

# Statistics 452: Statistical Learning and Prediction

## Chapter 2: Statistical Learning

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2018-09-01

# Statistical Learning

## Example 1: Advertising Data

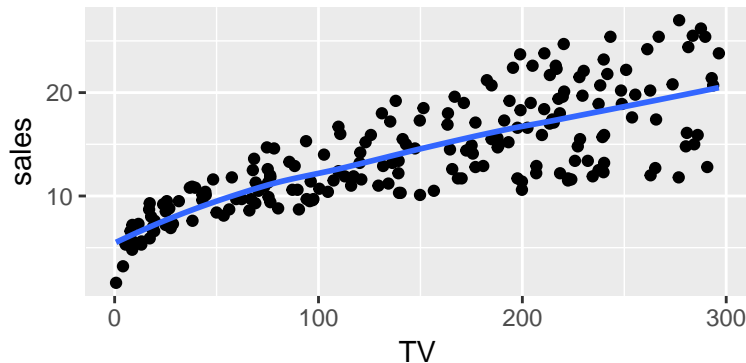
- Sales (in thousands of units), and advertising budgets in thousands of dollars for TV, radio and newspaper for 200 markets.

```
uu <- url("http://www-bcf.usc.edu/~gareth/ISL/Advertising.csv")
advert <- read.csv(uu,row.names=1)
head(advert)
```

```
##      TV radio newspaper sales
## 1 230.1  37.8      69.2  22.1
## 2  44.5  39.3      45.1  10.4
## 3  17.2  45.9      69.3   9.3
## 4 151.5  41.3      58.5  18.5
## 5 180.8  10.8      58.4  12.9
## 6   8.7  48.9      75.0   7.2
```

# Relationship Between Sales and TV

```
library(ggplot2)
ggplot(advert, aes(x=TV, y=sales)) +
  geom_point() + geom_smooth(se=FALSE)
```



- ▶ The smoother is not constrained to be linear, but is nearly so.
- ▶ What sort of return on investment do we get from increasing TV ads?

## Exercise

- ▶ Do similar scatterplots of Sales vs Radio and Sales vs Newspaper.
  - ▶ Try smoothing with an unconstrained smoother (default) and a linear smoother (`geom_smooth(method="lm")`)
  - ▶ Which medium provides the best return on investment?

# Terminology

- ▶ Advertising budgets  $X_1$ =TV,  $X_2$ =Radio and  $X_3$ =Newspaper are **inputs** or **explanatory variables** or **predictors** or **features**
  - ▶ Let  $X = (X_1, X_2, X_3)$ .
- ▶ Sales  $Y$  is the **output** or **response variable**

# Model

- ▶ A general model is

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

where

- ▶  $f$  is a fixed but unknown function that is the **systematic** component of the model
- ▶  $\epsilon$  is an error component, assumed to be independent of  $X$  and to have mean zero.

## Example 2: Income data

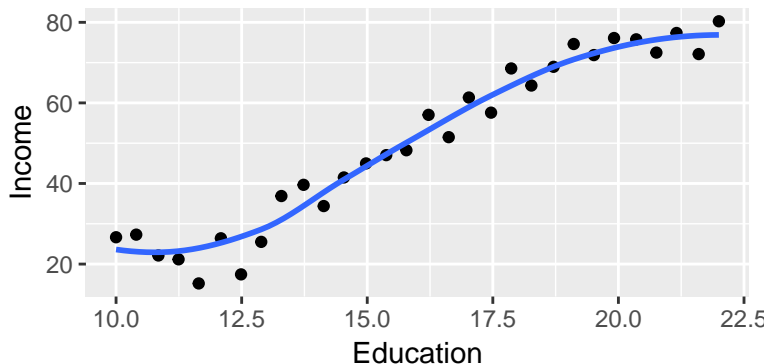
```
uu <- url("http://www-bcf.usc.edu/~gareth/ISL/Income1.csv")
income <- read.csv(uu,row.names=1)
head(income)
```

```
##      Education    Income
## 1  10.00000  26.65884
## 2  10.40134  27.30644
## 3  10.84281  22.13241
## 4  11.24415  21.16984
## 5  11.64548  15.19263
## 6  12.08696  26.39895
```



# Relationship Between Income and Education

```
ggplot(income, aes(x=Education, y=Income)) +  
  geom_point() + geom_smooth(se=FALSE)
```



- ▶ Here the relationship is non-linear.
- ▶ What is the effect of increasing education?
  - ▶ Depends; e.g., not much at low and high education

# Statistical Learning

- ▶ Approaches for
  - ▶ estimating  $f$
  - ▶ quantifying the accuracy of the estimate

# Why estimate $f(X)$ ?

- ▶ Two main goals:
  1. prediction
  2. inference

# Prediction

- ▶ Since the errors average to zero,  $f(X)$  is a reasonable prediction of a new  $Y$ .
- ▶ Notation: Let  $\hat{f}$  denote an estimate of  $f$  and  $\hat{Y}$  an estimate of  $Y$ .
- ▶ Based on  $\hat{f}$  the estimate of  $Y$  is

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

- ▶ For prediction,  $\hat{f}$  can be a “black box”.
  - ▶ We do not really care about the details of  $\hat{f}$ , only that its predictions  $\hat{Y}$  are accurate.

# Accuracy of $\hat{Y}$

- ▶ There are two components
  - ▶ reducible error –  $\hat{f}$  as an imperfect estimate of  $f$
  - ▶ irreducible error – the model includes the pure error component  $\epsilon$ , which cannot be predicted using  $X$  (assumed independent)
- ▶ We will study methods for estimating  $f$  that try to minimize the reducible error.

# Inference

- ▶ Or, should our goal be to “open the box” and see what’s inside?
  - ▶ See first 4:30 of TED talk by Barbara Englehardt:  
<https://www.youtube.com/watch?v=uC3SfnbCXmw>
- ▶ We may want to understand the relationship between  $X$  and  $Y$ .
  - ▶ If there are many explanatory variables, can we find a few important variables that explain the most variation in the response?
  - ▶ What is the nature of relationships: positive/negative, linear/non-linear?

# How to estimate $f(X)$

- ▶ Methods can be classified as either
  - ▶ parametric, or
  - ▶ non-parametric
- ▶ In either case, we will use **training data** to train our method how to estimate  $f$ .
- ▶ Notation: Let  $x_i = (x_{i1}, \dots, x_{ip})$  denote the observed predictors and  $y_i$  the response for the  $i$ th of  $n$  independent observations.
  - ▶ Then the training data are  $\{(x_1, y_1), \dots, (x_n, y_n)\}$

# Parametric Methods

- ▶ Two steps:

1. Specify a form for  $f$  that depends on a finite number of parameters
2. Use the training data to estimate the parameters.

- ▶ Example:

1. A linear model  $f(X) = \beta_0 + \beta_1 X_1 + \dots, + \beta_p X_p$ .
2. Use the method of least squares to estimate  $\beta_0, \beta_1, \dots, \beta_p$ .



# Drawbacks of Parametric Methods

- ▶ The true  $f$  may not be well-approximated by the functional form we choose for our parametric model.
- ▶ We can choose a very flexible parametric family, but if too flexible we may **overfit**; i.e., the fitted model may follow the error terms.

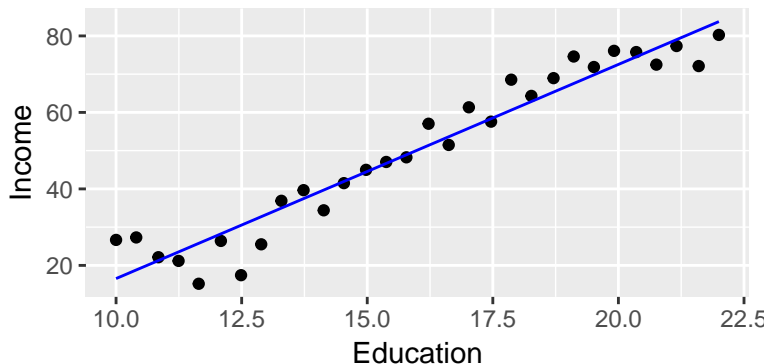
## Example: Income data

- Try using powers of Education to predict Income

```
ifit<- lm(Income ~ Education, data=income)
# grid of Education values
nGrid <- 100
rEd <- with(income,range(Education))
newEd = seq(from=rEd[1],to=rEd[2],length=nGrid)
# Predict income from ifit
newdat <- data.frame(Education = newEd)
pIncome <- predict(ifit,newdata=newdat)
incomePred <- data.frame(Income = pIncome, Education = newEd)
```

## Graph the fitted model

```
ggplot(income, aes(x=Education, y=Income)) + geom_point() +  
  geom_line(data=incomePred, color="blue")
```



# Higher powers

- ▶ Repeat for powers of Education using `I()`; e.g., for a cubic fit

```
ifit<- lm(Income ~ Education + I(Education^2) + I(Education^3), data=income)  
# Now return to code to predict income from ifit and draw fit
```

- ▶ At some point, do you get the feeling you are just fitting noise?
  - ▶ Fact: If you fit a polynomial of degree 30 you would interpolate the data points.

# Non-parametric Methods

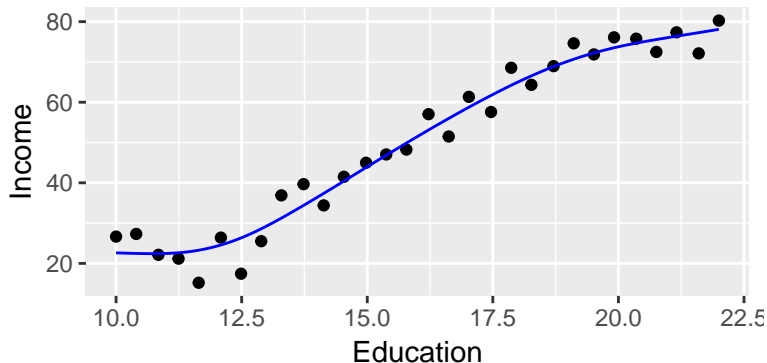
- ▶ An model-free specification of the functional form of  $f$ .
- ▶ Avoid over-fitting by limiting the roughness, or wigglyness of the fitted curve.

## Example: Smoothing spline

```
# install.packages("gam")
library(gam)
sfit <- gam(Income ~ s(Education),data=income)
# Predict income from sfit
pIncome <- predict(sfit,newdata=newdat)
incomePred <- data.frame(Income = pIncome, Education = newEd)
```

## Graph the fitted model

```
ggplot(income, aes(x=Education, y=Income)) + geom_point() +  
  geom_line(data=incomePred, color="blue")
```



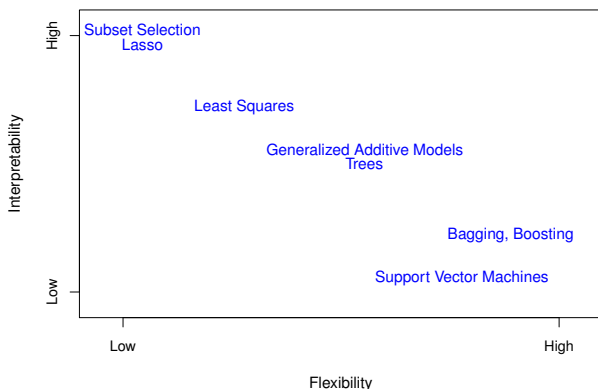
# Non-parametric Methods: Drawbacks

- ▶ The degree of smoothness was left at its default value – how do we choose this in general?
- ▶ Non-parametric methods require more data than a parametric method to train the model to obtain accurate estimates.



# Prediction Accuracy *versus* Interpretability

- ▶ Figure 2.7 of the text schematically represents the trade-off between prediction accuracy and model interpretability.



- ▶ The more flexible the model, the more accurate the predictions, but the less interpretable the model.
  - ▶ We will see this by comparing methods as we go.

# Supervised *versus* Unsupervised Learning

- ▶ When we have measured a response variable the problem is said to be supervised (Chapters 3-9).
- ▶ When there is no response, the problem is unsupervised (Chapter 10).
  - ▶ We observe  $x_i$ ;  $i = 1, \dots, n$  and are looking to understand the relationship between the variables, or between the observations (cluster analysis)
  - ▶ Cluster analysis is sometimes phrases in terms of looking for a latent (not observed) categorical variable underlying groups in the data.

# Regression *versus* Classification

- ▶ Regression methods specify models for the conditional mean of the outcome given values of the explanatory variables.
  - ▶ Generally, the aim of supervised learning with a quantitative response is regression.
- ▶ In classification problems we aim to predict which class an observation belongs to, rather than its mean outcome.
- ▶ Some approaches are both; e.g., logistic regression.
  - ▶ The outcome may be binary (diseased, not diseased) and we can use a fitted model to classify future observations.
  - ▶ But the model fits the mean response given values of the explanatory variables and so is a regression.

## Assessing Model Accuracy

# Quality of Fit in Regression: MSE

- In regression problems, a popular measure of the quality of a fitted model is the mean squared error (MSE), defined as

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

# The Training MSE

- ▶ However, we are not especially interested in the MSE from the training data (the training MSE in equation 1).
  - ▶ Recall the fact that a high enough polynomial regression can interpolate (see also the wiggly smoothing splines in Figure 2.9 of the text).
  - ▶ If all we cared about was training MSE, we'd fit high-degree polynomials.
  - ▶ But these would overfit and would give poor predictions of new responses.

# The Test MSE

- ▶ Instead we are interested in the accuracy of the prediction of new data, called test data. If the training observations  $\{(x_1, y_1), \dots, (x_n, y_n)\}$  are used to produce  $\hat{f}$ , and we had a large number of test observations  $(x_0, y_0)$ , the test MSE

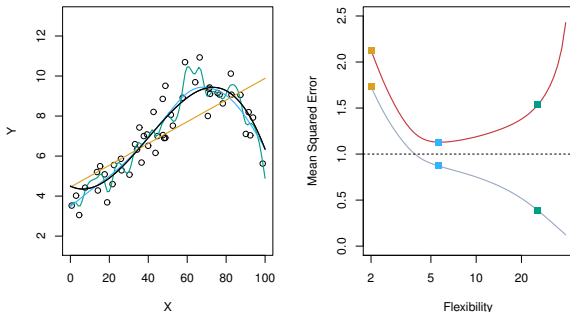
$$\text{Ave}((y_0 - \hat{f}(x_0))^2)$$

reflects how well  $\hat{f}$  predicts new observations.

- ▶ We would like to develop methods that minimize the test MSE.
- ▶ **Cross validation** (CV) is a tool to estimate the test MSE.

# Training *versus* Test MSE

- ▶ Text, simulated data example, Figure 2.9



- ▶ The black line is the curve used to simulate data (circles) and the other lines are fitted curves of different flexibility (smoothing splines, Chapter 7).
- ▶ In the right panel, the grey line is the training MSE and the red is the test MSE.
  - ▶ The “U” shape of the test MSE is typical and reflects the bias-variance trade-off.



# Bias-Variance Tradeoff

- ▶ For fixed  $x_0$  and  $y_0$ , the expected test MSE  $E(y_0 - \hat{f}(x_0))^2$ , obtained by averaging over repeated estimations of  $f$ , can be decomposed as

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

where

- ▶  $\text{Var}(\hat{f}(x_0))$  is the variance (spread) of the predictions,
  - ▶  $\text{Bias}(\hat{f}(x_0))$  is the bias (systematic departure from truth) of the predictions, and
  - ▶  $\text{Var}(\epsilon)$  is the irreducible error term that is beyond our control
- ▶ Generally, the more flexible the method for estimating  $f$  the higher the variance and the lower the bias.
    - ▶ Initially as we increase flexibility, the variance increase is offset by a decrease in bias, and the test MSE decreases.
    - ▶ At some point though the variance increase exceeds the decrease in bias and the expected test MSE increases.

# Quality of Fit in Classification

- ▶ For categorical  $Y$ , the error rate is the proportion of mistaken classifications

$$\frac{1}{n} \sum_{i=1}^n I(y_i \neq \hat{y}_i) \quad (2)$$

where

- ▶  $\hat{y}_i$  is the predicted class label for the  $i$ th observation, and
  - ▶  $I(y_i \neq \hat{y}_i)$  is an indicator variable that is one if  $y_i \neq \hat{y}_i$  and zero if  $y_i = \hat{y}_i$ .
- ▶ Equation (2) is the training error rate. We are more interested in the test error rate:

$$\text{Ave}(I(y_0 \neq \hat{y}_0)) \quad (3)$$

where the average is over new  $(x_0, y_0)$ .

# The Bayes Classifier

- ▶ It can be shown that the test error (3) is minimized by the Bayes classifier.
- ▶ To a new  $x_0$  the Bayes classifier assigns class label  $j$  if  $P(Y = j|X = x_0)$  is the largest over all categories  $j$ .
- ▶ The resulting error rate is called the Bayes error rate – this is a lower bound on the test error rate.
  - ▶ This is analogous to the irreducible error from regression.
- ▶ We don't know the conditional probabilities  $P(Y = j|X = x_0)$  so the Bayes classifier is not practically useful.
  - ▶ Suggests we try to estimate the required conditional probabilities. This is the idea behind the K-nearest neighbors classifier (Chapter 4).

# Loss Functions

- ▶ Reference: Elements of Statistical Learning, Chapter 7.
- ▶ We measure the errors between  $Y$  and fit  $\hat{f}(X)$  by a loss function  $L(Y, \hat{f}(X))$ .

- ▶ For quantitative  $Y$  we mentioned squared error loss

$$L(Y, \hat{f}(X)) = (Y - \hat{f}(X))^2$$

which gave us the test MSE.

- ▶ For categorical response,  $G$ , we mentioned zero-one loss (misclassification error)

$$L(Y, \hat{f}(X)) = I(Y \neq \hat{f}(X))$$

which gave us the test error.

- ▶ In general, the test error is the average loss over a test set.