

Statistics 452: Statistical Learning and Prediction

Chapter 2: Statistical Learning

Brad Mcnenny

2017-09-01

Statistical Learning

Example 1: Advertising Data

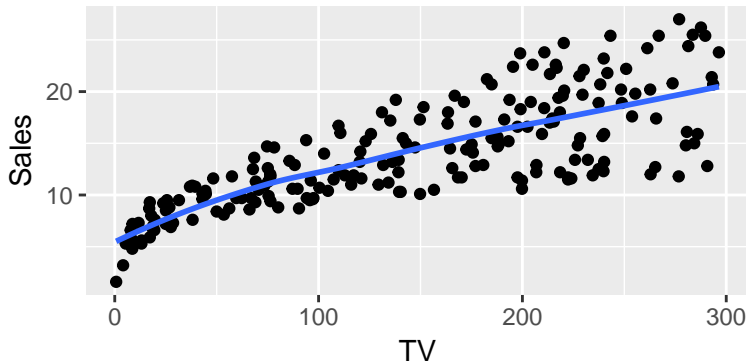
- Sales (in thousands of units), and advertising budgets in thousands of dollars for TV, radio and newspaper for 200 markets.

```
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
- ▶ ϵ is an error component, assumed to be independent of X and to have mean zero.

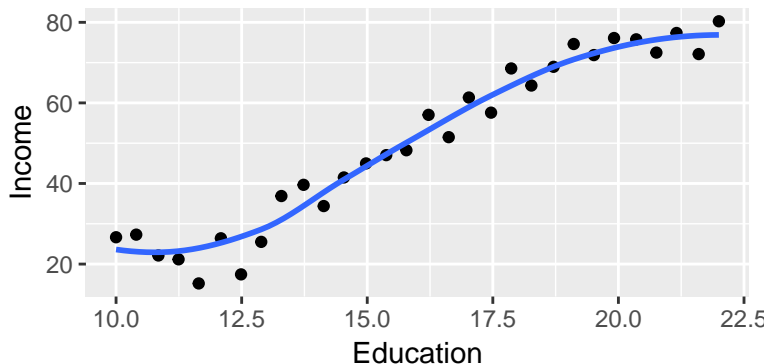
Example 2: Income data

```
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 ϵ , which cannot be predicted using X (assumed independent)
- ▶ We will study methods for estimating f that try to minimize the reducible error.

Inference

- ▶ Looking inside the black box.
- ▶ 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.

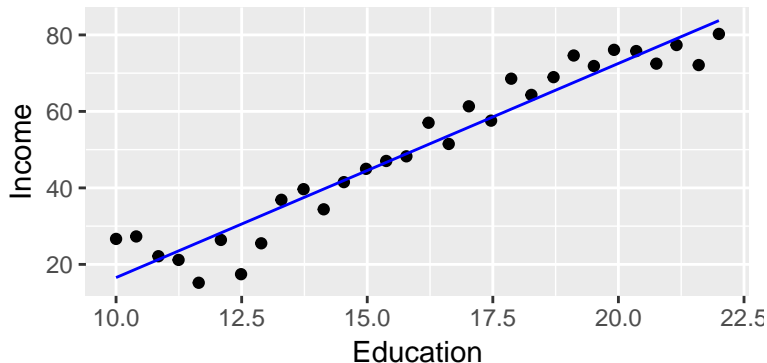
Example: Income data

- 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)
```

- ▶ 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

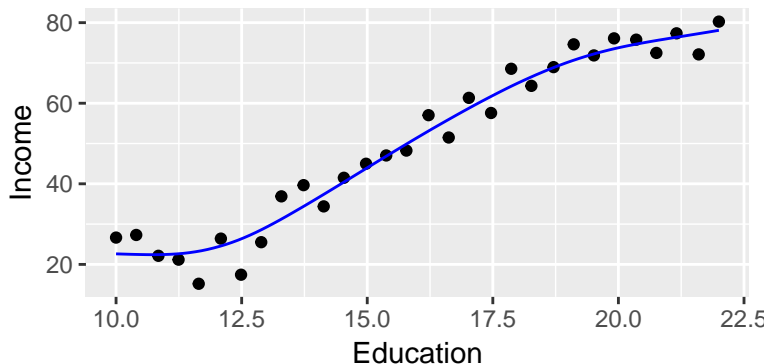
- ▶ An model-free specification of the functional form of f .
- ▶ Avoid over-fitting by limiting the roughness, or wigglyness of the fitted curve.

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

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

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.

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

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

for 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).