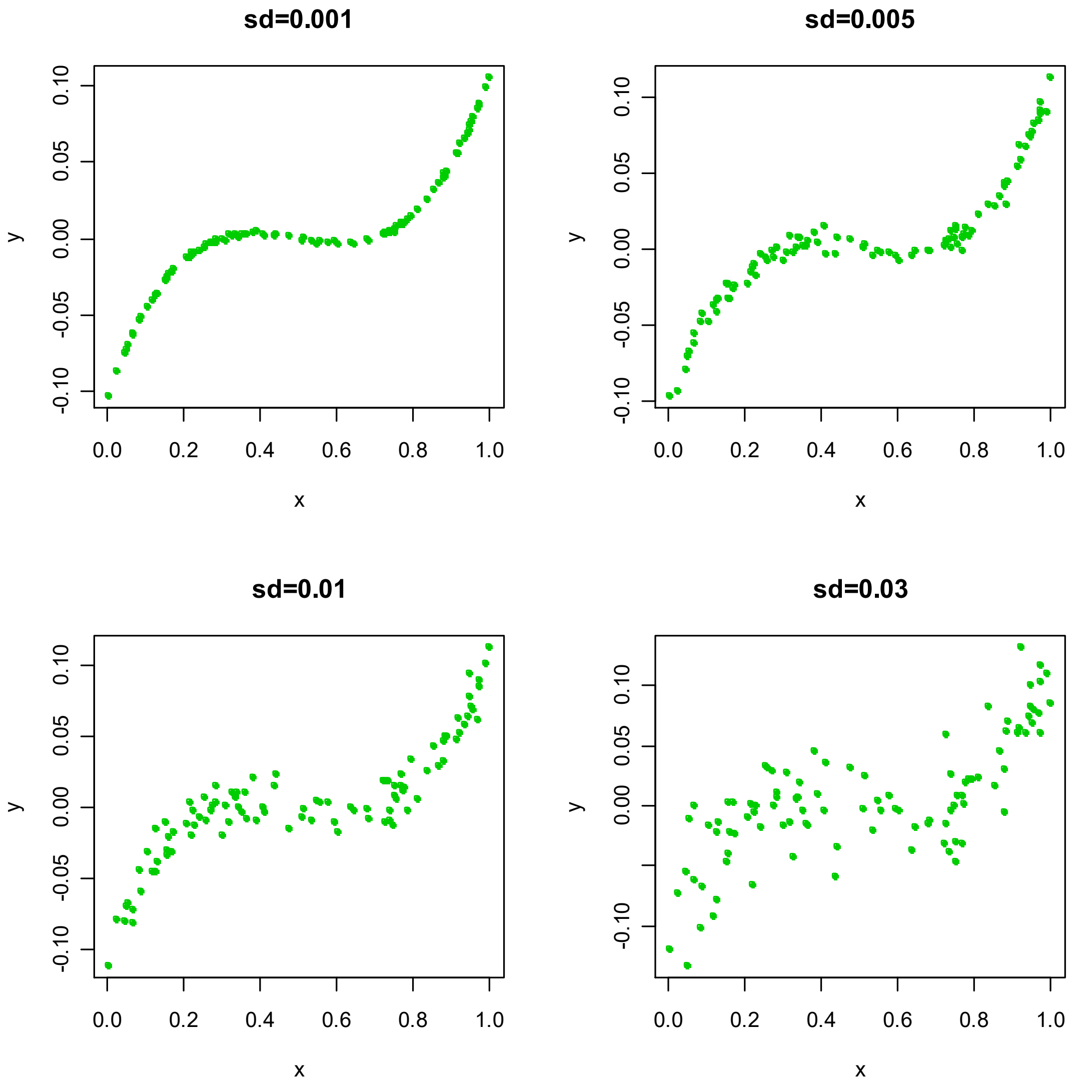
A simple example

- Assuming we know f (in red)

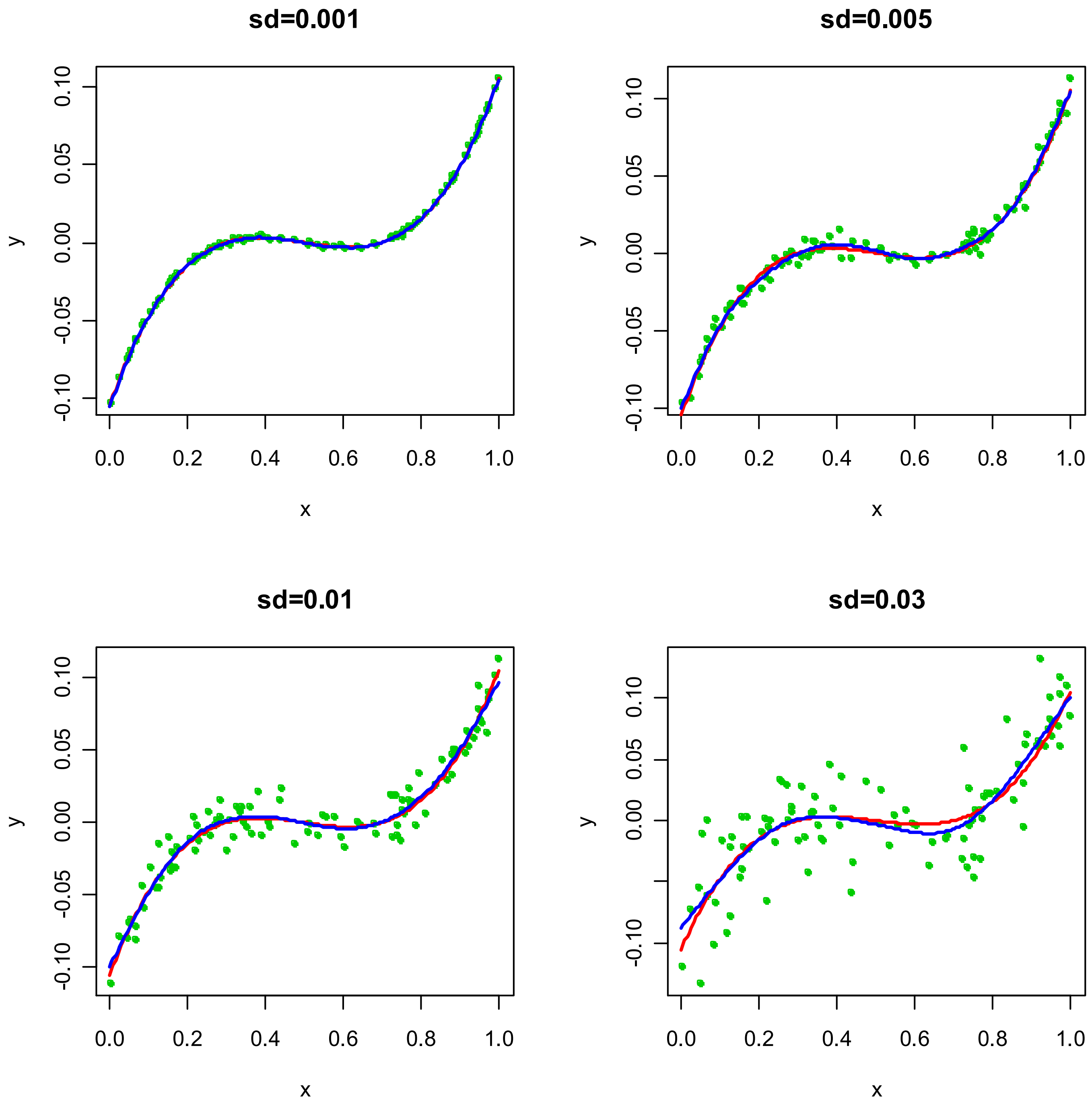


Different standard deviations of error

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

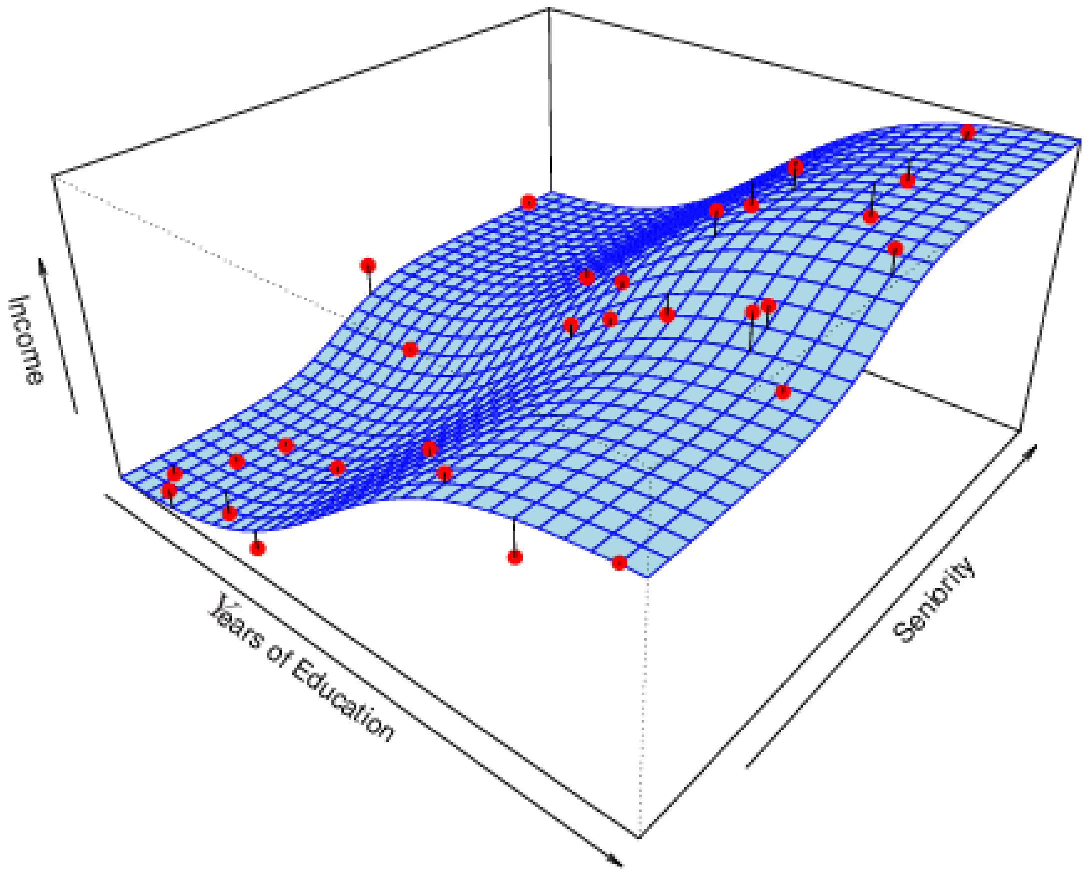


Different estimates for *f*



Income vs. Education and Seniority

Multidimensional **X**



1^{st} goal of learning: 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_i, based on a new value of $X_{i.}$

- 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^{nd} goal of learning: inference

- often we are interested in the type of relationship between Y and all the $X_{.j}$
- 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.?
  - For a given ($X_{i.}$, Y_i), which feature values x_{ij} are the most important to determine y_i?
- Sometimes more important than prediction, e.g., in medicine.
- 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**

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

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

Parametric methods

- They reduce 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.

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

More complicated and flexible models for *f* are often more realistic.

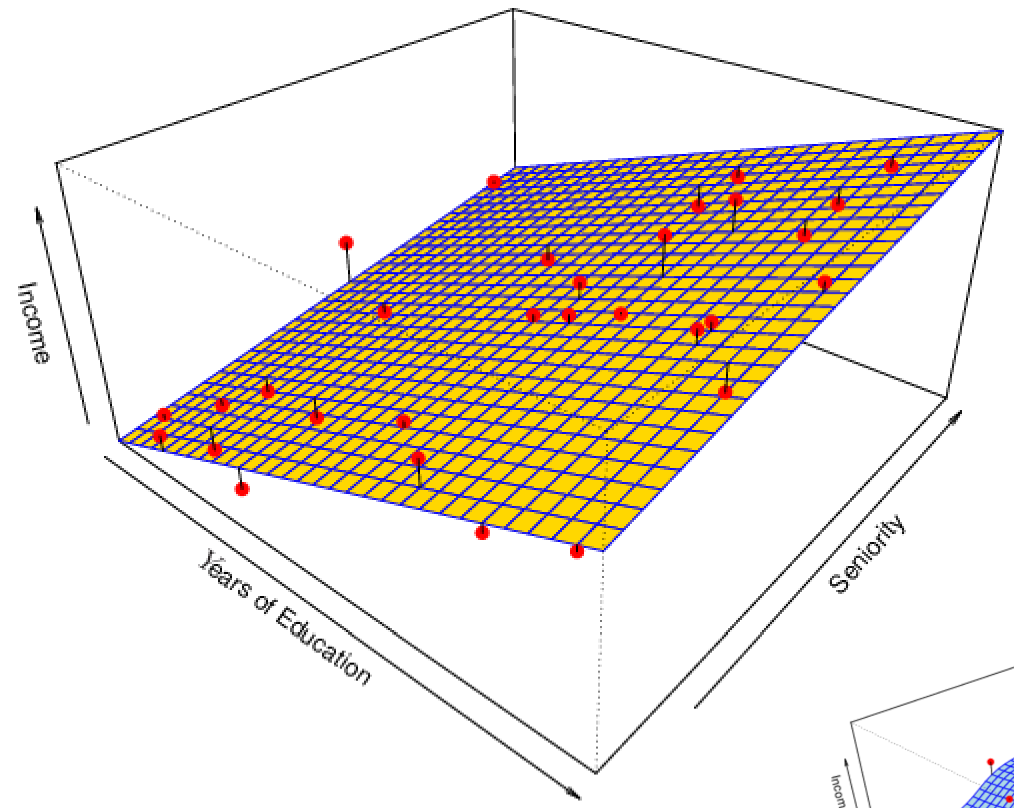
STEP 2:

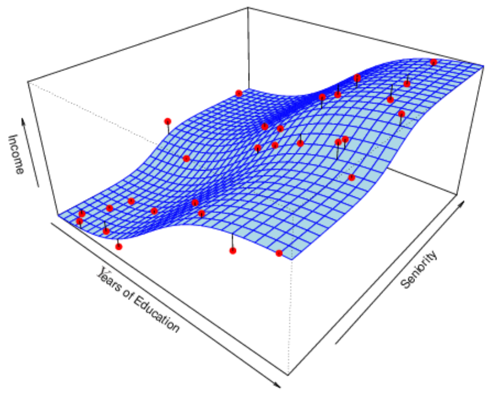
Use the training data to fit the model, i.e. estimate *f* or equivalently the unknown parameters such as β_0, β_1, β_2,…β_p

For linear model the most common method uses ordinary least squares (OLS).

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.





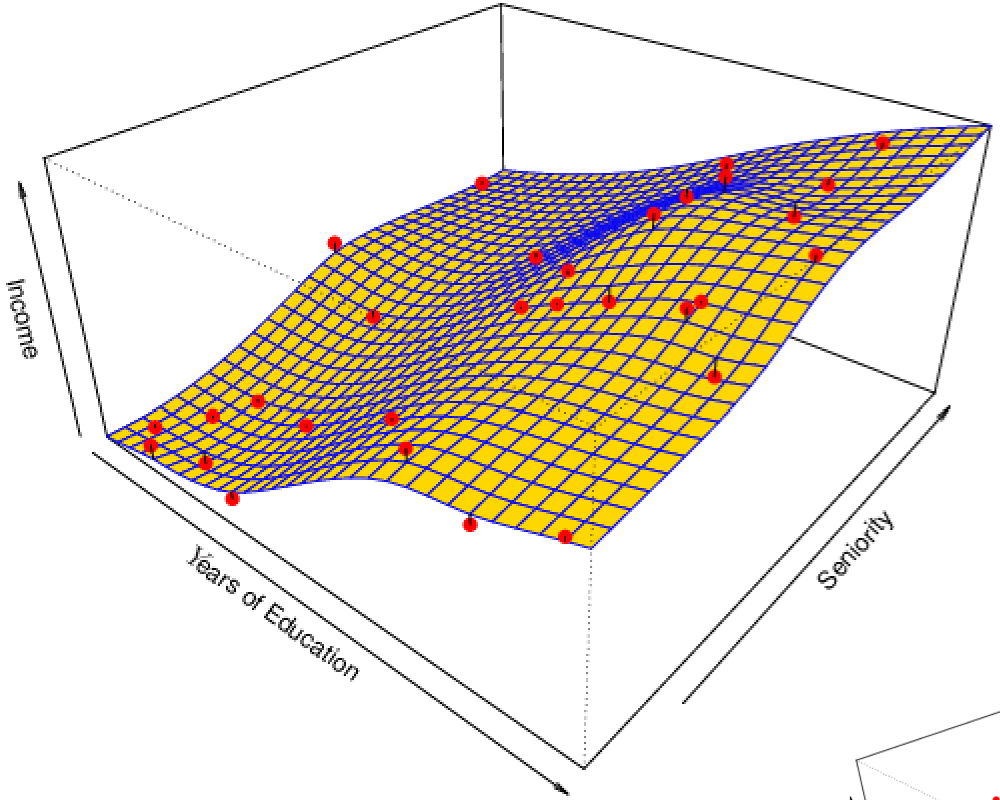
$$f = \beta_0 + \beta_1 \cdot Education + \beta_2 \cdot Seniority$$

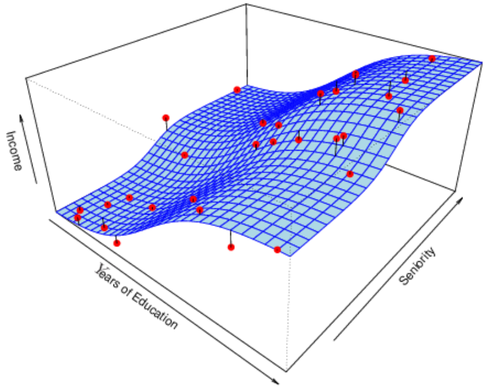
Non-parametric methods

- They do not make explicit assumptions about the functional form of *f*.
- <u>Advantage:</u> They accurately fit a wider range of possible shapes of *f*.
- <u>Disadvantage:</u> A large number of observations may be 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.





Trade-off between prediction accuracy and model interpretability

- Why not just use a more flexible method if it is more realistic?

Reason 1:

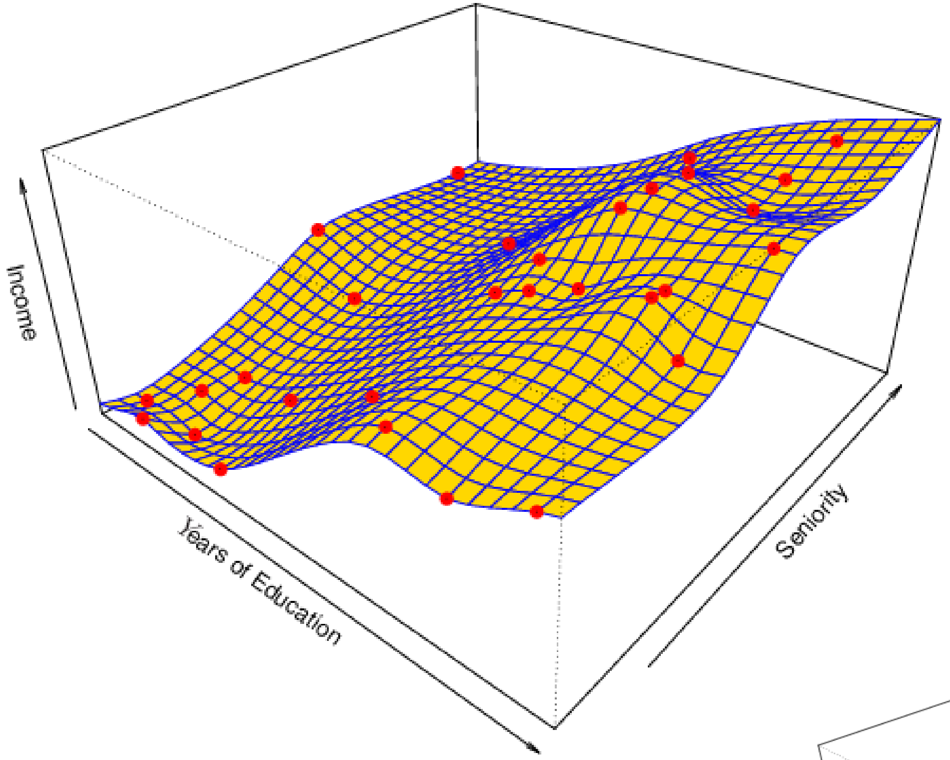
A simple method such as linear regression produces a model which is much easier to interpret (the inference part is better). For example, in a linear model, β_j is the average increase in Y for a one unit increase in X_j holding all other variables constant.

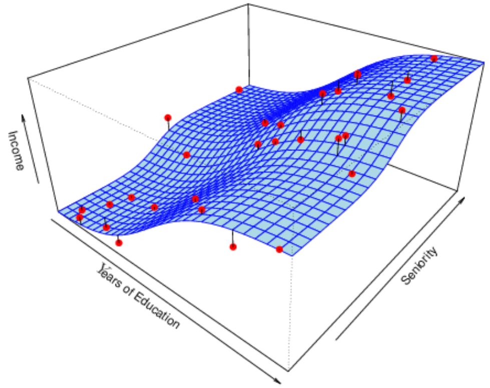
Reason 2:

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.

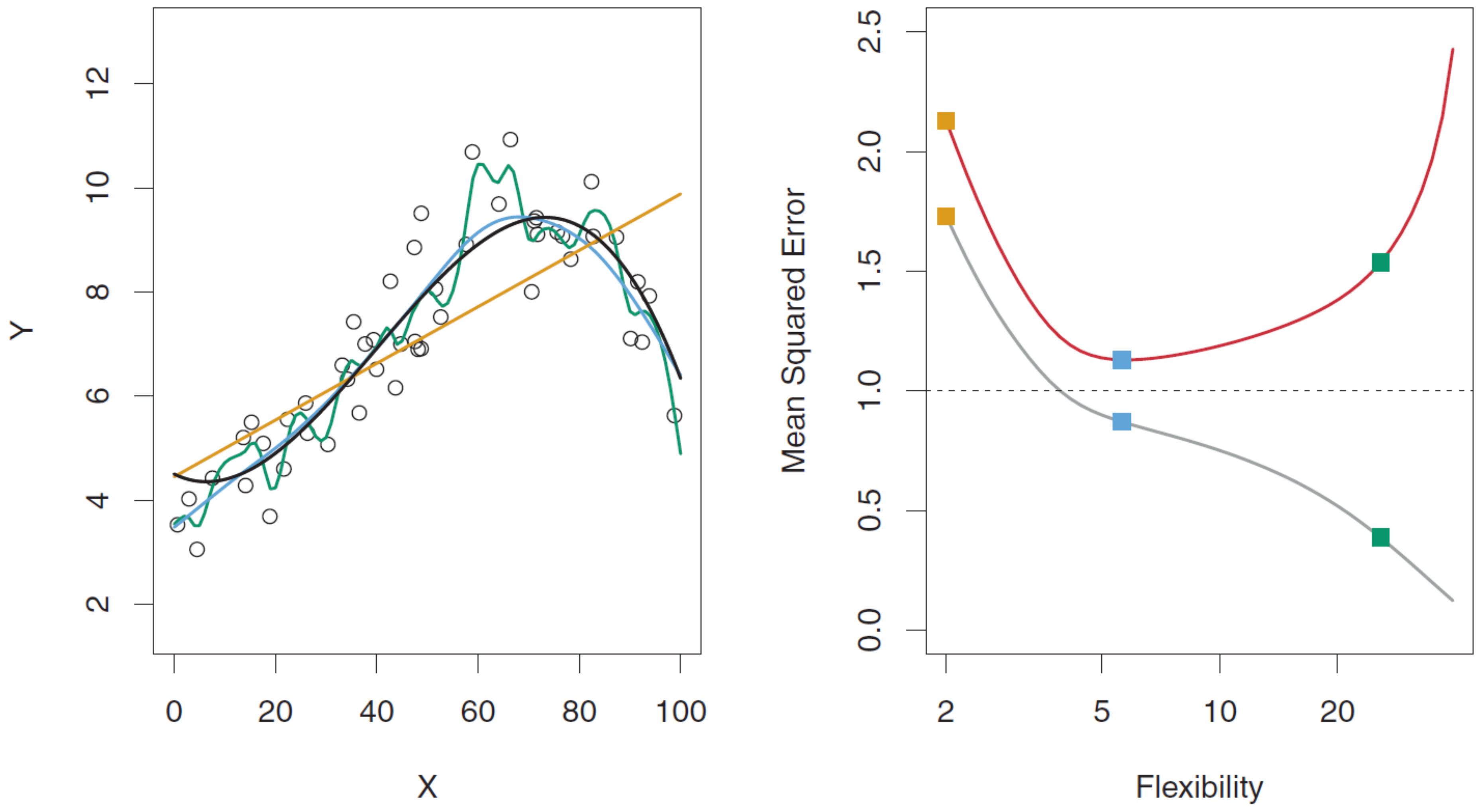
A poor estimate: overfitting

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





Goodness of fit for three models



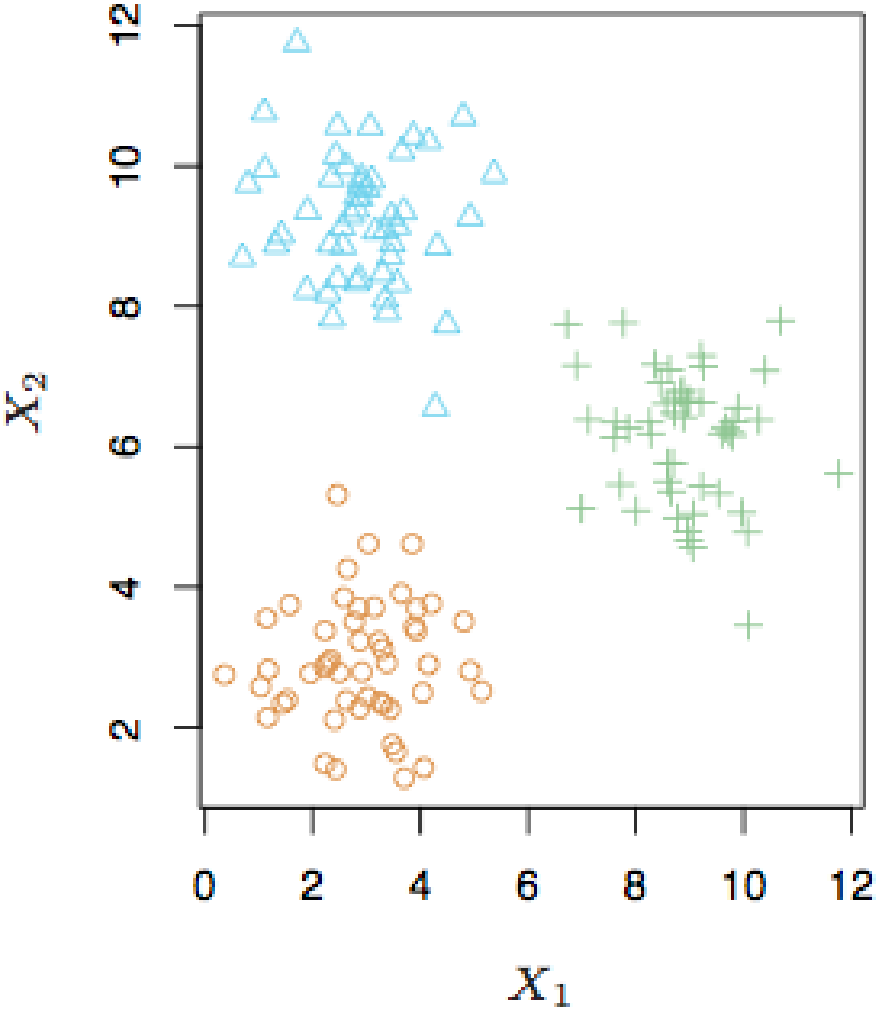
<u>LEFT</u>
Black: Truth
Orange: Linear Estimate
Blue: smoothing spline
Green: smoothing spline (more flexible)

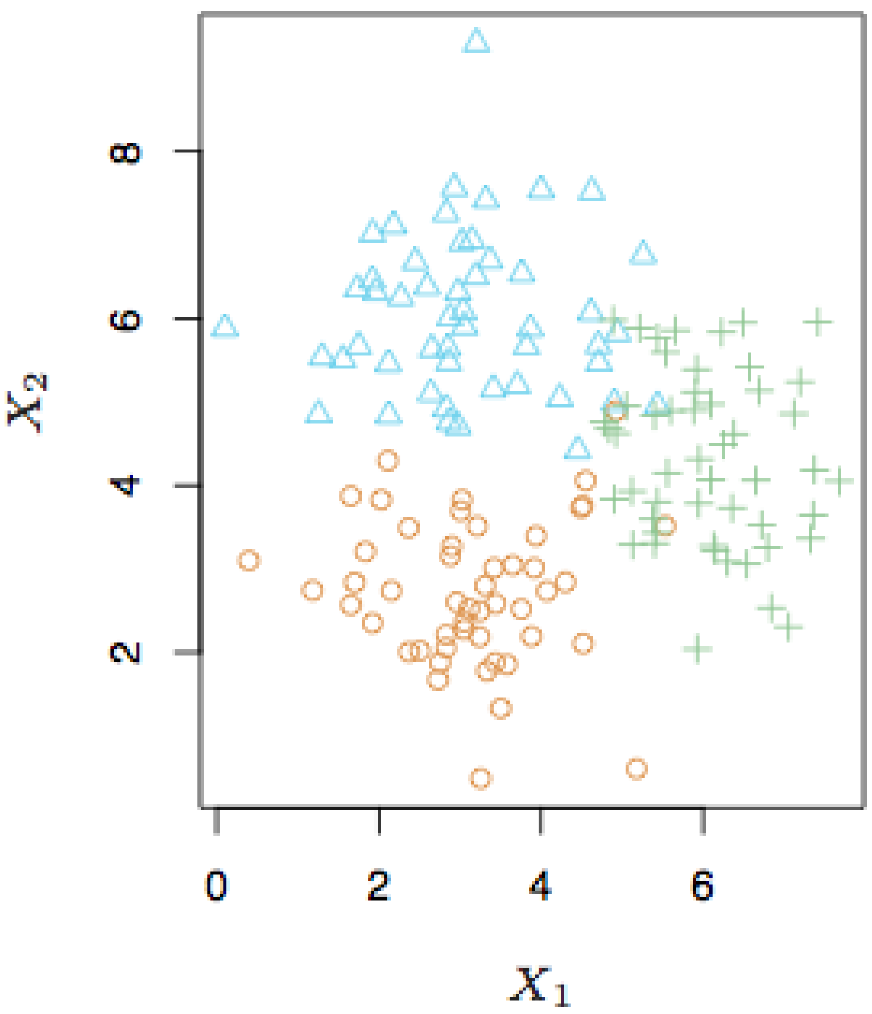
<u>RIGHT</u>
RED: Test MSE
Grey: Training MSE
Dashed: Minimum possible test MSE (irreducible error)

Supervised, unsupervised, semi-supervised, self-supervised, weakly-supervised learning 1/2

- We can divide learning problems into Supervised and Unsupervised situations
- Supervised learning:
  - Supervised Learning is where both the predictors, $\mathbf{X}_i$, and the response, Y_i, are observed.
  - e.g., linear regression
- Unsupervised learning:
  - In this situation only the $\mathbf{X}_i$'s are observed.
  - We need to use the $\mathbf{X}_i$'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.
    - Idea: Maximizing initra-cluster similarity & minimizing inter-cluster similarity
- Semi-supervised learning
  - only a small sample of labelled instances are observed but a large set of unlabeled instances
  - an initial supervised model is used to label unlabeled instances
  - the most reliable predictions are added to the training set for the next iteration of supervised learning

A simple clustering example





Supervised, unsupervised, semi-supervised, self-supervised, weakly-supervised learning 2/2

- Self-supervised learning
  - a mixture of supervised and unsupervised learning
  - learns from unlabeled data
  - the labels are obtained from related properties of the data itself, often leveraging the underlying structure in the data
  - usually predicts any unobserved or hidden part (or property) of the input from any observed or unhidden part of the input.
  - e.g., in NLP, we can hide part of a sentence and predict the hidden words from the remaining words
  - e.g., in video processing, we can predict past or future frames in a video (hidden data) from current ones (observed data)
- Weakly-supervised data
  - noisy, limited, or imprecise sources are used to provide supervision signal for labeling large amounts of training data to do supervised learning
  - reduces the burden of obtaining hand-labeled data sets, which can be costly or impractical
  - e.g., using a smart electricity meter to estimate household occupancy

Regression vs. classification

- Supervised learning problems can be further divided into
- Regression problems: Y is continuous/numerical. e.g.
    - Predicting the value of certain share on stock market
    - Predicting the value of a given house based on various inputs
    - The duration in years till cancer recurrence
- Classification problems: Y is categorical, e.g.,
    - Will the price of a share go up (U) or down (D)?
    - Is this email a SPAM or not?
    - Will the cancer recur?
    - What will be an outcome of a football match (Home, Away, or Draw)?
    - Credit card fraud detection, direct marketing, classifying stars, diseases, web-pages, etc.
    - Note that we mostly predict probabilities of the categories
- Some methods work well on both types of problem, e.g., neural networks or kNN

Data mining (analytics, science): on what kinds of data?

- Database-oriented data sets and applications
  - Relational database, data warehouse, transactional database
- Advanced data sets and advanced applications
  - Data streams and sensor data
  - Time-series data, temporal data, sequence data (incl. bio-sequences)
  - Structure data, graphs, social networks and multi-linked data
  - Object-relational databases
  - Heterogeneous databases and legacy databases
  - Spatial data and spatiotemporal data
  - Multimedia database
  - Text databases
  - The World-Wide Web

Association and correlation analysis

- Frequent patterns (or frequent itemsets)
  - What items are frequently purchased together in the supermarket?
- Association, correlation vs. causality
  - A typical association rule
    - Diaper → Beer [0.5%, 75%] (support, confidence)
  - Are strongly associated items also strongly correlated?
- How to mine such patterns and rules efficiently in large datasets?
- How to use such patterns for classification, clustering, and other applications?

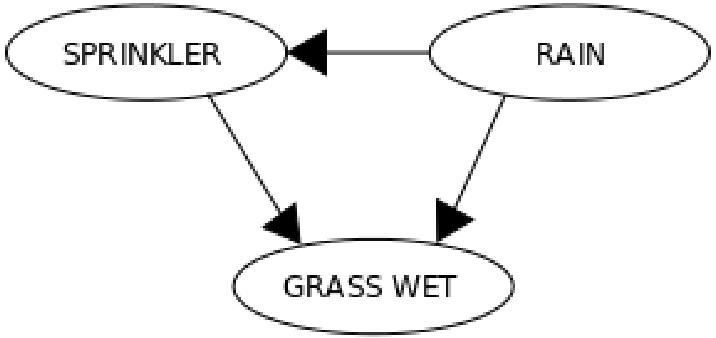
Outlier analysis

- Outlier: A data object that does not comply with the general behavior of the data
- Noise or exception? — One person’s garbage could be another person’s treasure
- Methods: byproduct of clustering or regression analysis, …
- Useful in fraud detection, rare events analysis

Relational learning

- Several variants:
  - Bayesian networks,
  - inductive logic programming
  - graph learning, e.g., link prediction

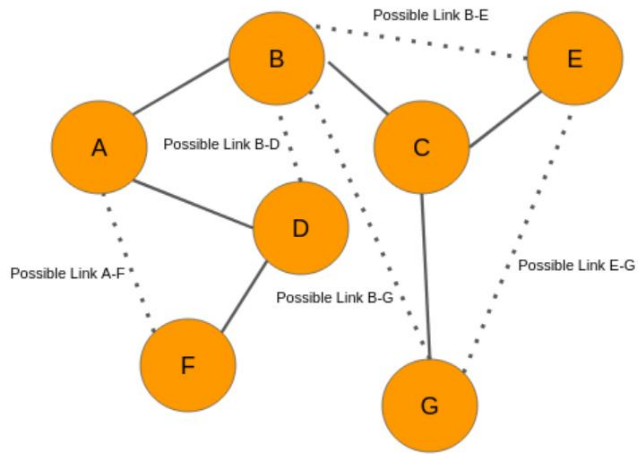
	SPRINKLER	
RAIN	T	F
F	0.4	0.6
T	0.01	0.99

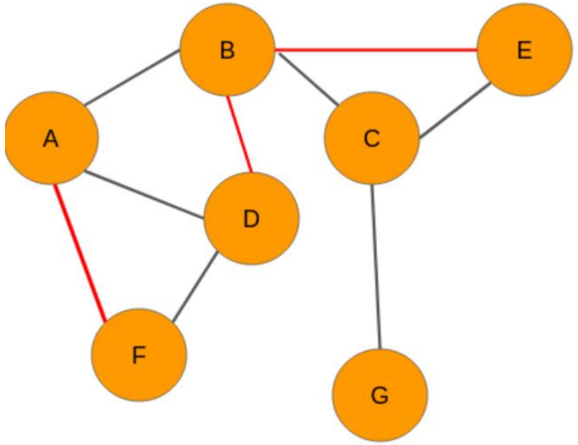


RAIN	
T	F
0.2	0.8

		GRASS WET	
SPRINKLER	RAIN	T	F
F	F	0.0	1.0
F	T	0.8	0.2
T	F	0.9	0.1
T	T	0.99	0.01

Notation	Example rule
Explicit	IF *Shape* = *triangle* ∧ *Color* = *red* ∧ *Size* = *big* THEN *Class* = *positive*
Formal	$Class = positive \leftarrow Shape = triangle \wedge Color = red \wedge Size = big$
Logical	`positive(X):-shape(X,triangle),color(X,red),size(X,big).`





Generalization as a search

- So far, we presented the “learning as an optimization” ML view
- Inductive learning: find a concept description that fits the data
- Example: rule sets as description language
  - Enormous but finite search space
- Simple solution:
  - enumerate the concept space
  - eliminate descriptions that do not fit examples
  - surviving descriptions contain target concept

Learning as optimization

- Usually the goal of classification is to minimize the test error
- Therefore, many learning algorithms solve optimization problems, e.g.,
  - linear regression minimizes squared error on the training set
  - AntMiner algorithms minimize the classification accuracy of decision rules on the training set using ACO
  - to find a good architecture of neural networks, GAs can be applied and minimize the prediction error on the validation set
  - most learning methods use optimization algorithms to minimize the implicitly or explicitly stated loss function, e.g., cross-entropy in neural network is minimized with gradient descent, where cross-entropy is a distance between two distributions, the predicted P and the true Q: $H(P, Q) = \sum_{x \in X} p(x) \log q(x)$

Criteria of success for ML

- No single best ML method (no free lunch theorem)
- How to select the best model?
  - measure the quality of fit, i.e. how well the predictions match the observed data
  - measure on previously unseen data (called test set). Why? Can we do it many times?
- In regression, the most popular measure is the mean squared error

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

where y_i is the true (observed) value of instance i, and $f(x_i)$ is its predicted value

- in classification, the *classification accuracy = 1 – error rate* is the most popular criterion

$$CA = \frac{1}{n}\sum_{i=1}^{n} I(y_i = f(x_i))$$

where $f(x_i)$ is the predicted category

- We will say more about this topic later

No-Free-Lunch theorem

- In the "no free lunch" metaphor,
  each "restaurant" (problem-solving procedure)
  has a "menu" associating
  each "lunch plate" (problem)
  with a "price" (the performance of the procedure in solving the problem).
- The menus of restaurants are identical except in one regard – the prices are shuffled from one restaurant to the next.
- For an omnivore who is as likely to order each plate as any other, the average cost of lunch does not depend on the choice of restaurant.
- But a vegan who goes to lunch regularly with a carnivore who seeks economy might pay a high average cost for lunch.
- To methodically reduce the average cost, one must use advance knowledge of
  - a) what one will order and
  - b) what the order will cost at various restaurants.
- That is, improvement of performance in problem-solving hinges on using prior information to match procedures to problems.

Consequences of the NFL theorem

If no information about the target function f(x) is provided:

- No classifier is better than some other in the general case.
- No classifier is better than random in the general case.

- ML practitioners possess implicit or explicit knowledge about the prices in different restaurants

- Meta-learning
- Automatic ML (AutoML)