Business 4720 - Class 12

Supervised Machine Learning using R

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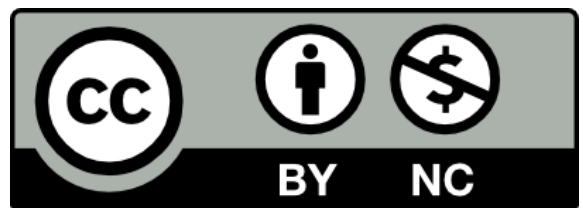

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This Class

What You Will Learn:

- Linear Regression Models in R
  - Linear regression
  - Lasso and Ridge regression
- Classification Models in R
  - Logistic Regression
  - K-NN

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Based On

Gareth James, Daniel Witten, Trevor Hastie and Robert Tibshirani: *An Introduction to Statistical Learning with Applications in R*. 2nd edition, corrected printing, June 2023. (ISLR2)

`https://www.statlearning.com`

Chapters 2, 3, 4, 5

Trevor Hastie, Robert Tibshirani, and Jerome Friedman: *The Elements of Statistical Learning*. 2nd edition, 12th corrected printing, 2017. (ESL)

`https://hastie.su.domains/ElemStatLearn/`

Chapters 2, 3, 4, 7

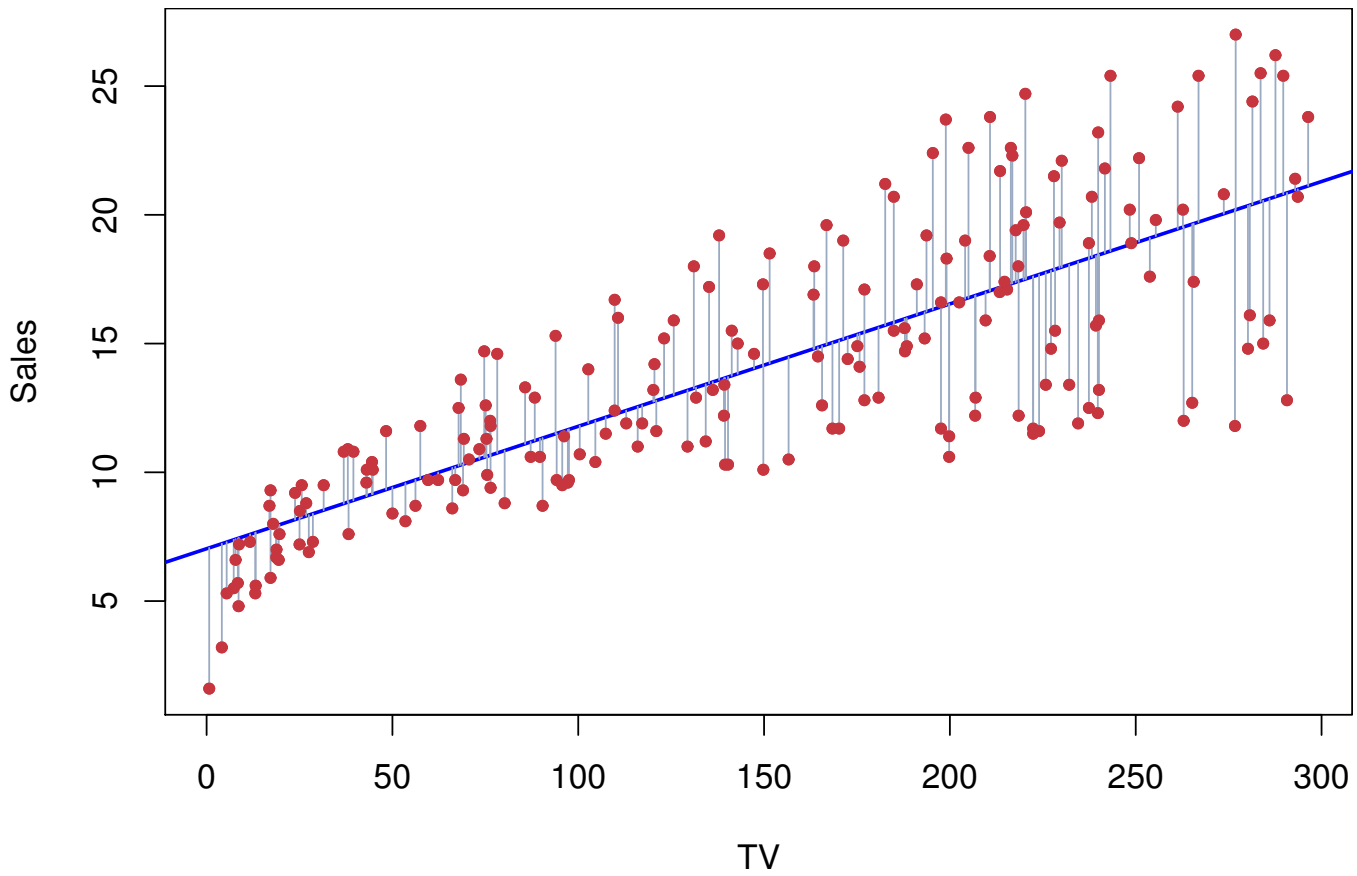
Kevin P. Murphy: *Probabilistic Machine Learning – An Introduction*. MIT Press 2022.

`https://probml.github.io/pml-book/book1.html`

Chapters 4, 6, 9, 10, 11

Linear Regression

$$Y = \beta_0 + \beta_1 X + \epsilon$$



Source: ISLR2 Figure 3.1

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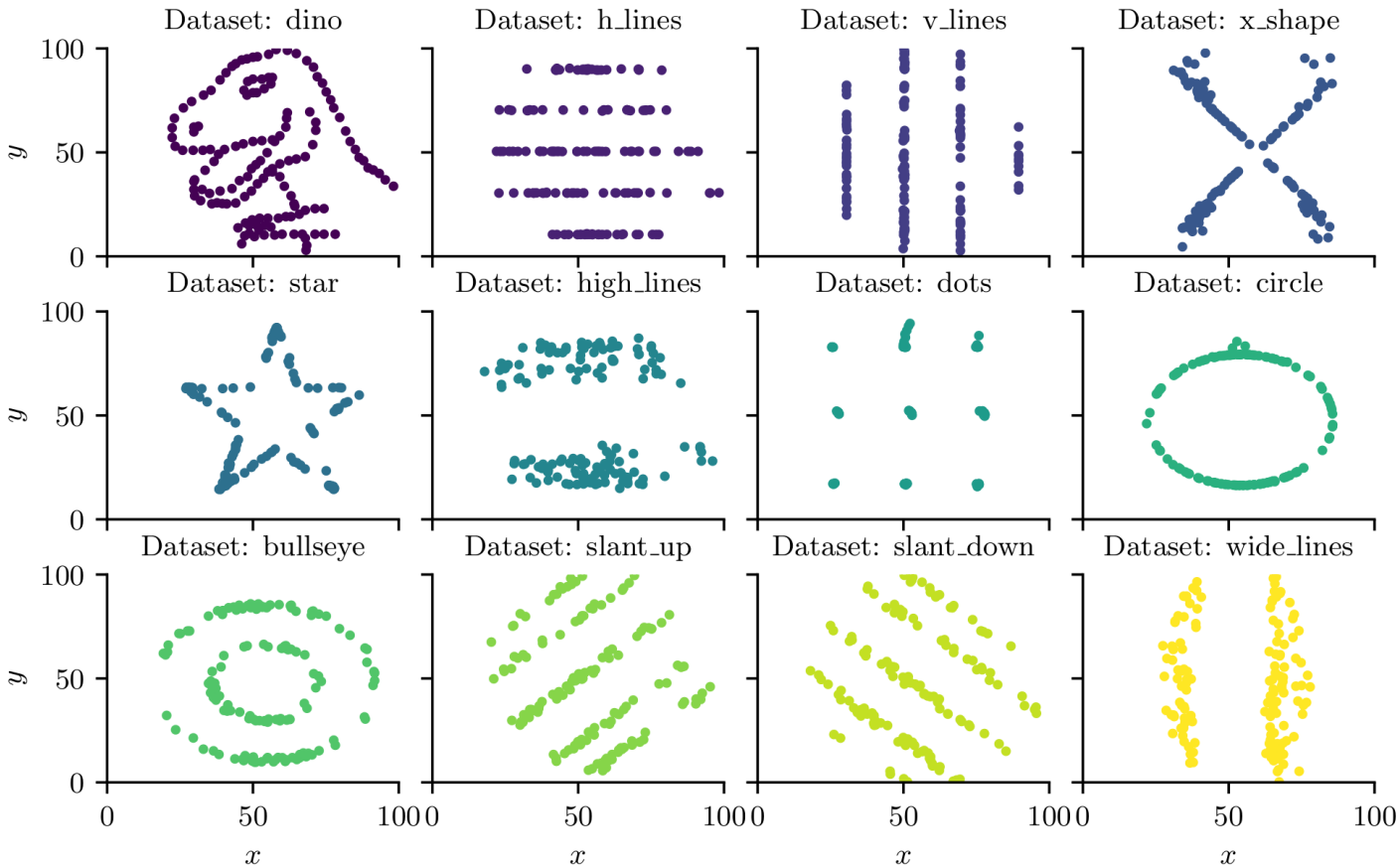
Ensure a Linear Model is Sensible



Source: Murphy Figure 2.6

The ”Datasaurus Dozen”: All datasets have the same correlation between the two variables!

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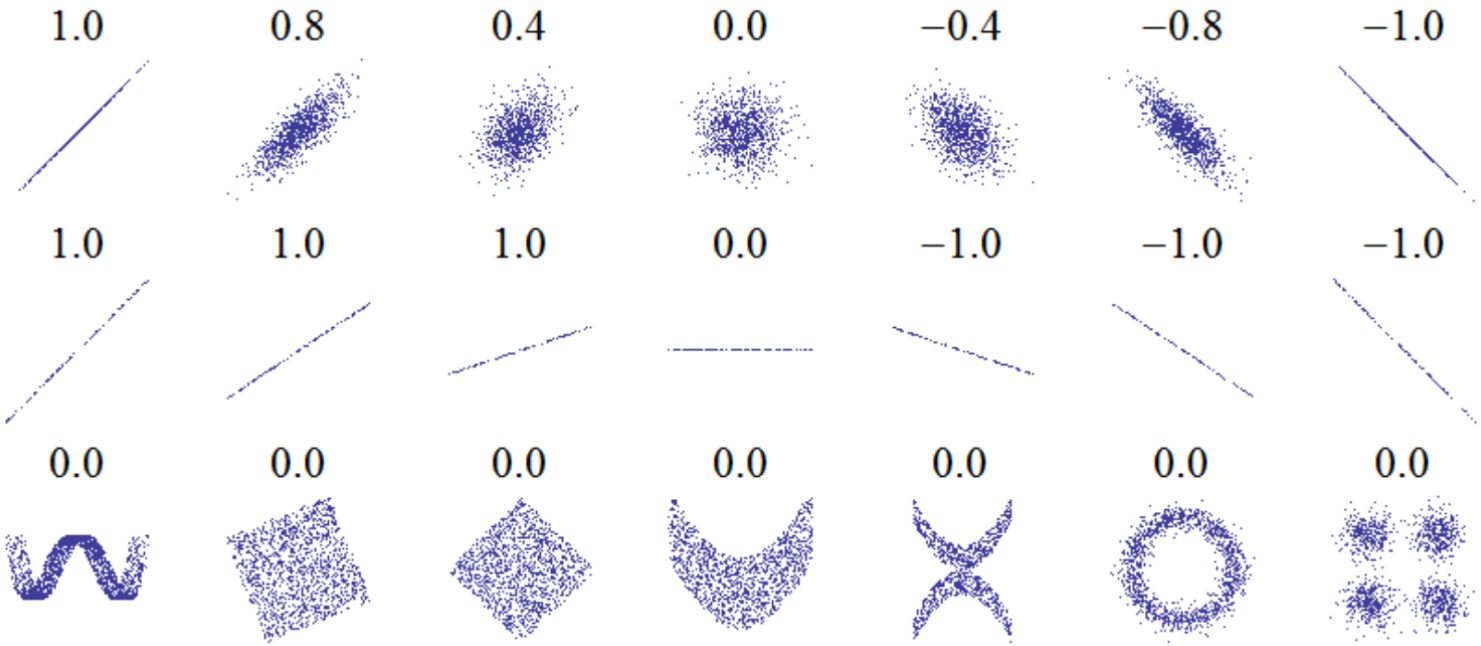
Ensure a Linear Model is Sensible



Source: Murphy Figure 3.1

Datasets with the same correlation (as indicated above each dataset) between two variables do not need to have the same regression slope!

Estimating Linear Regression [cont'd]

- Estimate $\hat{\beta}_0$ and $\hat{\beta}_1$ to minimize the mean squared error (MSE) or residual sum of square (RSS)

$$RSS = \sum_i \left(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i\right)^2 \qquad MSE = \frac{1}{n} RSS$$

- Analytically derivable *least squares estimates* are

$$\hat{\beta}_1 = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2}$$
$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

  where $\bar{x}$ and $\bar{y}$ are the sample means
- MSE ("L2 loss") is susceptible to outlier influence, the MAE ("L1 loss") is more robust

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Evaluating Linear Regression Models [cont'd]

- Estimates have *standard errors* that indicate uncertainty of the estimates
- A *t-test* can be used to determine if a parameter is statistically significant from a value V (typically $V = 0$) using the test statistic

$$t = \frac{\hat{\beta}_1 - V}{SE(\hat{\beta}_1)}$$

- The *p-value* is the probability that the parameter is non-zero, assuming the estimated model is true
- The R^2 value is the proportion of explained variance

$$R^2 = \frac{TSS - RSS}{TSS} = 1 - \frac{RSS}{TSS}$$

where $TSS = \sum_i (y_i - \bar{y})^2$ is the total sum of squares

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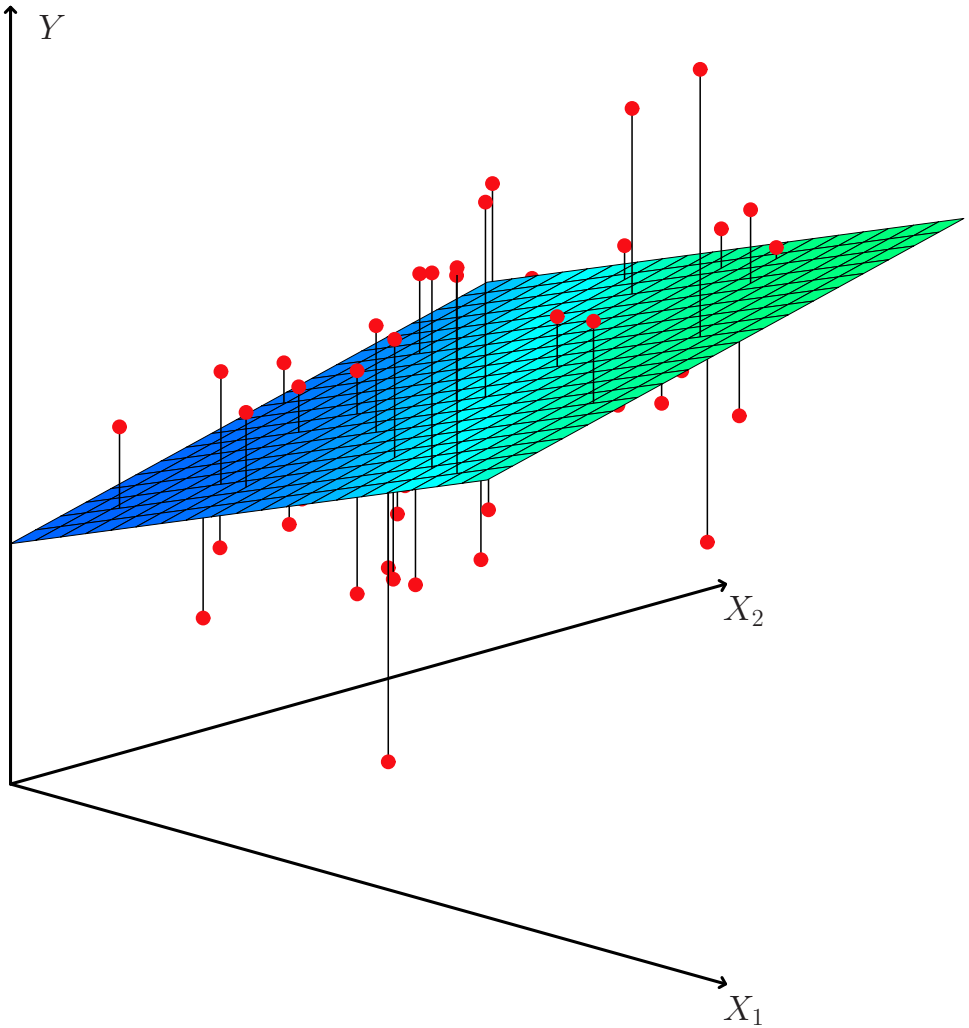
Generalization to Multiple Predictors



Source: ISLR2 Figure 3.4

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon$$

R^2 represents the correlation of Y and $\hat{Y}$

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Regression with Qualitative Predictors

- Qualitative predictors (*factors* with multiple, exclusive *levels*) can be used in linear regression models using **dummy variables**:

$$x_{i1} = \begin{cases} 1 & \text{level "a"} \\ 0 & \text{else} \end{cases}$$

$$x_{i2} = \begin{cases} 1 & \text{level "b"} \\ 0 & \text{else} \end{cases}$$

$$x_{i3} = \begin{cases} 1 & \text{level "c"} \\ 0 & \text{else} \end{cases}$$

- Note: $x_{i1} = x_{i2} = x_{i3} = 0$ represents level d!
- "Contrasts" determine how factor levels are coded using dummy variables

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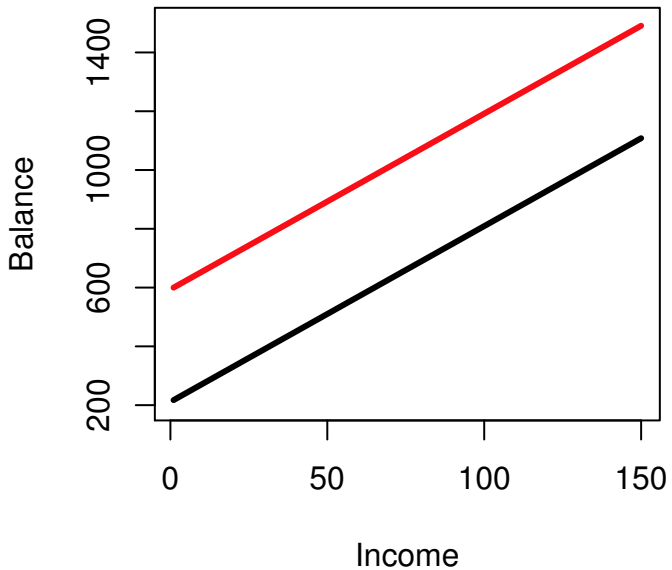
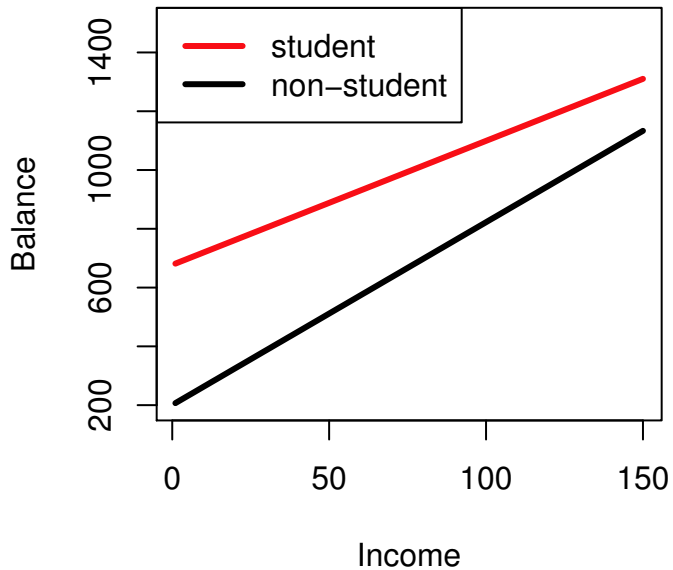
Inputs, Predictors, and Polynomials

- Example:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_2 + \beta_4 X_1 X_2 + \epsilon$$

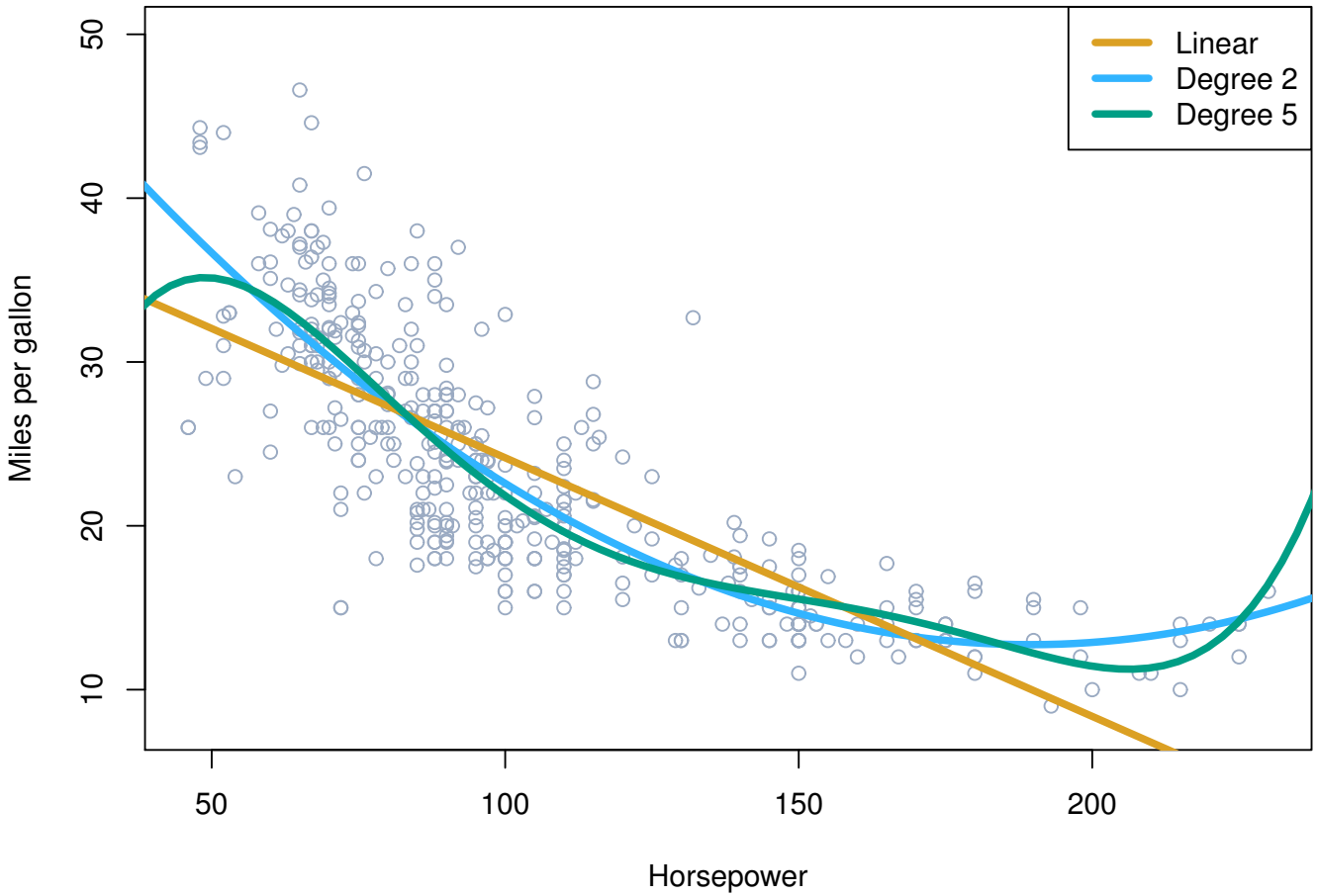
- Still linear in β_j
- Two *inputs* X_1 and X_2
- Four *predictors* or *features*: X_1, X_1^2, X_2, $X_1 X_2$
- **Main effects** β_1 and β_3, **interaction effect** β_4, and a degree-2 polynomial





Source:
ISLR2
Figure 3.7

Multiple Regression with Polynomial Expansion



Source: ISLR2 Figure 3.8

Multiple Linear Regression in R

The 'Boston' data set contains housing values in Boston in variable `medv` (median value). Examine the data:

```
# Functions and data from the textbook # 'Modern
# Applied Statistics with S'
library(MASS)

# Data sets from the textbook 'Introduction to
# Statistical Learning with Applications in R'
library(ISLR2)

# Get a description of the data
?Boston

# Get a summary and first few rows
summary(Boston)
head(Boston)

# Bivariate scatterplots
plot(Boston)
```

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Multiple Linear Regression in R [cont'd]

Fit a simple model, examine the results, and make predictions:

```
# Fit a model with intercept only
fitted.model <- lm(medv ~ 1, data=Boston)
summary(fitted.model)

# Fit a model with predictor lstat
fitted.model <- lm(medv ~ lstat, data=Boston)
summary(fitted.model)

# Plot the data and the regression line
plot(medv ~ lstat, data=Boston)
abline(fitted.model, lwd=3, col='red')

# Plot the residuals against predicted values
plot(predict(fitted.model), residuals(fitted.model))

# Predict three new observations of lstat
predict(fitted.model, data.frame(lstat=c(5, 10, 15)),
   interval='confidence')
```

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Multiple Linear Regression in R [cont'd]

Build more complex models:

```
# Add another predictor
fitted.model <- lm(medv ~ lstat + age, data=Boston)

# Add all main effects
fitted.model <- lm(medv ~ ., data=Boston)

# Add interaction terms
fitted.model <- lm(medv ~ lstat + age + lstat:age,
   data=Boston)

# Shorter and equivalent
fitted.model <- lm(medv ~ lstat*age, data=Boston)
summary(fitted.model)
```

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Multiple Linear Regression in R [cont'd]

Add polynomial terms:

```
# Add a polynomial term; use the I(.) function
# for any data transformations, such as log(),
# or exp() or sqrt() as well as polynomials
fitted.model <- lm(medv ~ lstat + I(lstat^2),
   data=Boston)
summary(fitted.model)

# Add all polynomial terms up to degree 5
fitted.model <- lm(medv ~ poly(lstat, 5), data=Boston)
# Note the coefficients for the polynomials
# in the summary
summary(fitted.model)
```

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Multiple Linear Regression in R [cont'd]

Categorical predictors ("factors") using dummy variables:

```
?Carseats
```

Identify factor/categorical variables and their levels:

```
is.factor(Carseats$ShelveLoc)
levels(Carseats$ShelveLoc)
levels(Carseats$Urban)
levels(Carseats$US)
```

Contrasts show the dummy variables created (columns) and the values they take for different factor levels (row):

```
contrasts(Carseats$ShelveLoc)
contrasts(Carseats$US)
```

Fit the model:

```
summary(lm(Sales ~ . , data=Carseats))
```

Hands-On Exercises

(Source: ISLR2 Chapter 3)

Use the `Auto` data set from the ISLR2 library with `mpg` as the target.

1. Perform a linear regression with `horsepower` as predictor
2. Is there a relationship between the predictor and target? What form and how strong?
3. What is the predicted `mpg` value for a `horsepower` of 98?
4. Plot the response and predictor. Use the `abline()` function to add the regression line
5. Produce a scatterplot of all variables
6. Perform a linear regression of all main effects (except for the variable `name`), then remove non-significant predictors
7. Use the `*` and `:` symbols to add interaction effects. Retain only significant ones
8. Add transformations of the predictors (using the `I(.)` function) such as $\log(X)$, $\sqrt{X}$, X^2.

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Hands-On Exercises

(Source: ISLR2 Chapter 3)

Use the `Carseats` data set from the ISLR2 library with `Sales` as the target.

1. Perform a linear regression with `Price`, `Urban` and `US` as predictors
2. Interpret the coefficients. Tip: Some variables are categorical
3. Remove non-significant predictors
4. How well do the two models fit the data?
5. Determine the 95% confidence intervals for the coefficients of each model.
6. (How) does the importance of predictors change?

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Cross-Validation in R – Holdout Sample

Validation set approach:

```
# Set the seed for the pseudo-random
# number generator (RNG)
set.seed(1)

# Randomly use half the Auto data as training sample
train.idx <- sample(nrow(Auto), nrow(Auto)/2)
train.data <- Auto[train.idx,]
test.data <- Auto[-train.idx,]

# Fit model to (train model on) a subset
fitted.model <- lm(mpg ~ horsepower, data=train.data)

# Calculate the validation data MSE.
mean((test.data$mpg-predict(fitted.model,test.data))^2)

# Calculate the training MSE, first from residuals,
# then by explicitly predicting the training data
mean(summary(fitted.model)$residuals^2)
mean((train.data$mpg-predict(fitted.model,train.data))^2)
```

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Cross-Validation in R – Leave One Out CV

- The `glm()` function fits *Generalized Linear Models* using maximum-likelihood estimation, not RSS minimization. They yield identical solutions for ”ordinary” linear models but MLE is more flexible and can be used on a wide range of models.
- The use of `glm()` is identical to that of `lm()` for ”ordinary” linear models; the `boot` package provides cross-validation for `glm` models
- **Tip:** LOOCV is K-Fold CV with $K = N$

```
library(boot)

# Fit a model with glm and show its summary
glm.fit <- glm(mpg ~ horsepower, data=Auto)
summary(glm.fit)

# LOOCV is k-fold CV where k equals N, num of obs
cv.err <- cv.glm(Auto, glm.fit, K=nrow(Auto))
cv.err$delta[1]
```

Cross-Validation in R – K-Fold CV

K-Fold Cross-Validation using the `glm` function

```
cv.err <- cv.glm(Auto, glm.fit, K=10)
cv.err$delta[1]
```

Example: Use cross-validation to compare different models:

```
set.seed(17)
cv.err <- rep(0, 5)
for(i in 1:10) {
  glm.fit <- glm(mpg ~ poly(horsepower,i), data=Auto)
  cv.err[i] <- cv.glm(Auto, glm.fit, K=10)$delta[1]
}
cv.err
```

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Hands-On Exercises – Cross-Validation

Consider the Boston housing data set `Boston`.

1. Fit a regression model using `medv` as target, and `age`, `lstat`, and `ptratio` as predictors
2. Using the validation set approach, compute the test error of this model. Perform the following steps
   - 2.1 Split the data set using 75% for training and 25% for testing
   - 2.2 Fit the model to training data
   - 2.3 Predict the target for the testing data
   - 2.4 Compute the test error
3. Repeat the previous step 3 times, using different splits. How do the results change?
4. Average the test error of the four splits.
5. Include `dis` as predictor. Does it reduce the test error?
6. Calculate the test error estimate using LOOCV. Compare your result to that of step 4.
7. Calculate the test error estimate using 4-fold cross-validation. Compare the estimate to that of step 4

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Shrinkage Methods

Goals

- Avoid overfitting
- Reduce variance
- ”Shrink” regression coefficients towards zero
- Penalize coefficients that are ”too high”
- Type of ”regularization”

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Ridge Regression

a.k.a Tikhonov Regularization

$$\text{Minimize} \quad RSS + \lambda \sum_{j=1}^{p} \beta_j^2 = RSS + \lambda ||\beta||_2^2$$

- L2 regularizer (it penalizes the L2 norm of β)
- Parameter λ controls the amount of shrinkage
- Larger λ reduce variance but increase bias
- Not scale invariant: Standardize predictors

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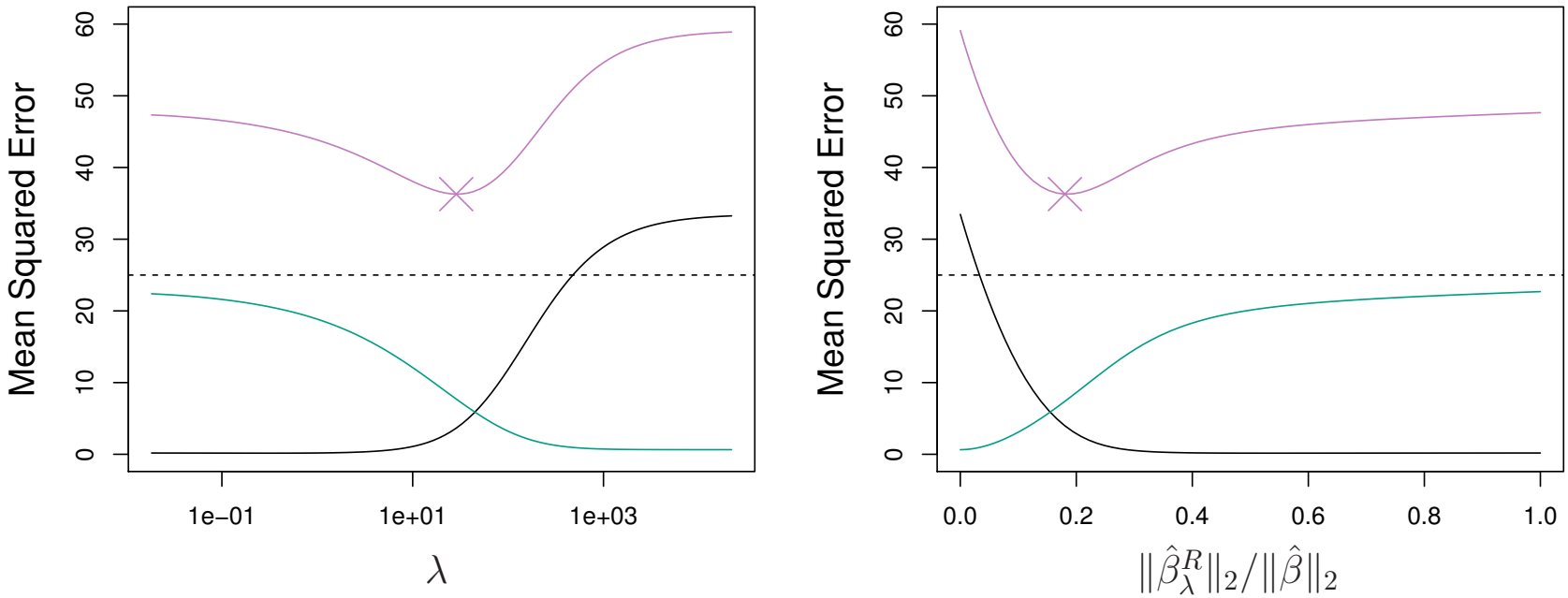
Ridge Regression

a.k.a Tikhonov Regularization



Source: ISLR2 Figure 6.5

- Bias
- Variance
- MSE

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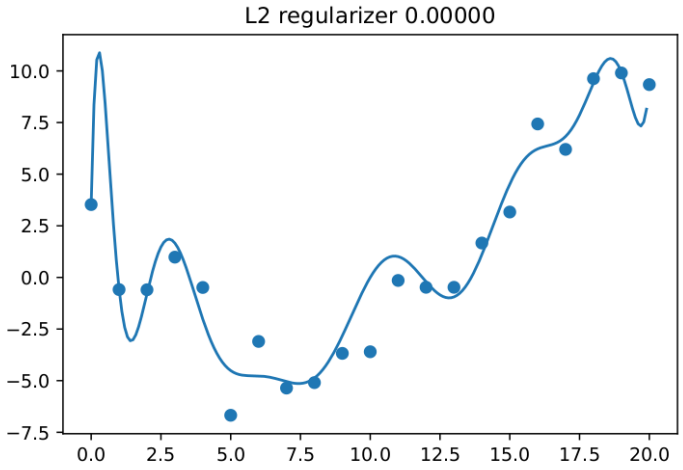
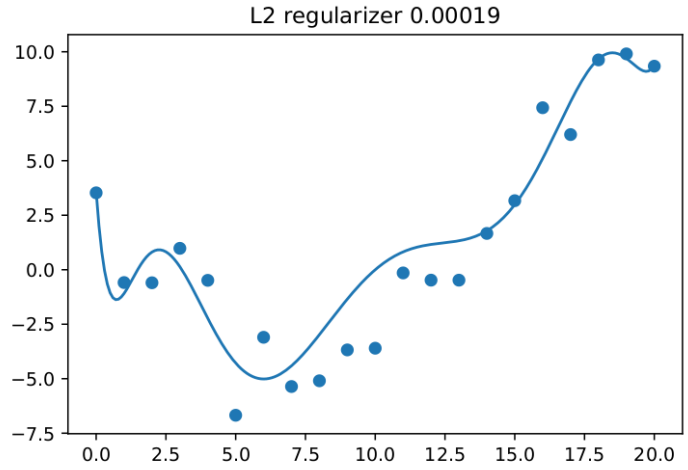
Ridge Regression Example

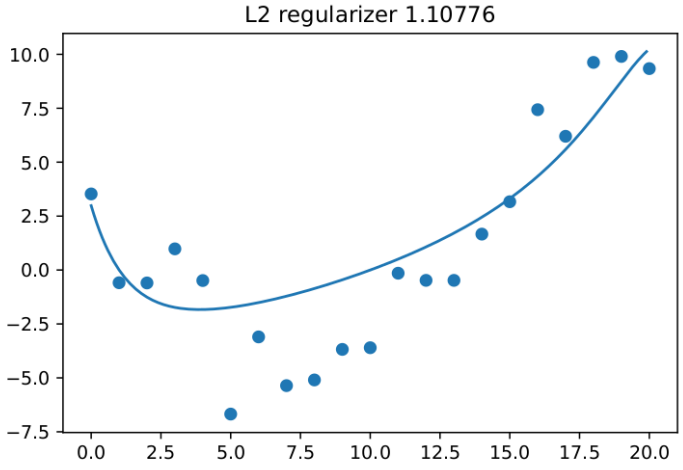
Fitting a Degree 14 Polynomial



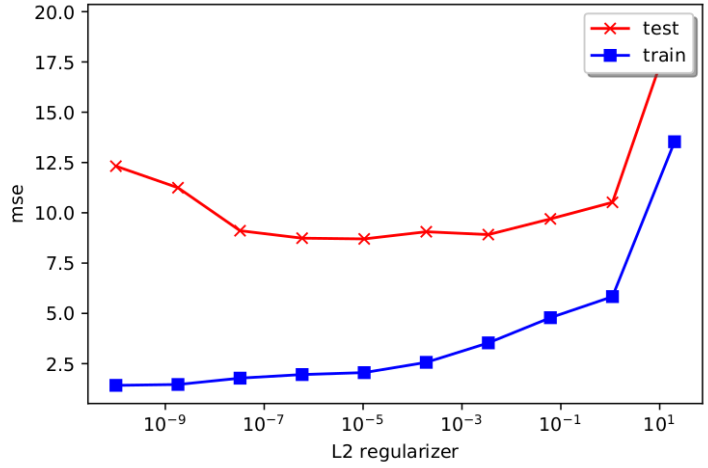
(a)



(b)



(c)



(d)

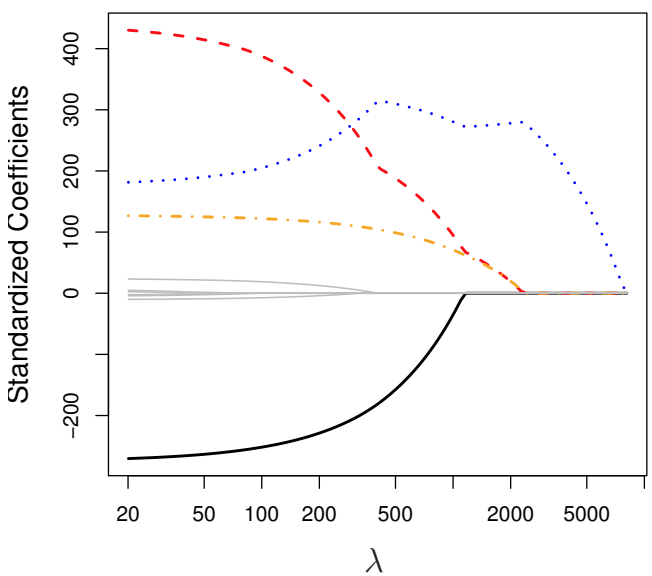
Source: Murphy Figure 4.5

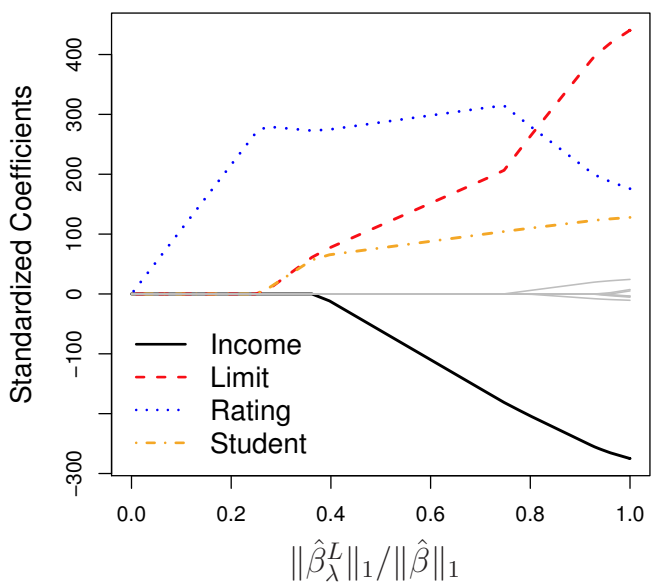
Lasso regression

"Least Absolute Shrinkage and Selection Operator"

$$\text{Minimize} \quad RSS + \lambda \sum_{j=1}^{p} |\beta_j| = RSS + \lambda ||\beta||_1$$

- L1 regularizer (it penalizes the L1 norm of β)
- Lasso may exclude variables by forcing their β_j to 0
- Parsimonious, more interpretable models than ridge regression





Source: ISLR2
Figure 6.6

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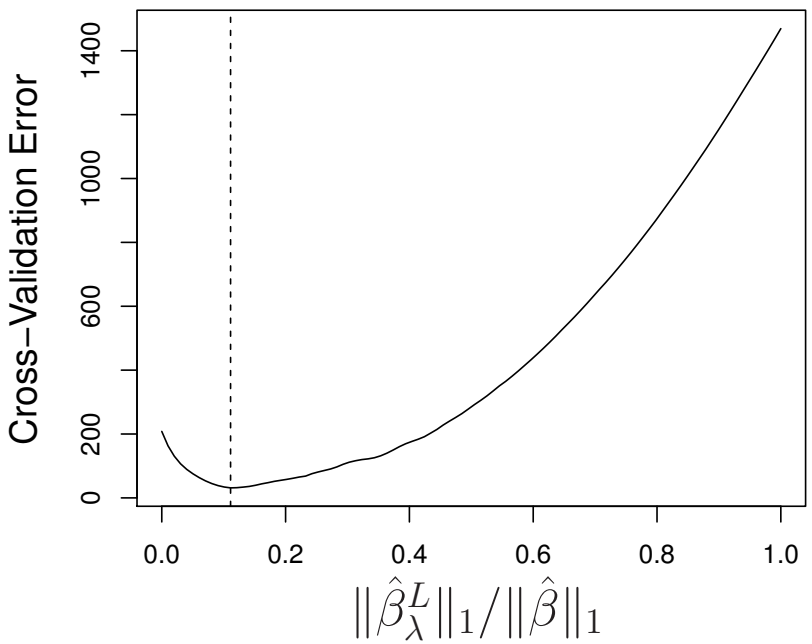
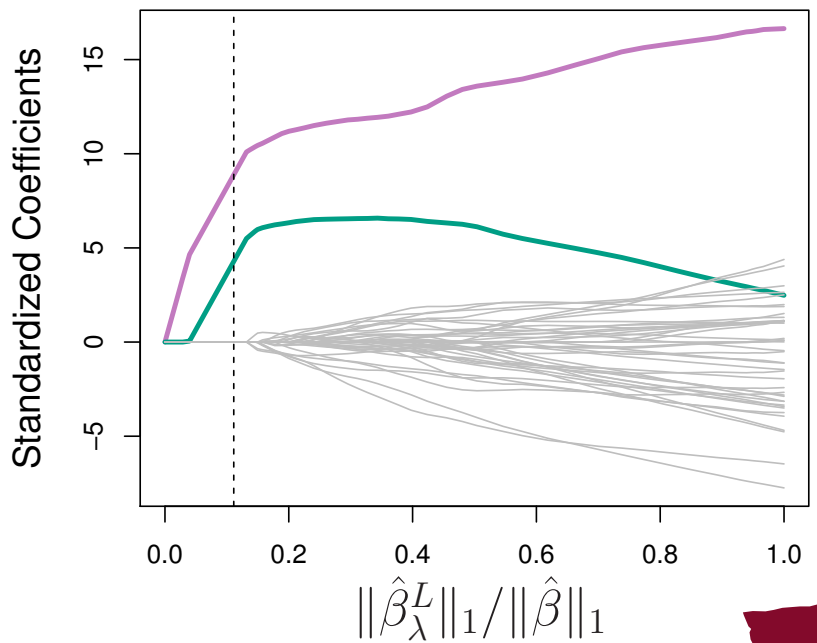
Selecting the Tuning Parameter

Grid Search

- Define a ”grid” of tuning parameters (e.g. λ) to search
- Cross-validate models for each point in the grid (each value of λ)
- Fit the final model to the optimal cross-validated error





Source: ISLR2 Figure 6.13

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Elastic Net

The Elastic Net penalty is a mix of L1-norm $||\beta||_1$ and L2-norm $||\beta||_2^2$ penalties, defined by α:

$$\lambda \left(\alpha ||\beta||_1 + (1 - \alpha) ||\beta||_2^2 \right)$$

- $\alpha = 0$: Ridge regression
- $\alpha = 1$: Lasso

The `glmnet()` function in the `glmnet` library uses the Elastic Net regularization method.

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Ridge Regression in R

Use the `Hitters` data set to model `Salary` as outcome and other variables as predictors.

```
library(ISLR2)
library(glmnet)

# Remove missing values
Hitters <- na.omit(ISLR2::Hitters)
```

The `glmnet()` function requires separate *x* and *y* values, instead of a formula. To create dummy variables for categorical variables, use the `model.matrix` function:

```
# Create dummy variables for categorical variables
# Remove intercept from model
x <- model.matrix(Salary ~ ., Hitters)[, -1]
y <- Hitters$Salary
```

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Ridge Regression in R [cont'd]

Set up a sequence of λ to try and fit the model for each λ:

```
# Set up the sequence of lambda values to try
grid <- 10^seq(from=10, to=-2, length=100)
print(grid)
ridge.model <- glmnet(x, y, alpha=0, lambda=grid)
```

Examine some results:

```
# Select the 50th lambda value
ridge.model$lambda[50]
coef(ridge.model)[, 50]
L2.norm = sqrt(sum(coef(ridge.model)[-1, 50]^2))

# Select the 60th lambda value
ridge.model$lambda[60]
coef(ridge.model)[, 60]
L2.norm = sqrt(sum(coef(ridge.model)[-1, 60]^2))
```

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Ridge Regression in R [cont'd]

Identify the optimal λ using cross-validation. First, create holdout test data set:

```
# Randomly split the Hitters data
train.idx <- sample(nrow(Hitters), nrow(Hitters)/2)
x.train <- x[train.idx,]
x.test <- x[-train.idx,]
y.train <- y[train.idx]
y.test <- y[-train.idx]
```

Use the training set for cross-validation:

```
# 5-fold cross-valiation, use MSE as metric
cv.out <- cv.glmnet(x.train, y.train, alpha=0,
   nfolds=5, type.measure='mse')
```

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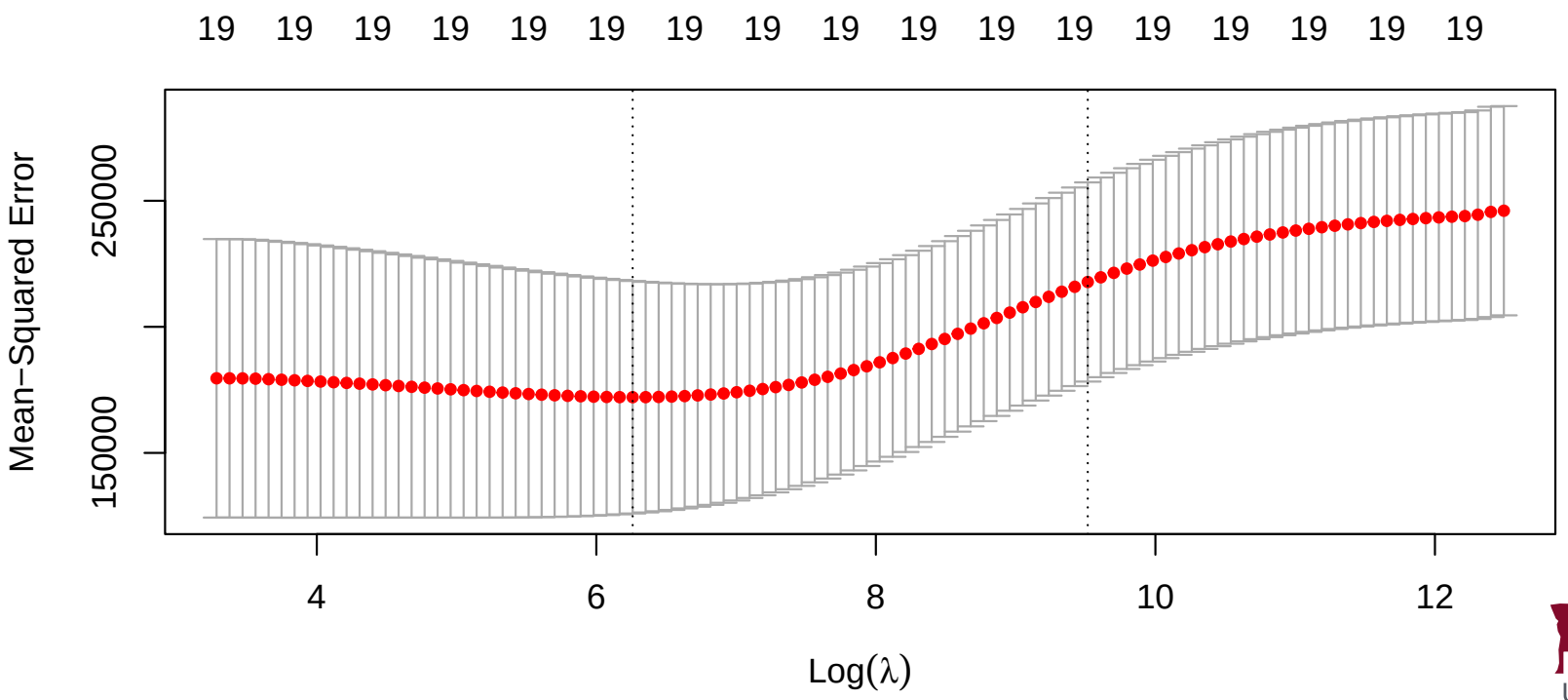
Ridge Regression in R [cont'd]

Show the optimal lambda, the MSE measure, the SE of MSE and the number of non-zero coefficients. Also shown the largest lambda within one SE of the optimal lambda.

```
print(cv.out)
plot(cv.out)
lambda.opt <- cv.out$lambda.min
```



Ridge Regression in R – Prediction

Fit test data:

```
ridge.test <- glmnet(x.test, y.test, alpha=0)
```

Compare regression coefficients between ridge using optimal λ and unpenalized least squares:

```
# Show the coefficients at optimal lambda
predict(ridge.test, type='coefficients', s=lambda.opt)
# Compare to unpenalized least-squares fit
coef(lm.fit(x.test, y.test))
```

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Ridge Regression in R – Prediction

Predict values for the test data set:

```
predictions <- predict(ridge.test, type='response',
                       s=lambda.opt, newx=x.test)
```

Calculate test MSE to compare to the CV optimal MSE above:

```
mean((predictions - y.test)^2)
```

Recall, the CV cross-validated error on the training set is an estimate/approximation of the real test error.

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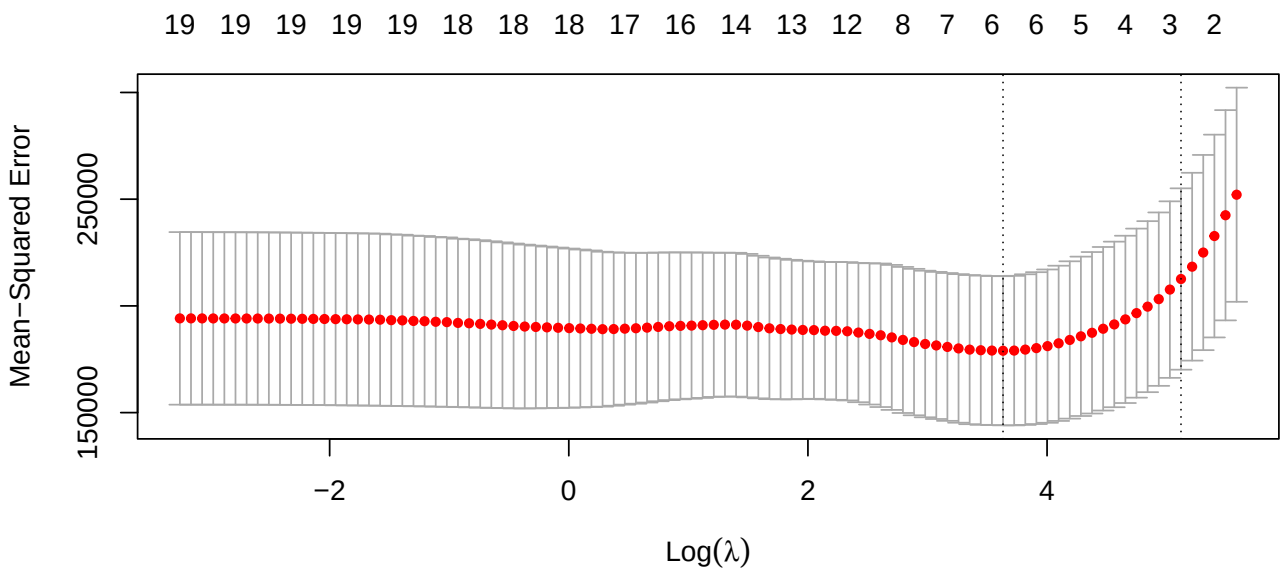
The Lasso in R

Identify the optimal λ using cross-validation:

```
# Set alpha to 1 for lasso
cv.out <- cv.glmnet(x.train, y.train, alpha=1,
   nfolds=5, type.measure='mse')
print(cv.out)
plot(cv.out)
lambda.opt <- cv.out$lambda.min
```

Note the number of non-zero coefficients in the result:



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The Lasso in R – Prediction

Fit test data:

```
lasso.test <- glmnet(x.test, y.test, alpha=1)
```

Compare regression coefficients between Lasso using optimal λ and unpenalized least squares:

```
# Show the coefficients at optimal lambda, note the
# many zero coefficients
predict(lasso.test, type='coefficients', s=lambda.opt)
# Compare to unpenalized least-squares fit
coef(lm.fit(x.test, y.test))
```

Predict values for the test data set and compute test MSE

```
predictions <- predict(lasso.test, type='response',
                       s=lambda.opt, newx=x.test)
mean((predictions - y.test)^2)
```

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Hands-On Exercises – Shrinkage Methods

Source: ISLR2, Chapter 6

Predict the number of applications received using the other variables in the `College` dataset

1. Split the data set into a training and a test set
2. Fit an unpenalized linear model on the training set. Report the test error.
3. Fit a ridge regression model on the training set, with λ chosen by cross-validation. Report the test error.
4. Fit a lasso model on the training set, with λ chosen by cross-validation. Report the test error.
5. Compare and conrast the results

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Hands-On Exercises – Shrinkage Methods

Source: ISLR2, Chapter 6

Predict the per-capita crime rate in the `Boston` data set using the other variables.

1. Split the data set into a training and a test set
2. Fit an unpenalized linear model on the training set. Report the test error.
3. Fit a ridge regression model on the training set, with λ chosen by cross-validation. Report the test error.
4. Fit a lasso model on the training set, with λ chosen by cross-validation. Report the test error.
5. Compare and conrast the results

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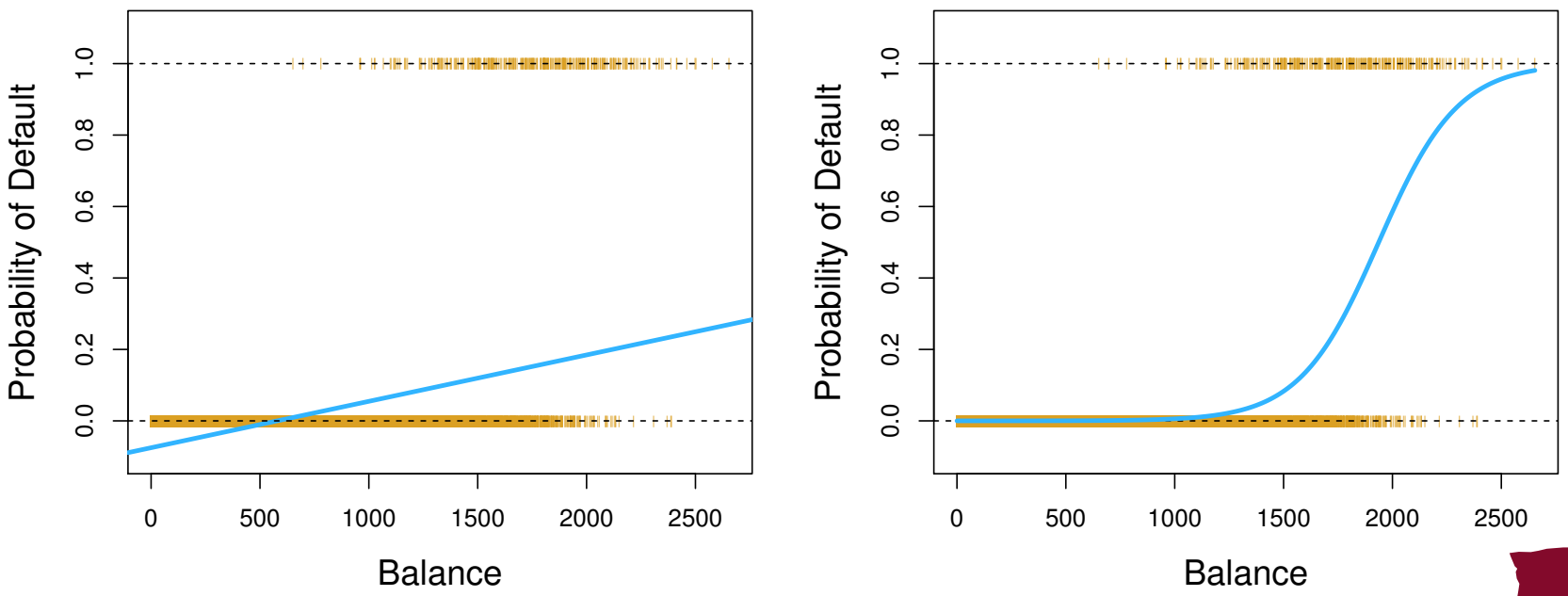
Classification

- Qualitative (categorical) outcome
- Estimate/predict probabilities of class membership
- **Problem**: Linear combinations of predictors are not limited to $[0, 1]$
- **Solution**: ”Link” function that transforms the weighted sum of predictors



Source: ISLR2 Figure 4.2

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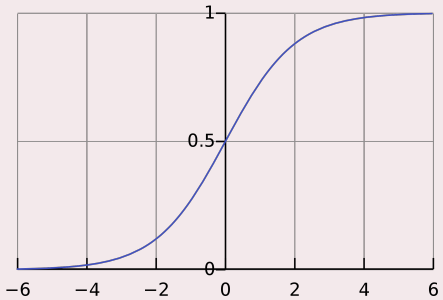
Logistic Regression

Logistic / Sigmoid Function

$$\sigma(x) = \frac{1}{1+e^{-x}} = \frac{e^x}{1+e^x}$$
$$= 1 - \sigma(-x)$$



Binary Case (Binomial Logistic Regression)

$$p(X) = \sigma(\beta_0 + \beta_1 X) = \frac{e^{\beta_0+\beta_1 X}}{1+e^{\beta_0+\beta_1 X}}$$

$$\Rightarrow \quad \frac{p(X)}{1-p(X)} = e^{\beta_0+\beta_1 X} \qquad \textbf{"Odds"}$$

$$\Rightarrow \quad \log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X \qquad \textbf{"Log-Odds", "Logits"}$$

Logistic Regression [cont'd]

Predictions

Given estimates $\hat{\beta}_0$ and $\hat{\beta}_1$, use the link function to predict probabilities:

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 X}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 X}}$$

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Logistic Regression [cont'd]

- Multiple p predictors: **Multiple Linear Regression**
- Multiple K classes: **Multinomial Logistic Regression**
- Multiple n labels: **Multi-label Classification**

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Multinomial Logistic Regression

$$\log\left(\frac{\Pr(Y=k|X=x)}{\Pr(Y=K|X=x)}\right) = \beta_{k0} + \beta_{k1}x_1 + \cdots + \beta_{kp}x_p \ , k < K$$

Exponentiating and rearranging:

$$\Pr(Y=k|X=x) = \Pr(Y=K|X=x)e^{\beta_{k0}+\beta_{k1}x_1+\cdots+\beta_{kp}x_p} \ , k < K$$

Because probabilities must sum to 1:

$$\begin{aligned}\Pr(Y=K|X=x) &= 1 - \sum_{l=1}^{K-1} \Pr(Y=l|X=x) \\ &= 1 - \sum_{l=1}^{K-1} \Pr(Y=K|X=x)e^{\beta_{k0}+\beta_{k1}x_1+\cdots+\beta_{kp}x_p}\end{aligned}$$

$$\Rightarrow \Pr(Y=K|X=x) = \frac{1}{1+\sum_{l=1}^{K-1} e^{\beta_{k0}+\beta_{k1}x_1+\cdots+\beta_{kp}x_p}}$$

$$\Rightarrow \Pr(Y=k|X=x) = \frac{e^{\beta_{k0}+\beta_{k1}x_1+\cdots+\beta_{kp}x_p}}{1+\sum_{l=1}^{K-1} e^{\beta_{l0}+\beta_{l1}x_1+\cdots+\beta_{lp}x_p}} \ , \ k < K$$

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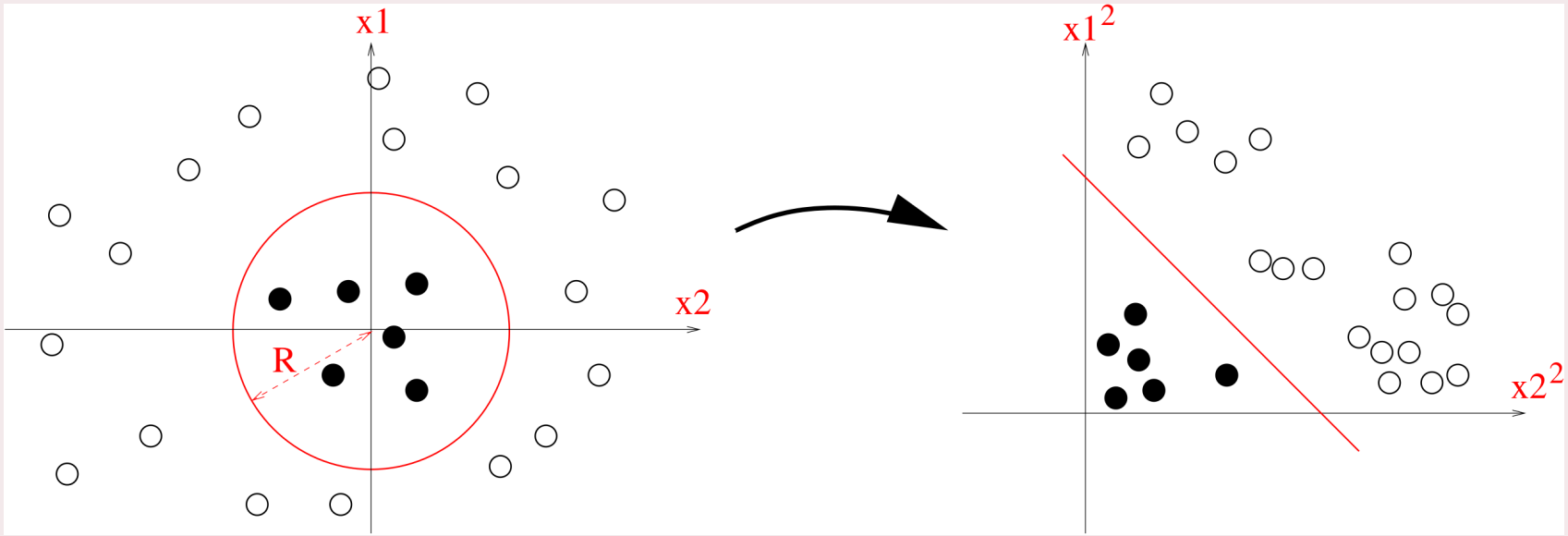
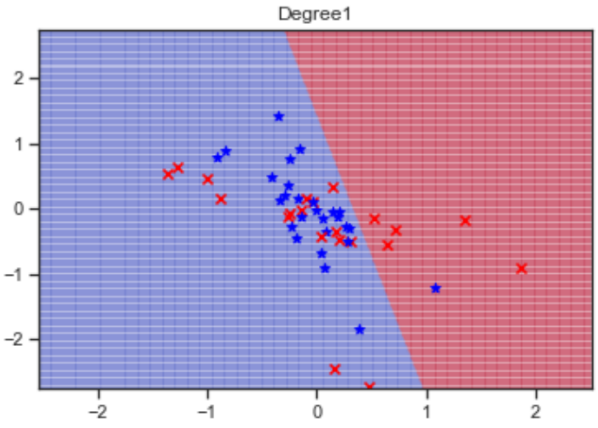
Logistic Regression with Polynomial Expansion

Transforming Decision Boundaries

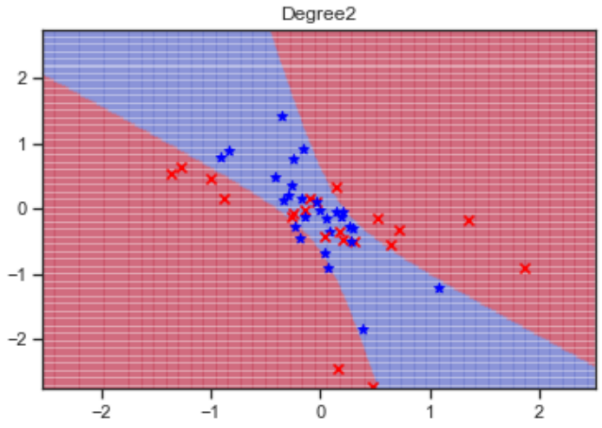


Source: Murphy Figure 10.3

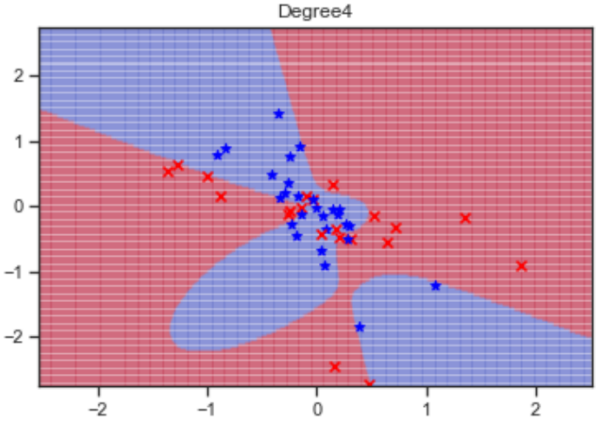
Logistic Regression with Polynomial Expansion [cont'd]



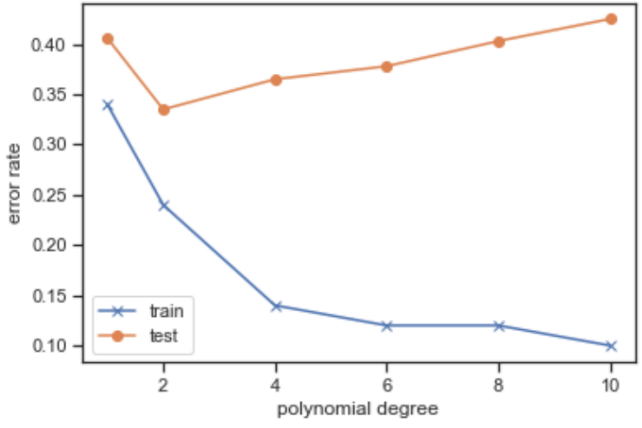
(a)



(b)



(c)



(d)

Source: Murphy Figure 10.4

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Logistic Regression in R

Use the stock market data set `Smarket` to predict the binary outcome `Direction` (the direction of market changes, up or down) using prior returns as predictors:

```
library(ISLR2)
?Smarket
```

Contrasts show how factor levels are encoded using dummy variables:

```
contrasts(Smarket$Direction)
```

Note the `family` argument for the `glm` function:

```
logreg.fitted <-
   glm(Direction~Lag1+Lag2+Lag3+Lag4+Lag5+Volume,
                 data=Smarket,
                 family=binomial(link='logit'))
summary(logreg.fitted)
```

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Logistic Regression in R – Prediction

Predict logits for training set:

```
logreg.logits <-
   predict(logreg.fitted, newdata = Smarket)
```

Predict probabilities for training set:

```
# Predict probabilities for training test
logreg.probabilities <-
   predict(logreg.fitted, newdata = Smarket,
           type='response')
```

Predict categorical outcomes:

```
# Predict 'up' or 'down' based on probabilities
# and a fixed threshold
pred.direction <- rep('Down', nrow(Smarket))
pred.direction[logreg.probabilities > .5] <- 'Up'
```

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Logistic Regression in R – Prediction

```r
# Compute confusion matrix
logreg.cm <- table(pred.direction, Smarket$Direction)
print(logreg.cm)

# Compute accuracy
mean(pred.direction == Smarket$Direction)
```

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Logistic Regression in R – Holdout Set

Split data to train and test set. Because this is time-dependent data, split by time to avoid mixing past and future data:

```
train.data <- Smarket[Smarket$Year < 2005,]
test.data <- Smarket[!(Smarket$Year < 2005),]
```

Fit using training set:

```
logreg.fitted <-
   glm(Direction~Lag1+Lag2+Lag3+Lag4+Lag5+Volume,
   data=train.data, family=binomial(link='logit'))
```

Predict probabilities for test data and classify:

```
logreg.probabilities <- predict(logreg.fitted,
    newdata = test.data, type='response')
pred.direction <- rep('Down', nrow(test.data))
pred.direction[logreg.probabilities > .5] <- 'Up'
```

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Logistic Regression in R – Holdout Set

Compute confusion matrix and accuracy for test data:

```
logreg.cm <- table(pred.direction, test.data$Direction)
print(logreg.cm)
mean(pred.direction == test.data$Direction)
```

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Logistic Regression in R – Evaluation

Using the ROCR library for classifier evaluation:

```
library(ROCR)

# A prediction object collects predicted
# probabilities and true labels
pred.obj <- prediction(logreg.probabilities,
                       test.data$Direction)

# Get some classifier performance metrics
# ROCR varies the threshold.
plot(performance(pred.obj, 'acc'))
plot(performance(pred.obj, 'prec'))
plot(performance(pred.obj, 'rec'))
plot(performance(pred.obj, 'f'))
performance(pred.obj, 'auc')@y.values[[1]]
```

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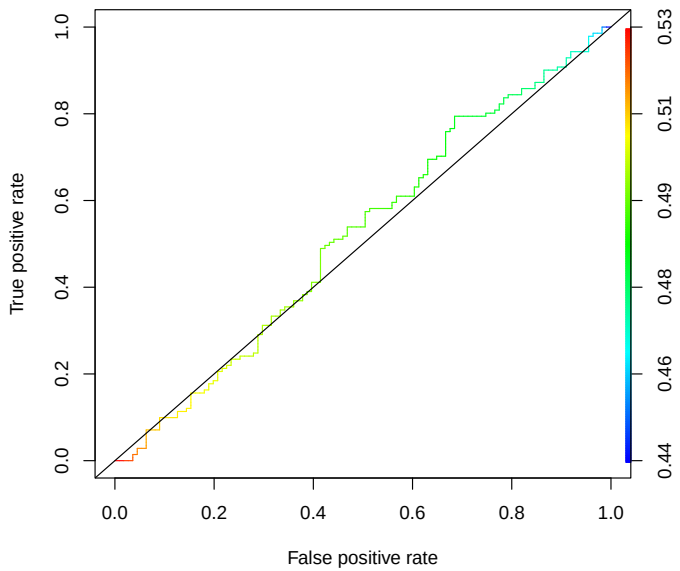
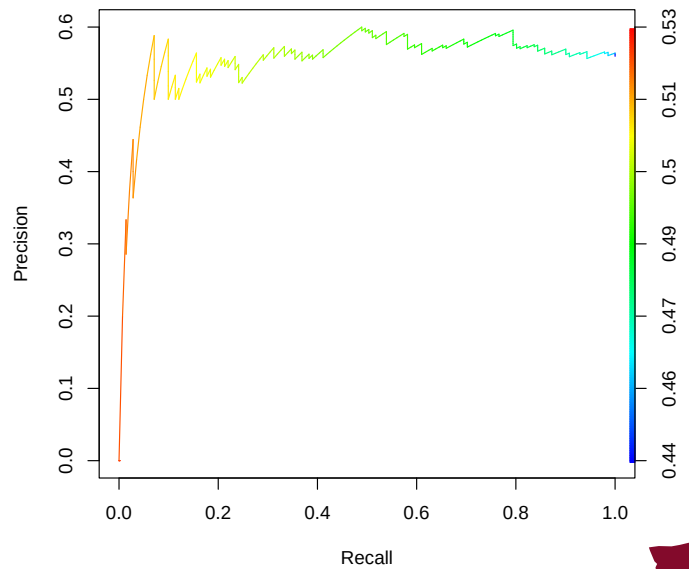
Logistic Regression in R – Evaluation

continued . . .

```
# ROC - True positive rate versus false positive rate
plot(performance(pred.obj, 'tpr', 'fpr'), colorize=T)
abline(0, 1)
# Precision/Recall plot
plot(performance(pred.obj, 'prec', 'rec'), colorize=T)
```





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Naive Bayes Classifier

- **Bayes Theorem**:

$$\begin{aligned}\Pr(Y = c\,|X) &= \frac{p(X|Y = c)\,p(Y = c)}{p(X)} \\ &= \frac{p(X|Y = c)\,p(Y = c)}{\sum_{l=1}^{K} p(X|Y = l)\,p(Y = l)}\end{aligned}$$

- **Naive Bayes Assumption**: Within each class c, the D predictors are independent:

$$\begin{aligned}p(X|Y = c) &= p(x_1|Y = c) \times p(x_2|Y = c) \times \cdots \\ &\quad \times p(x_D|Y = c) \\ &= \prod_{d=1}^{D} p(x_d|Y = c)\end{aligned}$$

- **Posterior probability**:

$$p(Y = c|X) = \frac{\left(\prod_{d=1}^{D} p(x_d|Y = c)\right)\, p(Y = c)}{\left(\sum_{l=1}^{K} \prod_{d=1}^{D} p(x_d|Y = l)\right)\, p(Y = l)}$$

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Naive Bayes Classifier in R

Naive Bayes using the `naiveBayes` function in the `e1071` library:

```
library(e1071)

# Fit using same syntax as glm
nb.fitted <-
    naiveBayes(Direction~Lag1+Lag2, data=train.data)
# Output contains prior and conditional
# probabilities (and their SD)
nb.fitted
```

Predict class membership and compute confusion matrix:

```
nb.predictions <- predict(nb.fitted, test.data)
nb.cm <- table(nb.predictions, test.data$Direction)
print(nb.cm)
```

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Naive Bayes Classifier in R – Evaluation

Evaluate the classifier:

```
# Predict probabilities (for use with ROCR)
nb.probabilities <-
     predict(nb.fitted, test.data, type='raw')
# Create an ROCR prediction object
nb.pred.obj <- prediction(nb.probabilities[,'Up'],
                          test.data$Direction)
```

Assess ROC and AUC:

```
# Generate an ROC plot
plot(performance(nb.pred.obj, 'tpr', 'fpr'),
          colorize=T)
abline(0, 1)

# Compute the AUC
performance(nb.pred.obj, 'auc')@y.values[[1]]
```

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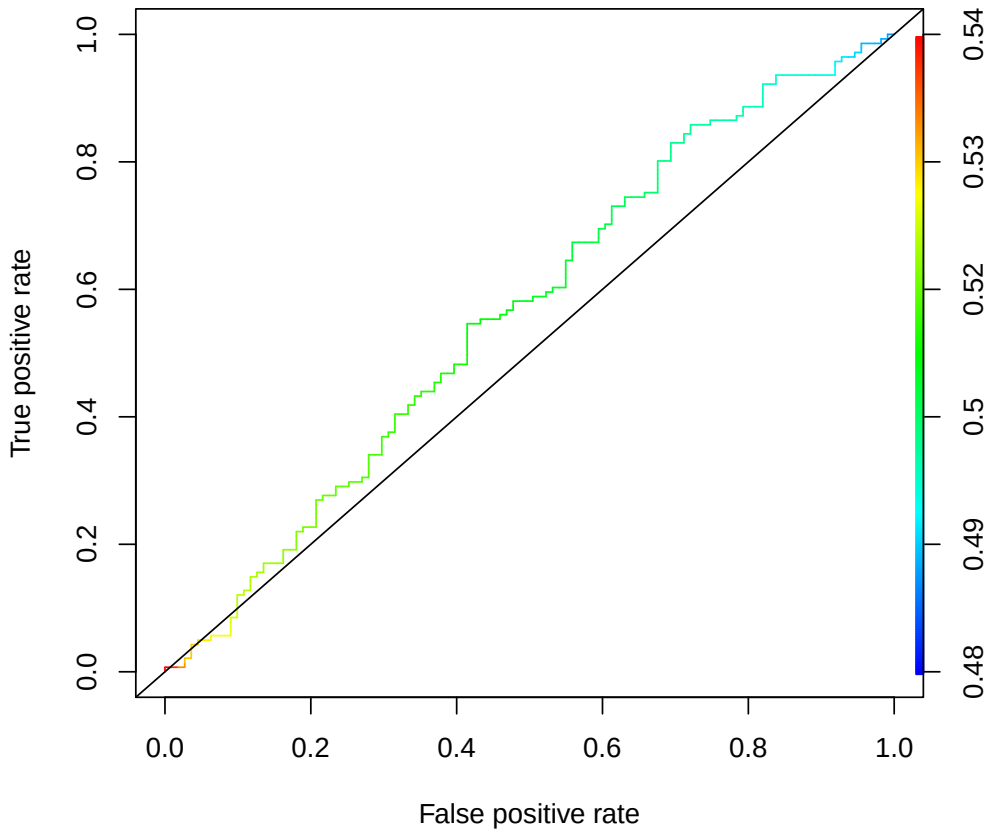
Naive Bayes Classifier in R – Evaluation



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KNN Classification in R

Using the `knn` function from the `class` library:

```
library(class)
```

Use only two predictors:

```
train.x <- cbind(train.data$Lag1, train.data$Lag2)
test.x <- cbind(test.data$Lag1, test.data$Lag2)
train.y <- train.data$Direction
test.y <- test.data$Direction
```

Make predictions from training set for test set, given true classes of training set ($k = 3$ and return probabilities):

```
knn.pred <- knn(train.x, test.x, train.y, k=3, prob=T)
```

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KNN Classification in R

Evaluate the classifier against test data:

```
# Confusion matrix
table(knn.pred, test.y)
# Accuracy
mean(knn.pred == test.y)
```

Save class probabilities of the majority class:

```
knn.probs <- attributes(knn.pred)$prob
```

Compute class probabilities of the minority class:

```
knn.class.probs <- knn.probs
knn.class.probs[knn.pred=='Down'] <-
                    1-knn.probs[knn.pred=='Down']
```

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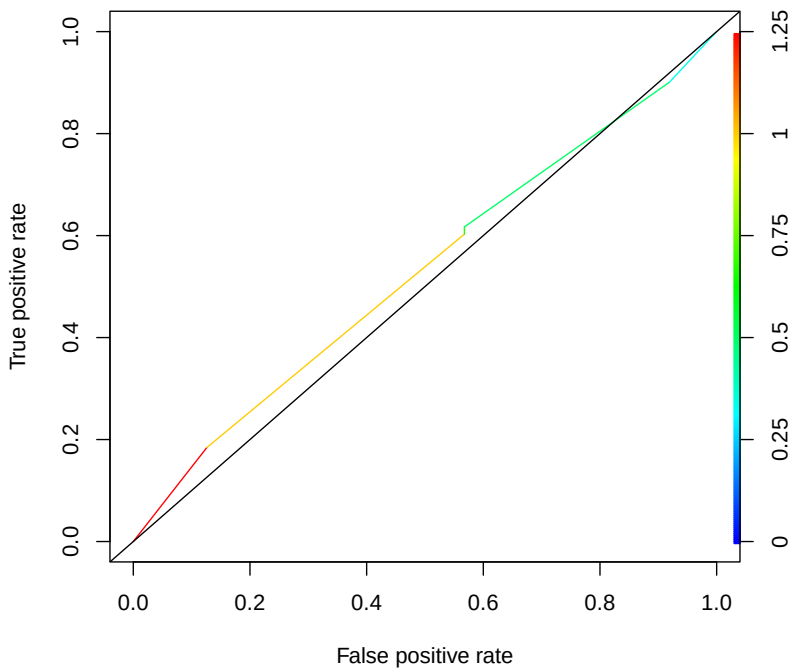
KNN Classification in R [cont'd]

Use ROCR functions to evaluate classifier:

```
knn.pred.obj <-
      prediction(knn.class.probs, test.data$Direction)
plot(performance(knn.pred.obj, 'tpr', 'fpr'),
                 colorize=T)
abline(0, 1)
performance(knn.pred.obj, 'auc')@y.values[[1]]
```



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Hands-On Exercises

Source: ISLR2, Chapter 4

Use the `Weekly` data set in the `ISLR2` package.

1. Use the full data set to perform a logisttic regression with `Direction` as target. Which predictors are statistically significant?
2. Compute the confusion matrix and accuracy.
3. Use the 1990 to 2008 data for a training set and the 2009/2010 for a test set. Fit a logistic regression model with `Lag2` as the only predictor.
4. Repeat (3) using Naive Bayes
5. Repeat (3) using KNN with $K = 1$
6. Which model provides the best results on this data?

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Hands-On Exercises

Source: ISLR2, Chapter 4

Use the `Auto` data set in the `ISLR2` package.

1. Create a binary variable, `mpg01` that contains a 1 if `mpg` is above its median, 0 otherwise. *Tip*: Use the `median()` function. Add the new variable to the data frame.
2. Split the data set into training and test set
3. Perform a logistic regression on the training data to predict `mpg01` from the other features. What is the test error of this model?
4. Repeat (3) using Naive Bayes
5. Repeat (3) using KNN with different values of K. What value of K performs best?

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Hands-On Exercises

Source: ISLR2, Chapter 4

Using the `Boston` data set in the `ISLR2` library, fit classification models to predict whether a given census tract has a crime rate above or below the median.

1. Create a new binary variable `crime01` that is 1 is `crime` is above its median, and 0 otherwise. Combine this variable with the data frame. *Tip*: Use the `median()` function for this.
2. Split your data set into a training and test data set
3. Fit logistic regression, Naive Bayes, and KNN (with different K)
4. Describe your findings in terms of prediction error, precision, recall, F1 and AUC

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