# Introduction to Machine Learning

Session 1b: General Introduction

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# Outline

# What is Machine Learning?

## Learning

The process of converting experience into expertise or knowledge.

## Machine Learning

Machine learning is automated learning. We program computers so that they can learn and improve based on input available to them.

- The input to a learning algorithm is training data, representing experience.
- The output of a learning algorithm is expertise, which we then use to perform some task.
- A successful learning algorithm should be able to progress from individual examples to broader generalization.

(Shalev-Shwartz and Ben-David 2014, 19f.)

# When Do We Need Machine Learning?

When do we rely on machine learning rather than directly programing computers to carry out the task at hand?

- **Complex tasks:** Tasks that we do not understand well enough to extract a well-defined program from our expertise (e.g., analysis of large and complex data, driving).
- **Tasks that change over time:** Machine learning tools are, by nature, adaptive to the changes in the environment they interact with (e.g., spam detection, speech recognition).

# Supervised Versus Unsupervised Learning

## Supervised Learning

- Data: for every observation $i = 1, \ldots, n$, we observe a vector of inputs $\mathbf{x}_i$ and a response $y_i$.
- Goal: fit a model that relates response $y_i$ to $\mathbf{x}_i$ in order to accurately predict the response for future observations.
- If $Y$ is quantitative, then this problem is a regression problem; if $Y$ is categorical, then it is a classification problem.

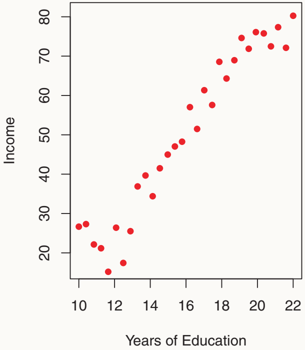
## Unsupervised Learning

- Data: for every observation $i = 1, \ldots, n$, we observe a vector of inputs $\mathbf{x}_i$ but no associated response $y_i$.
- Goal: learning about relationships between the inputs or between the observations.

# Supervised Learning

# Fundamental Problem

Suppose $Y = f(X) + \varepsilon$, where $X \perp\!\!\!\perp \varepsilon$ and $E[\varepsilon] = 0$. Goal is to estimate $f$ based on observed data $(X, Y)$.




(Source: James et al. 2013, 17)

# Fundamental Problem

- Given estimate $\hat{f}$ and inputs $X$, we can predict $\hat{Y} = \hat{f}(X)$.
- How accurate is $\hat{Y}$ as a prediction for $Y$?
- For fixed $\hat{f}$ and $X$,

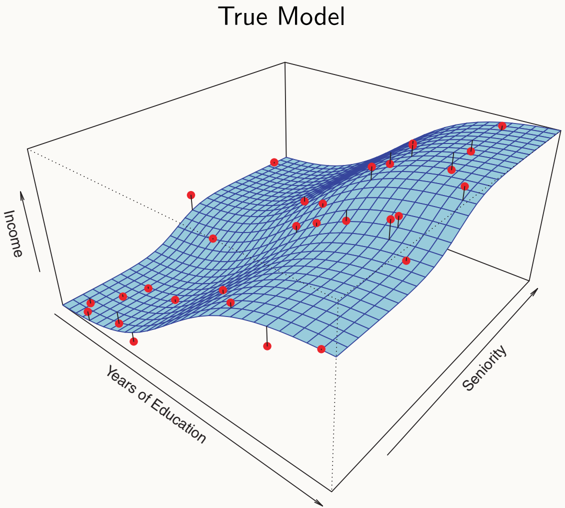
$$\begin{aligned} E\left[(Y - \hat{Y})^2\right] &= E\left[\left(f(X) + \varepsilon - \hat{f}(X)\right)^2\right] \\ &= \underbrace{\left[f(X) - \hat{f}(X)\right]^2}_{\text{reducible}} + \underbrace{Var\left[\varepsilon\right]}_{\text{irreducible}} \end{aligned} \tag{1}$$

- Our goal is to estimate $f$ so as to minimize the reducible error.

# How Do We Estimate $f$?

- Our goal is to apply a machine learning method to training data in order to estimate the unknown $f$.
- Training data consist of $\{(\mathbf{x}_i, y_i)\}_{i=1,\ldots,n}$, where $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ip})^T$.
- There are a range of methods for estimating $f$, some more and some less flexible with regard to the functional form of $f$.
- Flexible methods can fit a wider range of possible functional forms for $f$, but this comes at the cost of a greater potential for overfitting.

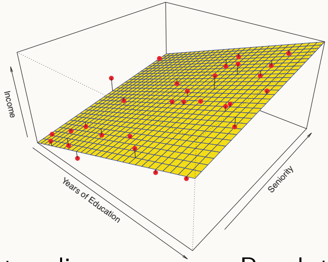
# Example: $f$ Estimated by Methods with Different Flexibility



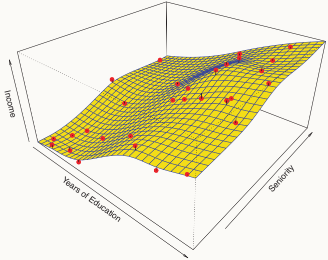

(Source: James et al. 2013, 18)

# Example: $f$ Estimated by Methods with Different Flexibility

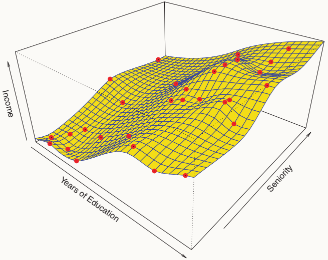
Linear model fit by least squares




Smooth thin-plate spline




Rough thin-plate spline




(Source: James et al. 2013, 22ff.)