# Regression (Chapter 11)

**Setup:** Have data on two quantitative variables — X and Y — on a sample of n subjects.

**Q:** Is there any association between X and Y? What kind?

### **Scatterplot:**

- Plot y against x
- Look for the **trend** in the plot a smooth curve that shows how the average value of Y changes with x
- Trend may be linear or non-linear
- If there is a trend, then the two variables are associated. In this case, x may be used to predict y
- Trend may be strong or weak. It is strong if the points are tightly clustered around the trend (small scatter)
- No trend: No association i.e., the variables are independent, and x is not helpful for predicting y.

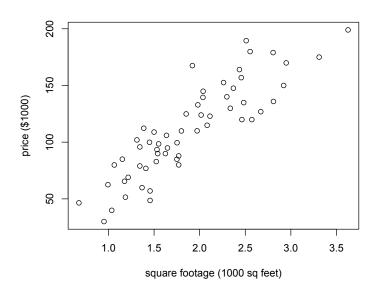
### Example: House price data

```
house <- read.table(file="house_price.txt", sep=",",
header=T)
> head(house)
   size price
1 0.951 30.00
2 1.036 39.90
3 0.676 46.50
4 1,456 48,60
5 1.186 51.50
6 1.456 56.99
>
> str(house)
'data.frame': 58 obs. of 2 variables:
 $ size : num 0.951 1.036 0.676 1.456 1.186 ...
```

```
$ price: num 30 39.9 46.5 48.6 51.5 ...
>

# Make a scatterplot

plot(house$size, house$price,
    xlab="square footage (1000 sq feet)",
ylab="price ($1000)")
```



# Overall pattern in a scatterplot

 $\mathbf{T}$ 

Form:	
Direction:	
Strength - assess the scatter of the points:	

## Correlation Coefficient

**Population correlation:** A measure of **linear** relationship between X and Y. It is defined as,

$$\rho = \frac{\operatorname{cov}(X, Y)}{\operatorname{sd}(X)\operatorname{sd}(Y)},$$

where  $cov(X, Y) = E\{(X - E(X))(Y - E(Y))\}\$  is covariance between X and Y.

**Sample correlation**: Estimator of  $\rho$ . It is defined as

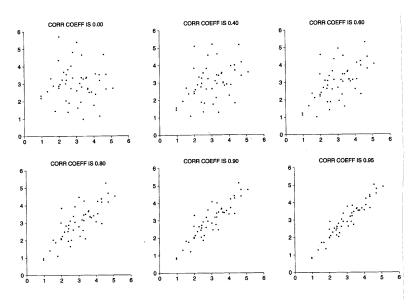
$$r = \frac{S_{xy}}{S_x S_y},$$

where

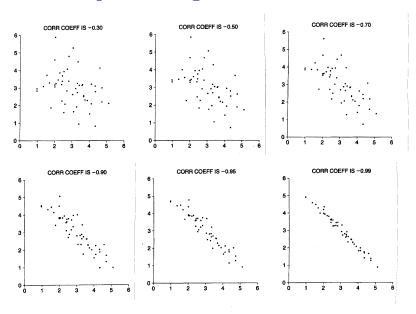
## Properties of $\rho$ and r:

- Range between -1 to 1
- Sign tells us
- Absolute value tells us
- Perfect correlation:
- Unit free
- No change if X and Y are interchanged or if X is replaced by aX + b and/or Y is replaced by cY + d, where a and c have the same sign. The sign will reverse if a and c have different signs.
- Zero correlation: **No linear** relationship. But there may be non-linear relationship.
- Independent X and Y: zero correlation, but the converse may not be true

# **Examples of Positive Correlation**



# **Examples of Negative Correlation**



# Caution: Non-linear relationships

Ex: Scatter plot of speed and mileage (miles per gallon) of an automobile.

### More non-linear patterns:

You can always compute r — but it doesn't makes sense for curve patters.

**Lesson**: Correlation only measures the strength of **linear** association — i.e., how close the points are to a straight line.

## Caution: Outliers

The position of an outlier relative to the rest of the ("cloud") of points determines how it affects r. Outliers may decrease or increase the value of r.

**Note**: Just knowing the value of r will give no information about whether outliers are present. That's why it is important to look at scatterplots.

# Simple Linear Regression

**Setup:** Have data  $(X_i, Y_i)$ , i = 1, ..., n, on two quantitative variables X & Y. Their scatterplot shows a linear relationship. Need an equation that would allow us to predict Y from X.

**Response variable** (Y): variable to be predicted (or modeled), aka, *dependent variable*.

**Predictor** (X): variable used to predict Y, aka, independent or explanatory variable or covariate.

**Regression model**: A function that models mean response — E(Y|X=x) — as a function of x

Simple linear regression:  $E(Y|X=x) = \beta_0 + \beta_1 x$ 

- Assumes mean response changes linearly with x
- $\beta_0$ : intercept E(Y|X=0)
- $\beta_1$ : slope rate of change of mean response. It represents the change in mean when x increases by 1 unit.

- The regression coefficients are estimated from data.
- Let  $(\hat{\beta}_0, \hat{\beta}_1)$  = estimator of  $(\beta_0, \beta_1)$ .

**Observed response:**  $Y_i$  when  $X = x_i$ , i = 1, ..., n.

Fitted response:  $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 x$ 

- Estimated mean response when X = x
- Response predicted by the regression line
- $(\hat{Y}, x)$  falls on the regression line
- Fitted values:  $\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ , i = 1, ..., n.

Residuals:  $e_i = Y_i - \hat{Y}_i$ , i = 1, ..., n.

- $\bullet$  Vertical distance between observed and predicted Y's
- Error in prediction
- Large residuals: observed and fitted Ys are too far

Least squares method for estimating coefficients: Find  $(\hat{\beta}_0, \hat{\beta}_1)$  that minimize the sum of squares of residuals

$$\sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2.$$

- Results in the **line of best fit** the line is such that the fitted Ys are "closest" to the observed Ys
- Fitted regression line:  $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 x$
- Other criteria possible, e.g., minimizing  $\sum_{i=1}^{n} |e_i|$ , but the resulting estimates don't have simple expressions

To minimize  $\sum_{i=1}^{n} e_i^2$  wrt  $(\beta_0, \beta_1)$ , solve the **normal equations** 

$$\frac{\partial \sum_{i=1}^{n} e_i^2}{\partial \beta_0} = 0, \quad \frac{\partial \sum_{i=1}^{n} e_i^2}{\partial \beta_1} = 0,$$

resulting in the least squares estimates

$$\hat{\beta}_0 = \overline{Y} - \hat{\beta}_1 \overline{x}, \quad \hat{\beta}_1 = rS_y/S_x,$$

where r is sample correlation, and  $S_x$  and  $S_y$  are standard deviations of x and y samples, respectively.

#### Recall that:

$$S_x^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \overline{x})^2, \quad S_y^2 = \frac{1}{n-1} \sum_{i=1}^n (y_i - \overline{y})^2,$$
$$r = \frac{\frac{1}{n-1} \sum_{i=1}^n (x_i - \overline{x})(y_i - \overline{y})}{S_x S_y}$$

## The fitted regression line

Fitted regression line:  $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 x$ . Plugging-in  $\hat{\beta}_0$  and  $\hat{\beta}_1$ ,

$$\hat{Y} =$$
 $=$ 

implying that

$$\frac{\hat{Y} - \overline{Y}}{S_y} = r \frac{(x - \overline{x})}{S_x}.$$

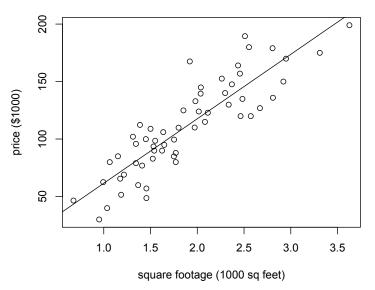
- If x is 1 SD away from its mean  $\overline{x}$ ,  $\hat{Y}$  is r SD away from its mean  $\overline{Y}$ . Since  $|r| \leq 1$ , this means  $\hat{Y}$  is closer to  $\overline{Y}$  (in units of SD) than x is to  $\overline{x}$  regression toward mean.
- The fitted line passes through the points  $(\overline{x}, \overline{y})$ .
- The sign of slope  $\hat{\beta}_1$  is same as the sign of r.
- The sum of residuals,  $\sum_{i=1}^{n} e_i =$
- The average of fitted values,  $(1/n)\sum_{i=1}^{n} \hat{Y}_{i} =$

Ex: Let's get the fitted line for the house price data and add it to the scatterplot.

```
x <- house$size
y <- house$price
# Get the fitted regression line
> (house.reg <- lm (y ~ x))
Call:
lm(formula = y ~x)
Coefficients:
(Intercept)
                       X
      5.432
                56.083
>
# Does R do what we expect it to do?
> c(mean(x), sd(x), mean(y), sd(y), cor(x,y))
```

```
[1]
      1.8829655 0.6316624 111.0344483 40.4431900
0.8759374
>
> cor(x,y)*sd(y)/sd(x)
[1] 56.08328
> mean(y)-(cor(x,y)*sd(y)/sd(x))*mean(x)
[1] 5.431568
>
# Add the line to the plot
plot(x, y, xlab="square footage (1000 sq feet)",
ylab="price ($1000)")
abline(house.reg)
```

## Fitted regression for house price data



The estimated regression coefficients are:

$$\hat{\beta}_0 = 5.432, \ \hat{\beta}_1 = 56.083$$

**Q:** How do we interpret these coefficients? What is the predicted price of a house that is 3200 square feet?

**Issue:** How well does the fitted regression line describe the data?

## **Approach 1:** Consider $r^2$ .

• High  $r^2$  (and hence |r|)  $\Longrightarrow$  points are tightly clustered around the line  $\Longrightarrow$  predicted Ys are close to observed Ys  $\Longrightarrow$  residuals are small  $\Longrightarrow$  fit is good

**Approach 2:** Consider the variability in Ys explained by regression. To understand this, let's think about why the house prices are different. This is because the houses may have

- different square-footage
- different locations
- different years of sale
- other known/unknown reasons

# Analysis of Variance (ANOVA)

- Total variability in Ys:  $SS_{TOT} = \sum_{i=1}^{n} (Y_i \overline{Y})^2 = (n-1)S_y^2$  total SS
- A part of SS<sub>TOT</sub> is explained by the fitted regression:  $SS_{REG} = \sum_{i=1}^{n} (\hat{Y}_i \overline{Y})^2$  SS due to regression
- The rest is error variability:  $SS_{ERR} = SS_{TOT} SS_{REG} = \sum_{i=1}^{n} e_i^2$  error SS
- ANOVA Identity:  $SS_{TOT} = SS_{REG} + SS_{ERR}$ .

This suggests proportion of total variation explained,

$$R^2 = \frac{\text{SS}_{\text{REG}}}{\text{SS}_{\text{TOT}}}$$

as a measure of **goodness of fit** of the fitted regression.

- Also called **coefficient of determination**
- Between 0 and 1, with high values suggesting a good fit.



## Simple linear regression $(E(Y|x) = \beta_0 + \beta_1 x)$

- $\bullet SS_{TOT} = (n-1)S_y^2$
- $SS_{REG} = r^2(n-1)S_y^2$
- $SS_{ERR} = (1 r^2)(n 1)S_y^2$
- $R^2 = r^2$  a reasonable measure from Approach 1 also.

**Ex:** For house price data:  $r^2 = 0.88^2 \approx 0.77$ 

# Alternative form for a regression model

**Regression model**: Models mean response — E(Y|X=x) — as a function of x

Alternative form:  $Y = E(Y|X = x) + \epsilon$ 

- E(Y|x) is modeled as before
- $\epsilon = Y E(Y|X = x) = \text{error}$  a catchall for everything that causes the observed response to differ from its mean e.g., random variability, effect of missing predictors, etc.
- $E(\epsilon) = 0$ ,  $var(\epsilon) = \sigma^2$

Model for data:  $Y_i = E(Y_i|X=x_i) + \epsilon_i, i = 1, ..., n$ 

Regression assumptions: The errors  $\epsilon_i$  have mean zero, variance  $\sigma^2$ , and are independent. No additional assumptions are needed to estimate regression coefficients by least squares.

Additional assumption: Errors follow a normal distribution — needed for testing hypotheses and constructing confidence intervals. This means

$$\epsilon_i \sim \text{i.i.d. } N(0, \sigma^2), \ i = 1, \dots, n$$

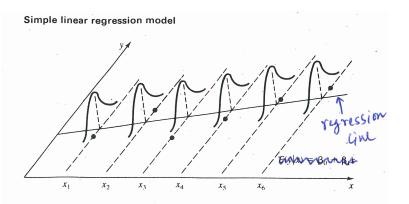
# Simple Linear Regression with Normality

Assumed model:  $Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$ ,  $\epsilon_i \sim \text{ i.i.d. } N(0, \sigma^2)$ , i = 1, ..., n.

**Note:** The values  $x_1, \ldots, x_n$  of predictor X are known and fixed (i.e., non-random), and are assumed to be measured without error.

### Properties:

- $E(Y_i|x_i) =$
- $\operatorname{var}(Y_i|x_i) =$
- $Y_i|x_i \sim \text{ independent } N(\beta_0 + \beta_1 x_i, \sigma^2)$



- The least squares estimators  $(\hat{\beta}_0, \hat{\beta}_1)$  of  $(\beta_0, \beta_1)$  are also maximum likelihood estimators.
- $\hat{\beta}_1 \sim N\left(\beta_1, \sigma^2/\{(n-1)S_x^2\}\right)$

•

- Define:  $\hat{\sigma}^2 = SS_{ERR}/(n-2)$ . Then,  $E(\hat{\sigma}^2) = \sigma^2$ .
- An unbiased estimator of  $\sigma^2$  is
- Note: The sample variance  $S_y^2$  is no longer unbiased for  $\sigma^2$ . This is because
- $SS_{\text{ERR}}/\sigma^2 = (n-2)\hat{\sigma}^2/\sigma^2$  follows a  $\chi^2$  distribution with (n-2) degrees of freedom.

**ANOVA table:** A standard summary of regression fit. Here we have "simple linear regression" — i.e., two regression coefficients,  $\beta_0$  and  $\beta_1$ .

Source	SS	d.f.	MS	F
Model	$SS_{ m REG}$	1	$MS_{\text{REG}} = \frac{SS_{\text{REG}}}{1}$	$\frac{MS_{\mathrm{REG}}}{MS_{\mathrm{ERR}}}$
Error	$SS_{ m ERR}$	n-2	$MS_{\text{ERR}} = \frac{SS_{\text{ERR}}}{n-2}$	Ditt
Total	$SS_{\mathrm{TOT}}$	n-1		

#### Recall that:

• 
$$SS_{TOT} = \sum_{i=1}^{n} (Y_i - \overline{Y})^2$$

• 
$$SS_{REG} = \sum_{i=1}^{n} (\hat{Y}_i - \overline{Y})^2$$

• 
$$SS_{ERR} = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2$$

# Inference about slope $\beta_1$

**Issue:** Is the predictor X "significant", i.e., does it really help in predicting the response Y?

**Approach 1:** Test  $H_0: \beta_1 = 0$  vs.  $H_1: \beta_1 \neq 0$ . This is equivalent to testing  $H_0: \rho = 0$  vs.  $H_1: \rho \neq 0$ . (Why?)

Test statistic:

#### Null distribution:

• A two-sided t-test.

 $100(1-\alpha)\%$  Confidence Interval for  $\beta_1$ :

Approach 2: Test for model significance. In simple linear regression, this is equivalent to testing  $H_0: \beta_1 = 0$  vs.  $H_1: \beta_1 \neq 0$ .

Test statistic:

$$F = \frac{MS_{\text{REG}}}{MS_{\text{ERR}}}$$

**Null distribution:** This F statistic follows an F distribution with numerator d.f. 1 and denominator d.f. n-2.

- An F-test.
- Equivalent to the t-test seen before because  $T^2 = F$  (verify).

### Model evaluation

**Issue:** Is the fitted model a good representation of the data?

**Approach:** Examine the residuals,  $e_i = Y_i - \hat{Y}_i$ , i = 1, ..., n, and verify the key assumptions, namely,

- Errors have mean zero and constant variance
- Errors are normally distributed
- Errors are independent often an issue when the data are collected over time.

### **Key Graphical Tools:**

- Residual plot: Plot of residuals  $e_i$  against fitted values  $\hat{Y}_i$ . In the ideal plot, the points are scattered around zero and there is no pattern. This verifies the first assumption.
- Normal QQ plot: This verifies the normality assumption.
- Time series plot: Plot  $e_i$  against i. In the ideal plot, there should be no dependence, which verifies the independence assumption. More sophisticated tools exist.

```
Ex: House price data, continued.
x <- house$size
y <- house$price
house.reg <- lm (y ~ x)
# ANOVA table
> (anova(house.reg))
Analysis of Variance Table
Response: y
          Df Sum Sq Mean Sq F value Pr(>F)
           1 71534 71534 184.62 < 2.2e-16 ***
х
Residuals 56 21698
                        387
Signif. codes: 0'***'0.001'**'0.01'*'0.05'.'0.1' '1
                                    4 D > 4 A > 4 B > 4 B > 9 Q P
```

```
# Testing for zero slope
> summary(house.reg)
Call:
lm(formula = y ~ x)
Residuals:
   Min
         1Q Median
                          3Q
                                 Max
-38.489 -14.512 -1.422 14.919 54.389
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept)
                     8.191 0.663
             5.432
                                        0.51
            56.083
                       4.128 13.587 <2e-16 ***
X
```

>

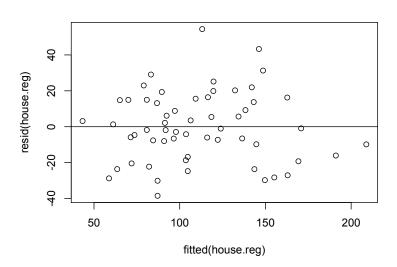
```
Signif. codes: 0'***'0.001'**'0.01'*'0.05'.'0.1' '1
Residual standard error: 19.68 on 56 degrees of freedom
Multiple R-squared: 0.7673, Adjusted R-squared: 0.7631
F-statistic: 184.6 on 1 and 56 DF, p-value: < 2.2e-16
>
# Confidence interval for slope
> confint(house.reg)
                2.5 % 97.5 %
(Intercept) -10.97619 21.83933
            47.81473 64.35183
X
>
# Prediction at a new x
```

```
x.new <- data.frame(x=3)
> (predict(house.reg, newdata=x.new))
       1
173.6814
# Use fitted(house.reg) to get the fitted values
# Use resid(house.reg) to get the residuals
# Residual plot
plot(fitted(house.reg), resid(house.reg))
abline(h=0)
# QQ plot
```

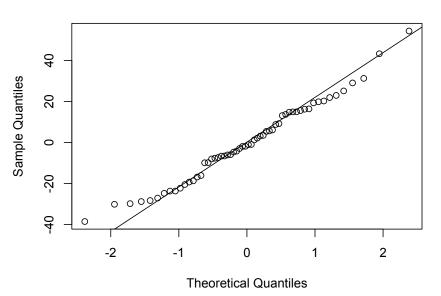
```
qqnorm(resid(house.reg))
qqline(resid(house.reg))

# Time series plot of residuals
plot(resid(house.reg), type="l")
abline(h=0)
```

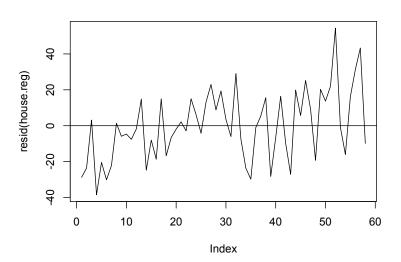
# Residual plot



## **Normal Q-Q Plot**



# Time series plot



# Multiple Linear Regression

Simple linear regression: One predictor — X

Multiple linear regression: Several predictors —  $X_1, \ldots, X_k$ 

## Linear (regression) model:

$$E(Y|X_1 = x_1, ..., X_k = x_k) = \beta_0 + \beta_1 x_1 + ... + \beta_k x_k$$
 — models **mean response** as a function of predictors

## Examples:

- $\bullet \ E(Y|x) = \beta_0 + \beta_1 x$
- $E(Y|\mathbf{x}) = \beta_0 + \beta_1 x + \beta_2 x^2$
- $E(Y|\mathbf{x}) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 (x_1 * x_2)$
- $E(\log(Y)|x) = \beta_0 + \beta_1 \log(x)$  —
- $E(Y|x) = \beta_0 + (\beta_1 x)^{-1}$  —

Note: "Linear" refers to linear in regression coefficients



Linear model:  $E(Y|\mathbf{x}) = \beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k$ 

Interpretation of k+1 regression coefficients:

- $\beta_0 = E(Y|\mathbf{x} = \mathbf{0})$  intercept
- $\beta_j = E(Y|x_1, \dots, x_j + 1, \dots, x_k) E(Y|x_1, \dots, x_j, \dots, x_k)$  slope of  $x_j$ , i.e., change in mean response when jth predictor increases by 1, while keeping other predictors fixed,  $j = 1, \dots, k$ .

**Data:** n independent subjects, ith subject gives  $(Y_i, X_{1i}, X_{2i}, \dots, X_{ki}), i = 1, \dots, n$ .

Linear model for data: For i = 1, ..., n,  $E(Y_i|x_{i1},...,x_{ik}) = \beta_0 + \beta_1 x_{i1} + ... + \beta_k x_{ik}$ 

## Alternative form: $Y_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_k x_{ik} + \epsilon_i$

## **Assumptions:**

- $E(\epsilon_i) = 0$ ,  $var(\epsilon_i) = \sigma^2$ , and  $\epsilon_i$  are independent.
- k + 1 < n i.e., have more observations than the number of regression coefficients
- The predictors are considered fixed and are measured without error

## These imply:

- $\bullet E(Y_i|x_{i1},\ldots,x_{ik}) =$
- $var(Y_i) =$
- $Y_1, \ldots, Y_n$  are independent.

## Linear Model in Matrix Notation

#### Define:

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}, \mathbf{X} = \begin{bmatrix} 1 & x_{11} & \dots & x_{1k} \\ 1 & x_{21} & \dots & x_{2k} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & \dots & x_{nk} \end{bmatrix}, \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}, \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

- $Y_i = BXi$
- Y =
- $E(\mathbf{Y}|\mathbf{X}) =$
- rank of X is full, i.e.,  $(\mathbf{X}'\mathbf{X})^{-1}$  exists.
- $\hat{\boldsymbol{\beta}} = \text{estimator of } \boldsymbol{\beta}$
- $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \text{fitted (or predicted) response}$

Predicted response when  $\mathbf{x} = \mathbf{x}_0$ :  $\hat{Y}_0 = \mathbf{x}_0' \hat{\boldsymbol{\beta}}$ 

# Least Squares Estimation of $\beta$

As before: Minimize  $\sum_{i=1}^{n} \epsilon_i^2$  with respect to  $\beta_0, \beta_1, \beta_k$  to get  $\hat{\beta}$ 

- Least squares estimator:  $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$
- Minimum value of  $\sum_{i=1}^{n} \epsilon_i^2$  is  $\sum_{i=1}^{n} (Y_i \hat{Y}_i)^2 = (\mathbf{Y} \hat{\mathbf{Y}})'(\mathbf{Y} \hat{\mathbf{Y}}) = SS_{\text{ERR}}$  error (or residual) sum of squares

## Properties of $\hat{\beta}$ :

- $\bullet$  Linear in  $\mathbf{Y}$
- Unbiased, i.e.,
- $\operatorname{var}(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$
- $\operatorname{var}(\hat{\beta}_0) = \sigma^2 \times \text{ first diagonal element of } (\mathbf{X}'\mathbf{X})^{-1}$
- $\operatorname{var}(\hat{\beta}_j) = \sigma^2 \times (j+1)$ th diagonal element of  $(\mathbf{X}'\mathbf{X})^{-1}$
- $\hat{\sigma}^2 = SS_{\text{ERR}}/(n-k-1) = MS_{\text{ERR}}$  is unbiased for  $\sigma^2$ .



## **ANOVA** table

#### As before:

• 
$$SS_{TOT} = \sum_{i=1}^{n} (Y_i - \overline{Y})^2 = (\mathbf{Y} - \overline{\mathbf{Y}})'(\mathbf{Y} - \overline{\mathbf{Y}})$$
, where  $\overline{\mathbf{Y}} = \overline{Y} \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$ 

- $SS_{REG} = \sum_{i=1}^{n} (\hat{Y}_i \overline{Y})^2 = (\hat{\mathbf{Y}} \overline{\mathbf{Y}})'(\hat{\mathbf{Y}} \overline{\mathbf{Y}})$
- $SS_{ERR} = \sum_{i=1}^{n} (Y_i \hat{Y}_i)^2 = (\mathbf{Y} \hat{\mathbf{Y}})'(\mathbf{Y} \hat{\mathbf{Y}})$

Source	SS	d.f.	MS	F
	$SS_{ m REG}$	k	$MS_{\text{REG}} = \frac{SS_{\text{REG}}}{k}$	$\frac{MS_{\mathrm{REG}}}{MS_{\mathrm{ERR}}}$
Error	$SS_{\mathrm{ERR}}$	n-k-1	$MS_{\text{ERR}} = \frac{SS_{\text{ERR}}^{n}}{n-k-1}$	Eltit
Total	$SS_{TOT}$	n-1		

Testing hypotheses: Additionally assume that  $\epsilon_i$  are normal, i.e.,  $\epsilon_i \sim$  independent  $N(0, \sigma^2)$ .

- Each  $\hat{\beta}_j$  follows a normal distribution
- $(n-k-1)\hat{\sigma}^2/\sigma^2$  follows a  $\chi^2_{n-k-1}$  distribution

## Testing significance of jth predictor:

$$H_0: \beta_j = 0 \text{ vs. } H_1: \beta_j \neq 0$$

- $H_0$ : Predictor  $X_j$  is not useful for predicting response after adjusting for the other predictors
- Test statistic:
- Null distribution:
- Rejection region:
- *p*-value:
- $100(1-\alpha)\%$  CI for  $\beta_j$ :



## Testing model significance:

$$H_0: \beta_1 = \ldots = \beta_k = 0$$
 vs.  $H_1:$  at least one  $\beta_j \neq 0$ 

- $H_0$ : None of the predictors is useful for predicting response
- Test statistic:
- Null distribution:
- Rejection region:
- $\bullet$  *p*-value:

Coefficient of determination: As before,

$$R^2 = \frac{SS_{\text{REG}}}{SS_{\text{TOT}}} = 1 - \frac{SS_{\text{ERR}}}{SS_{\text{TOT}}}$$

- $R^2$  = proportion of total variation explained by regression
- $R^2$  = square of correlation between  $(Y_i, \hat{Y}_i)$ , i = 1, ..., n can be verified
- When we add new predictors to the model,  $R^2$
- Even adding useless predictors will
- Not a fair criterion for comparing models with different numbers of predictors

## Beware of overfitting a model:

- Overfitting = Having too many predictors in the model
- An overfitted model will provide a good fit to the data at hand, but it will be terrible at predicting future observations.
- Estimated regression coefficients have large standard errors.
- See Figure 11.4 on page 369

## Adjusted $R^2$ :

$$R_{\text{adj}}^2 = 1 - \frac{SS_{\text{ERR}}/(n-k-1)}{SS_{\text{TOT}}/(n-1)}$$

- Unlike  $R^2$ ,  $R_{\text{adj}}^2$  rewards adding a predictor only if it reduces the error SS considerably
- Imagine adding a useless predictor. In this case,  $SS_{REG}$  and hence  $SS_{ERR}$  does not change. However,  $SS_{ERR}/(n-k-1)$  increases, which in turn decreases  $R_{adj}^2$
- A more fair measure of goodness-of-it than  $R^2$
- Can be used to compare two models with different numbers of predictors choose the model with the highest  $R_{\text{adj}}^2$

## Comparing two Nested Models

**Nested models:** Model 2 is nested within Model 1 if the predictors of Model 2 are a subset of predictors of Model 1.

**Issue:** How to compare two nested models?

Full model: Predictors  $X_1, \ldots, X_m$ 

**Reduced model:** Predictors  $X_1, \ldots, X_k$ , i.e., it does not have predictors  $X_{k+1}, \ldots, X_m$ 

**Hypotheses:**  $H_0: \beta_{k+1} = \ldots = \beta_m = 0$ , vs.,  $H_1:$  at least one slope  $\neq 0$ 

Extra sum of squares: Difference in variation explained by the two models

$$SS_{\text{EX}} = SS_{\text{REG}}(\text{full}) - SS_{\text{REG}}(\text{reduced})$$
  
=  $SS_{\text{ERR}}(\text{reduced}) - SS_{\text{ERR}}(\text{full})$ 

•  $SS_{\text{EX}}$  has m-k degrees of freedom. It equals the number of regression coefficients set to zero under  $H_0$ .

#### Test statistic:

$$F = \frac{MS_{EX}}{MS_{ERR}(full)} = \frac{SS_{EX}/(m-k)}{SS_{ERR}(full)/(n-m-1)}$$

#### Null distribution:

## Rejection region:

## p-value:

- aka "partial F-test"
- Used for designing stepwise model selection procedures (see pages 392-394)

**Example:** Home price data. These data come from a sample of homes sold in Maplewood, NJ in 2001.

```
# Read the home price data
```

```
home <- read.table("homeprice_multiple_predictors.txt",
sep=",", header=T)
> str(home)
```

```
'data.frame': 29 obs. of 7 variables:
$ list : num 80 151 310 295 339 ...
$ sale : num 118 151 300 275 340 ...
$ full : int 1 1 2 2 2 1 3 1 1 1 ...
$ half : int 0 0 1 1 0 1 0 1 2 0 ...
$ bedrooms : int 3 4 4 4 3 4 3 3 3 1 ...
$ rooms : int 6 7 9 8 7 8 7 7 7 3 ...
$ neighborhood: int 1 1 3 3 4 3 2 2 3 2 ...
```

```
# Attach the dataset in R's memory so that we can
# directly use the names of the variables
attach(home)
# Look at distributions of some predictors
> table(bedrooms)
bedrooms
1 2 3 4 5
1 3 16 8 1
> table(full)
full
1 2 3
13 11 5
```

```
> table(half)
half
 0 1 2
13 13 3
>
> table(neighborhood)
neighborhood
 1 2 3 4 5
 2 8 12 5 2
# Regress sale price on # bedrooms and neighborhood
fit1 <- lm(sale ~ bedrooms + neighborhood)</pre>
> summary(fit1)
Call:
```

```
lm(formula = sale ~ bedrooms + neighborhood)
```

#### Residuals:

```
Min 1Q Median 3Q Max -90.871 -39.861 0.636 28.815 107.660
```

#### Coefficients:

Signif. codes: 0'\*\*\*'0.001'\*\*'0.01'\*'0.05'.'0.1' '1

Residual standard error: 47.3 on 26 degrees of freedom Multiple R-squared: 0.8491, Adjusted R-squared: 0.8375 F-statistic: 73.16 on 2 and 26 DF, p-value: 2.1e-11 >

```
# Add # full and half baths
fit2 <- update(fit1, . ~ . + full + half)</pre>
```

> summary(fit2)

#### Call:

lm(formula = sale ~ bedrooms + neighborhood + full + half)

#### Residuals:

Min 1Q Median 3Q Max -56.554 -38.067 6.027 26.998 53.311

### Coefficients:

Estimate Std. Error t value Pr(>|t|)
(Intercept) -125.121 33.136 -3.776 0.000926 \*\*\*
bedrooms 29.513 10.091 2.925 0.007419 \*\*

```
9.669
neighborhood
             78.724
                                  8.142 2.31e-08 ***
full
              27.345 13.604 2.010 0.055785 .
half
            45.553 12.129 3.756 0.000974 ***
Signif. codes: 0'***'0.001'**'0.01'*'0.05'.'0.1' '1
Residual standard error: 38.79 on 24 degrees of freedom
Multiple R-squared: 0.9063, Adjusted R-squared: 0.8907
F-statistic: 58.05 on 4 and 24 DF, p-value: 5.425e-12
>
# Drop # full baths
fit3 <- update(fit2, . ~ . - full)</pre>
```

> summary(fit3)

Call:

```
lm(formula = sale ~ bedrooms + neighborhood + half)
```

#### Residuals:

```
Min 1Q Median 3Q Max -67.55 -42.27 7.17 26.93 68.83
```

#### Coefficients:

Signif. codes: 0'\*\*\*'0.001'\*\*'0.01'\*'0.05'.'0.1' '1

Residual standard error: 41.08 on 25 degrees of freedom Multiple R-squared: 0.8905, Adjusted R-squared: 0.8774 F-statistic: 67.8 on 3 and 25 DF, p-value: 3.808e-12

```
>
```

# Compare the nested models

Check {\tt ?anova.lm}

Important note: When comparing two models using anova the results are as expected from the partial F-test. However, when more than two models are compared using anova, the F-statistic and p-value may not be what we would like. The reason for this is that the F-statistic compares the mean SS for a row to the  $\mathrm{MS}_{ERR}$  for the largest model considered.

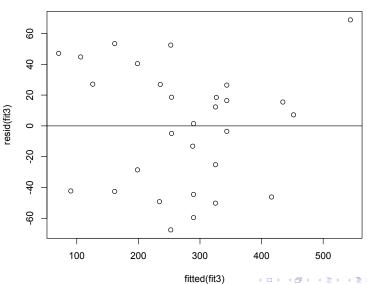
```
> anova(fit1, fit3, fit2)
Analysis of Variance Table
Model 1: sale ~ bedrooms + neighborhood
Model 2: sale ~ bedrooms + neighborhood + half
Model 3: sale ~ bedrooms + neighborhood + full + half
 Res.Df RSS Df Sum of Sq F Pr(>F)
1 26 58164
2 25 42194 1 15970.1 10.6132 0.003338 **
3 24 36114 1 6080.1 4.0406 0.055785 .
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 '
>
> anova(fit1, fit2)
Analysis of Variance Table
```

```
Model 1: sale ~ bedrooms + neighborhood
```

```
Model 2: sale ~ bedrooms + neighborhood + full + half
 Res.Df RSS Df Sum of Sq F Pr(>F)
1 26 58164
2 24 36114 2 22050 7.3269 0.003283 **
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 '
>
> anova(fit3, fit2)
Analysis of Variance Table
Model 1: sale ~ bedrooms + neighborhood + half
Model 2: sale ~ bedrooms + neighborhood + full + half
 Res.Df RSS Df Sum of Sq F Pr(>F)
1 25 42194
2 24 36114 1 6080.1 4.0406 0.05579 .
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 '
```

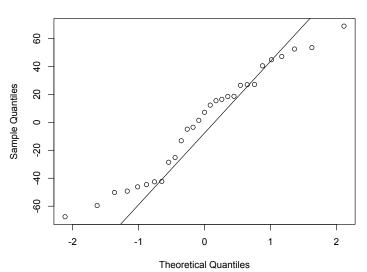
```
# Residual plot
plot(fitted(fit3), resid(fit3))
abline(h=0)
# QQ plot
qqnorm(resid(fit3))
qqline(resid(fit3))
```

# Residual plot



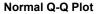
# Normal QQ plot

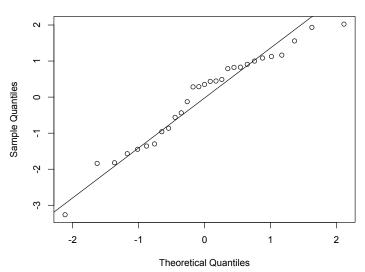
#### **Normal Q-Q Plot**



```
# Take sqrt(sale) rather than sale as response
fit4 <- update(fit3, sqrt(sale) ~ .)
# New QQ plot
qqnorm(resid(fit4))
qqline(resid(fit4))</pre>
```

## Normal QQ plot for transformed data





# Regression with categorical predictors

Categorical variable: Its values are categories (or attributes) with no particular order, e.g., race, OS, etc. The values should **not** be coded as 1, 2, 3, ..., unless R knows to treat the variable as a factor.

**Dummy variable:** A binary variable z with value 0 or 1

**Key idea:** Represent a categorical variable with C categories using C-1 dummy variables,  $z_1, \ldots, z_{C-1}$ . The model is

$$E(Y|\mathbf{z}) = \beta_0 + \gamma_1 z_1 + \ldots + \gamma_{C-1} z_{C-1}.$$

Base (or reference) category:  $z_1 = \ldots = z_{C-1} = 0$ .

**Ex 1:** OS with two categories — Windows and Mac.

## Ex 2: Race with three categories — White, Black and other.

- In general,  $\beta_0$  = mean for base category, and  $\beta_j$  = difference in means for category j and base category
- The regression model may have both numerical as well as categorical predictors.
- The model may have several categorical predictors.
- To test whether a categorical variable is significant, simultaneously test **all** corresponding slopes. In other words, the hypotheses are  $H_0: \gamma_1 = \ldots = \gamma_{C-1} = 0$ , vs.  $H_1:$  at least one non-zero slope, and they should be tested using an F-test with C-1 numerator d.f.

```
Example: Jane data.
# Read the Jane data
jane <- read.table("jane.csv", sep=",", header=T)</pre>
> str(jane)
'data.frame': 150 obs. of 3 variables:
 $ x : int 1 1 1 2 2 2 3 3 3 4 ...
$ color: Factor w/ 3 levels "blue", "green", ...: 3 1 2 3 1 3
$ y : num 24.9 12.3 16.6 25.2 12.1 ...
attach(jane)
> table(color)
color
blue green red
```

```
50 50
             50
# Include both x and color as predictors
fit1 <- lm(y~x+color)</pre>
# Note: color is already a factor variable. If this is
# numeric, then we need to write:
# fit1 <- lm(y~ x + factor(color))</pre>
> summary(fit1)
Call:
lm(formula = y ~ x + color)
Residuals:
     Min
               10 Median
                                  30
                                           Max
                                     ◆□ → ◆周 → ◆ ■ → ◆ ■ ・ ◆ ○ ○
```

#### Coefficients:

Signif. codes: 0'\*\*\*'0.001'\*\*'0.01'\*'0.05'.'0.1' '1

Residual standard error: 5.034 on 146 degrees of freedom Multiple R-squared: 0.898, Adjusted R-squared: 0.8959 F-statistic: 428.6 on 3 and 146 DF, p-value: < 2.2e-16 >

# Is color significant?

```
fit2 <- lm(y^x)
> anova(fit2, fit1)
Analysis of Variance Table
Model 1: y ~ x
Model 2: y ~ x + color
 Res.Df RSS Df Sum of Sq F Pr(>F)
1 148 4837.5
2 146 3700.4 2 1137.1 22.433 3.197e-09 ***
Signif. codes: 0'***'0.001'**'0.01'*'0.05'.'0.1' '1
>
```

**Q:** What is the predicted response for a subject with color=blue and x=2?