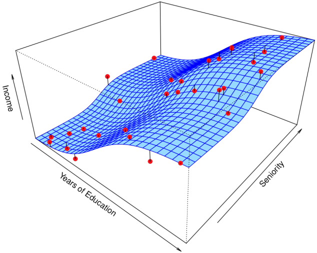
Statistical Machine Learning

Statistical Learning

Motivating Example

income dataset



Can we predict Income using these two variables?

$$\texttt{Income} \approx f(\texttt{Years of Education}, \texttt{Seniority})$$

Statistical Model

- here Sales is a response or target that we wish to predict. We generically refer to the response as Y.
- *Years of Education* is a feature, or input, or predictor; we name it X_1. Likewise name `Seniority` as X_2, and so on.
- We can refer to the input vector collectively as

$$X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix}$$

Now we write our model as

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

where ε captures all discrepancies

Why estimating f?

There are two main reasons that we may wish to estimate f: **prediction** and **inference**.

Prediction

- We can predict Y using $\hat{Y} = \hat{f}(X)$
- In this setting, $\hat{f}$ is often treated as a *black box*
- In general, $\hat{f}$ will not be a perfect estimate for f, and this inaccuracy will introduce some error.
  The accuracy of $\hat{Y}$ as a prediction for Y depends on two quantities, which we will call the *reducible error* and the *irreducible error*.
- For any estimate $f(x)$ of $f(x)$, we have

$$E[(Y - \hat{f}(X))^2|X = x] = \underbrace{E[f(X) - \hat{f}(X)]^2}_{\text{Reducible}} + \underbrace{Var(\varepsilon)}_{\text{Irreducible}}$$

Ideal Prediction

- The ideal $f(x) = E(Y|X = x)$ is called the regression function
- $f(x)$ is the function that minimizes $E[(Y - g(X))^2|X = x]$ over all functions g at all points $X = x$.

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 the relationship more complicated?

How to estimate f

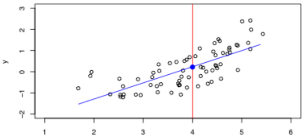
- Our goal is to apply a statistical learning method to the training data in order to estimate the unknown function f.
- In other words, we want to find a function $\hat{f}$ such that $Y \approx \hat{f}(X)$ for any observation (X, Y).
- Broadly speaking, most statistical learning methods for this task can be characterized as either *parametric* or *non-parametric*.

Parametric methods

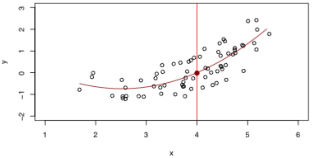
- The linear model is an important example of a parametric model:
$$f(X) = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p$$
- A linear model is specified in terms of $p + 1$ parameters
- We estimate the parameters by fitting the model to training data.
- Although it is almost never correct, a linear model often serves as a good and interpretable approximation to the unknown true function $f(X)$.

Linear models with higher order terms

A simple linear model $\hat{f}(X) = \beta_0 + \beta_1 X$ gives a reasonable fit here



A quadratic model $\hat{f}(X) = \beta_0 + \beta_1 X + \beta_2 X^2$ fits slightly better.



Non-parametric methods

- we know $E(Y|X = x)$ is the ideal estimator
- typically we have few if any data points with $X = x$ exactly.
  -so we cannot estimate $E(Y|X = x)$
- relax the definition and let

$$\hat{f}(x) = \text{Ave}(Y|X \in \mathcal{N}(x))$$

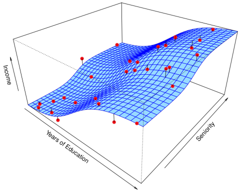
- $\mathcal{N}(x)$ is come neighborhood of x
- also called "local averaging"

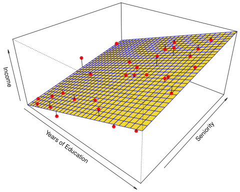
Curse of Dimensionality

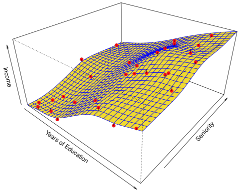
- Nearest neighbor averaging can be pretty good for small p — i.e. $p \leq 4$ and large n.
- We will discuss smoother versions, such as kernel and spline smoothing later in the course.
- Nearest neighbor methods can be lousy when p is large. Reason: the curse of dimensionality. Nearest neighbors tend to be far away in high dimensions.
- check http://en.wikipedia.org/wiki/Volume_of_an_n-ball

Parametric vs Non-Parametric methods

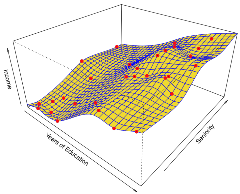
income data revisit







Overfitting

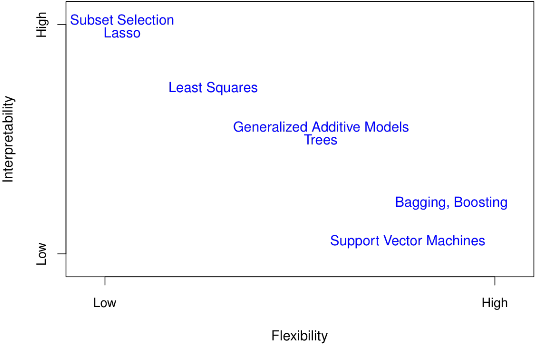


- The same thin-plate spline fit using a lower level of smoothness, allowing for a rougher fit.
- The resulting estimate fits the observed data perfectly!
- However, the spline fit shown is far more variable than the true function f.
- This is an example of overfitting the da

Prediction accuracy versus interpretability

- Linear models are easy to interpret; thin-plate splines are not.
- Good fit versus over-fit or under-fit.
- How do we know when the fit is just right?
- Parsimony versus black-box.
- We often prefer a simpler model involving fewer variables over a black-box predictor involving them all.

Various methods — Interpretability vs Flexibility



Assessing Model Accuracy

- Suppose we fit a model $f(x)$ to some training data $Tr = \{x_i, y_i\}_{i=1}^{n}$, and we wish to see how well it performs.
- We could compute the average squared prediction error over Tr

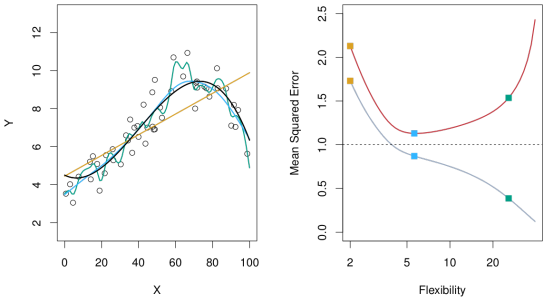
$$\text{MSE}_{Tr} = \text{Ave}_{i \in Tr}[y_i - \hat{f}(x_i)]^2$$

- This may be biased toward more overfit models.
- Instead we should, if possible, compute it using fresh test data $Te = \{x_i, y_i\}_{i=1,m}$

$$\text{MSE}_{Te} = \text{Ave}_{i \in Te}[y_i - \hat{f}(x_i)]^2$$

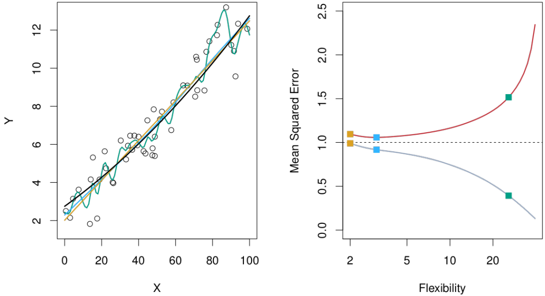
- also referred to "in-sample" and "out-of-sample" errors
- a.k.a. MSPE (P for prediction)

MSE_{Tr} vs MSE_{Te}



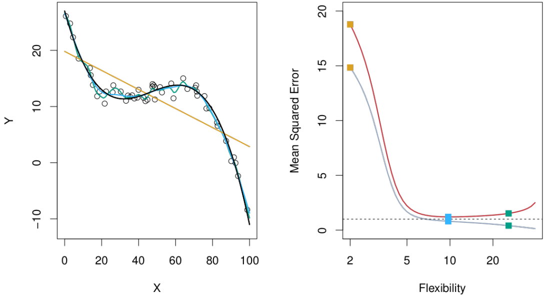
MSE_{Tr}: grey vs MSE_{Te}: red'

MSE_{Tr} vs MSE_{Te} - an almost linear function



MSE_{Tr}: grey vs MSE_{Te}: red'

MSE_{Tr} vs MSE_{Te} - a rough function



MSE_{Tr}: grey vs MSE_{Te}: red'

Bias-Variance trade offs

- Suppose we have fit a model $\hat{f}(x)$ to some training data Tr, and let (x_0, x_1) be a test observation drawn from the population. If the true model is

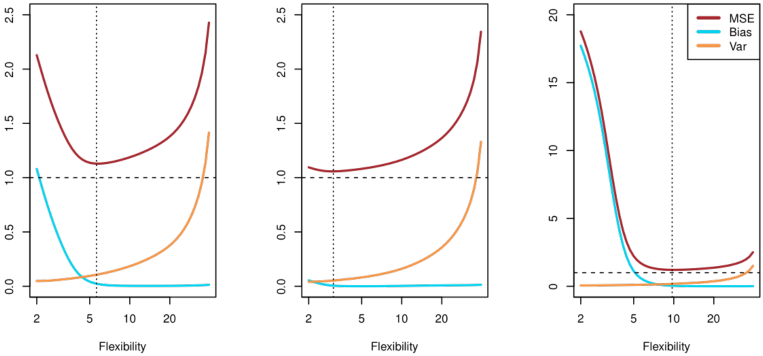
$$Y = f(X) + \varepsilon$$

- then

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = Var\left(\hat{f}(x_0)\right) + \left[Bias\left(\hat{f}(x_0)\right)\right]^2 + Var(\varepsilon)$$

- Typically as the flexibility of $\hat{f}$ increases, its variance increases, and its bias decreases. So choosing the flexibility based on average test error amounts to a bias-variance trade-off.

Previous example



curve vs almost linear vs rough