S&DS 355 / 365 / 565

(Schrodinger's Intro) Machine Learning and Data Mining

Linear Regression

Tuesday, September 3rd

Yale

365 + 355

For the next week, we will be merging both 365 and 355 classes.

365 vs 355

- 355 does not count towards the S&DS Major
- 365 = more math, harder topics, 355 = more programming

For today

- Linear regression
  - Estimation
  - Measures of fit
  - Inference
  - Several predictors
- Redux of part of last lecture

Why start here?

- Linear regression is foundation for more sophisticated topics:
  - Regularization: Ridge regression and lasso
  - Kernel methods: Support vector machines
  - Smoothing: Splines, generalized additive models, etc.

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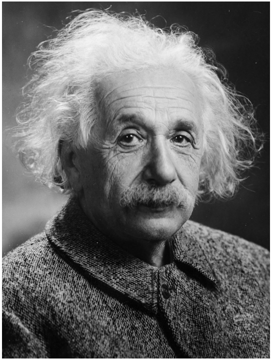
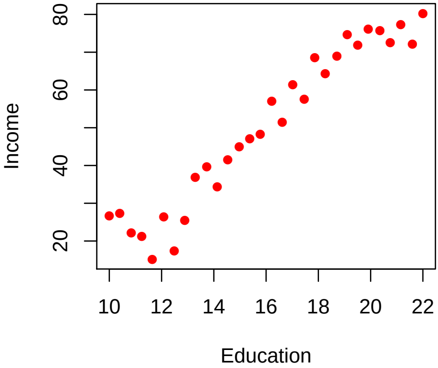
- Linear regression is foundation for more sophisticated topics:
  - Regularization: Ridge regression and lasso
  - Kernel methods: Support vector machines
  - Smoothing: Splines, generalized additive models, etc.
- Many advanced machine learning methods are generalizations or extensions of linear regression



Everything should be made as simple as possible, but no simpler.

https://en.wikiquote.org/wiki/Albert_Einstein

Simulated income dataset



Goal: Predict income(Y) using education (X).

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

$(x_1, y_1), (x_2, y_2), \ldots, (x_{30}, y_{30})$

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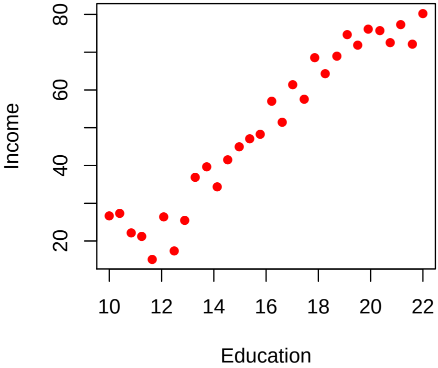

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Linear model:

$$f(X) = \beta_0 + \beta_1 X$$

$$\epsilon \sim N(0, \sigma^2)$$

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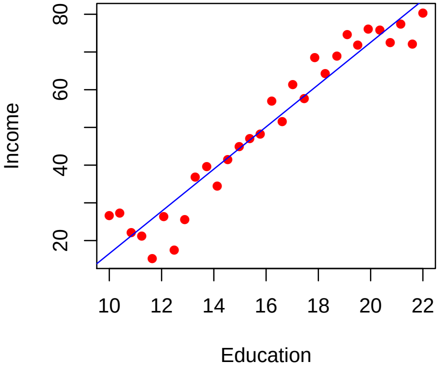

Goal: Predict income(Y) using education (X).

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

Linear model:

$$f(X) = \beta_0 + \beta_1 X$$

$$\epsilon \sim N(0, \sigma^2)$$

Find coefficients $\widehat{\beta}_0$ and $\widehat{\beta}_1$ s.t. $\widehat{Y} = \widehat{f}(X) = \widehat{\beta}_0 + \widehat{\beta}_1 X$ is reasonably close to Y.

Estimating the coefficients

For any $\widehat{\beta}_0, \widehat{\beta}_1$, we predict $\widehat{y}_i = \widehat{\beta}_0 + \widehat{\beta}_1 x_i$. We call these **fitted values.**

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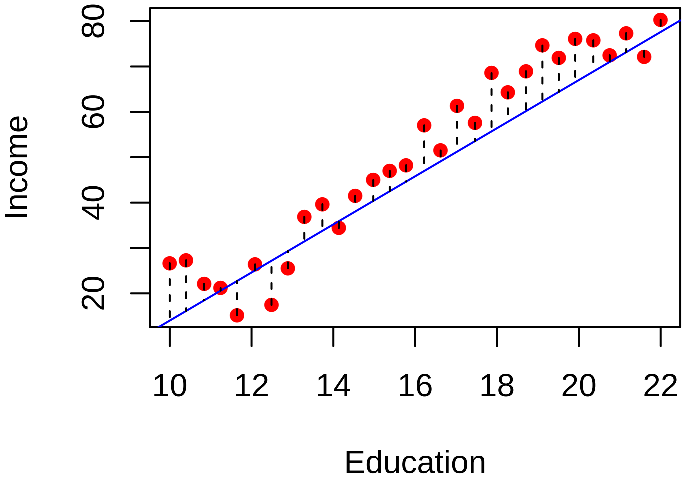
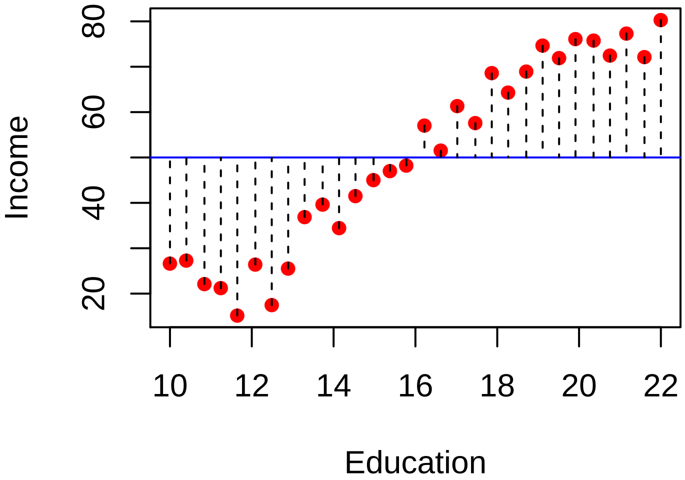
The **residual** $e_i = y_i - \widehat{y}_i$ is difference between the i-th observed value and its fitted value.

Some candidate lines (and residuals)



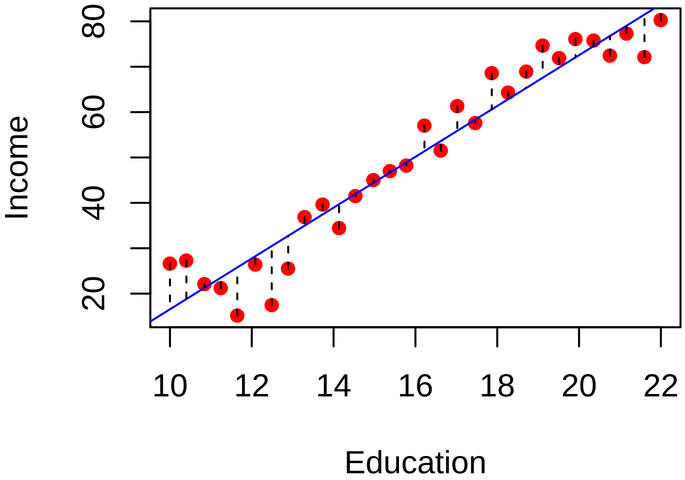
$$\widehat{\beta}_0 = -39, \widehat{\beta}_1 = 5.3$$

Some candidate lines (and residuals)



$\widehat{\beta}_0 = 50, \widehat{\beta}_1 = 0$

Some candidate lines (and residuals)



$\widehat{\beta}_0 = -39.4, \widehat{\beta}_1 = 5.6$

Estimating the coefficients

The **least squares** approach selects coefficients $\widehat{\beta}_0$ and $\widehat{\beta}_1$ that minimize the **residual sum of squares** (RSS):

$$RSS = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \widehat{y}_i)^2.$$

Estimating the coefficients

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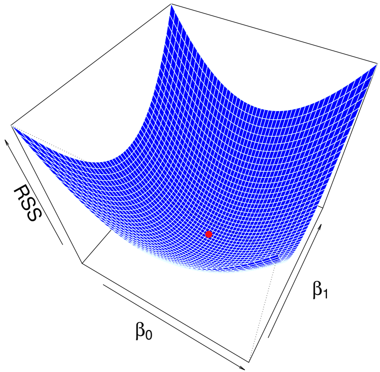
$$RSS(\beta_0, \beta_1) = \sum_{i=1}^{n} e_i^2 = (y_1 - \beta_0 - \beta_1 x_1)^2 + \cdots + (y_n - \beta_0 - \beta_1 x_n)^2.$$



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How do we find the minimum?

- $RSS(\beta_0, \beta_1)$ is convex.
- Take partial derivatives and set to 0:

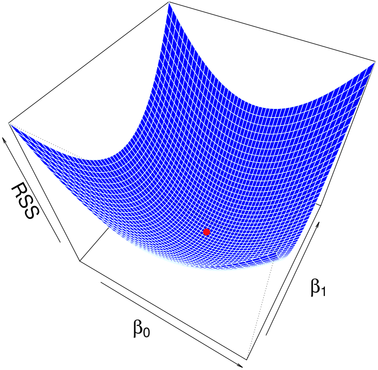
$$\frac{\partial RSS(\beta_0, \beta_1)}{\partial \beta_0} = \sum_{i=1}^{n} -2(y_i - \beta_0 - \beta_1 x_i) = 0$$

$$\frac{\partial RSS(\beta_0, \beta_1)}{\partial \beta_1} = \sum_{i=1}^{n} -2x_i(y_i - \beta_0 - \beta_1 x_i) = 0$$

Estimating the coefficients

The **least squares** approach selects coefficients $\widehat{\beta}_0$ and $\widehat{\beta}_1$ that minimize the **residual sum of squares** (RSS):

$$RSS(\beta_0, \beta_1) = \sum_{i=1}^{n} e_i^2 = (y_1 - \beta_0 - \beta_1 x_1)^2 + \cdots + (y_n - \beta_0 - \beta_1 x_n)^2.$$



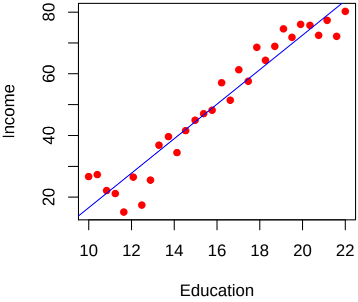
Minimum RSS is achieved at:

$$\widehat{\beta}_0 = \bar{y} - \widehat{\beta}_1 \bar{x},$$

$$\widehat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2},$$

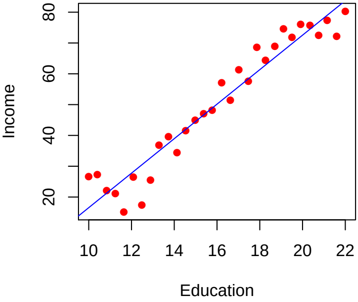
where $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$ and $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$.

Simulated income dataset



$$\widehat{\beta}_0 = -39.45 \qquad \widehat{\beta}_1 = 5.60$$

Simulated income dataset



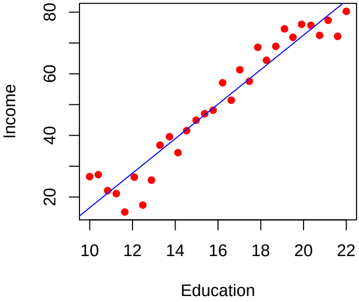
$$\widehat{\beta}_0 = -39.45 \qquad \widehat{\beta}_1 = 5.60$$

$$\widehat{y} = -39.45 + 5.60x$$

Interpretation:

- A one-year increase in education is associated with an increase in average income of 5.6 units.

Simulated income dataset



$$\widehat{\beta}_0 = -39.45 \qquad \widehat{\beta}_1 = 5.60$$

$$\widehat{Income} = -39.45 + 5.60 \cdot Education$$

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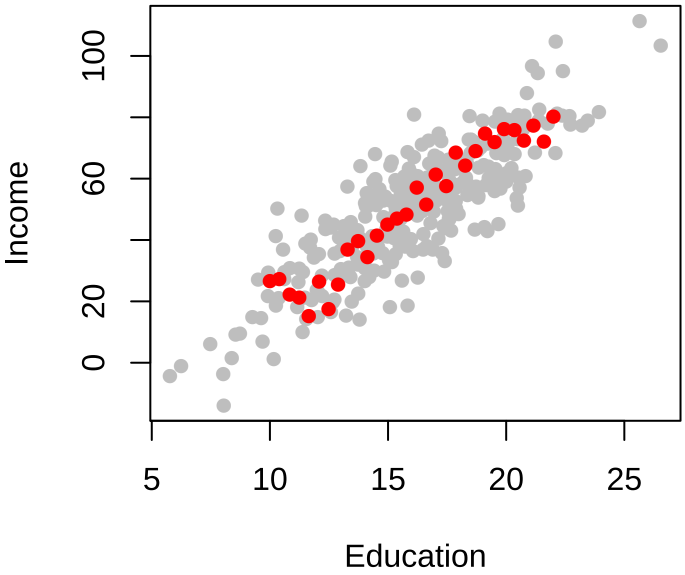
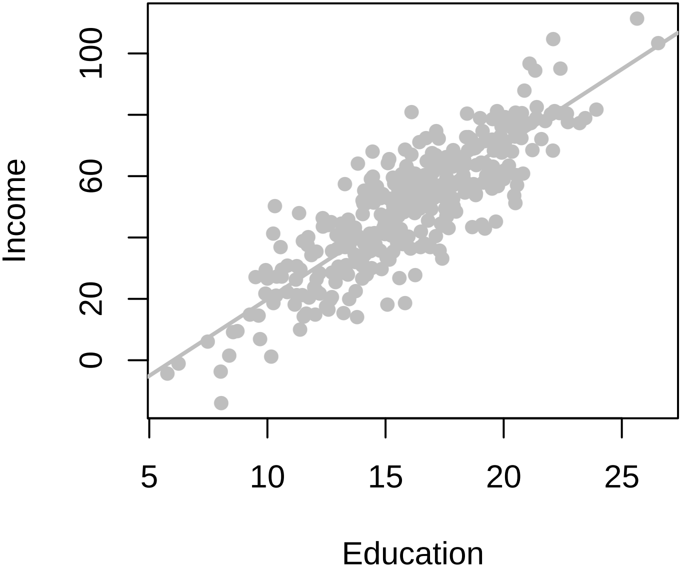
Population vs. sample



Population vs. sample



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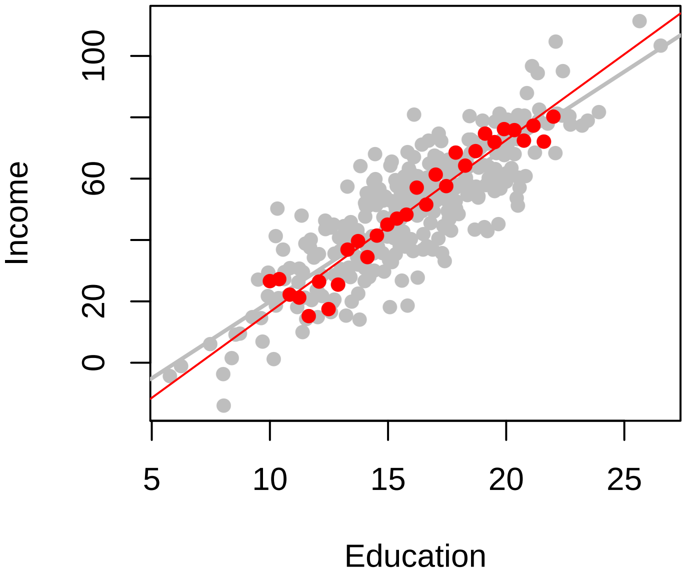
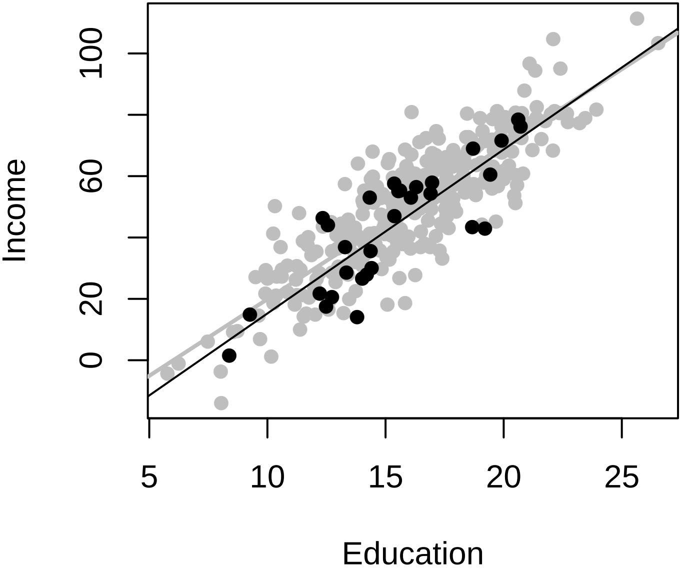


Different samples



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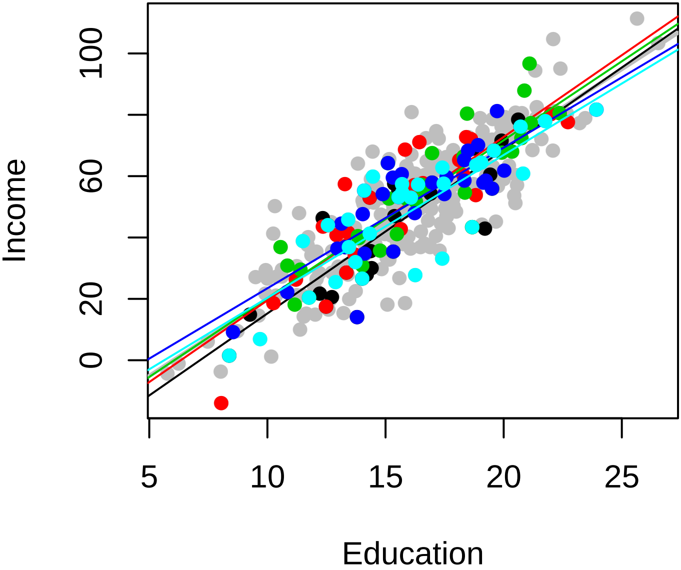

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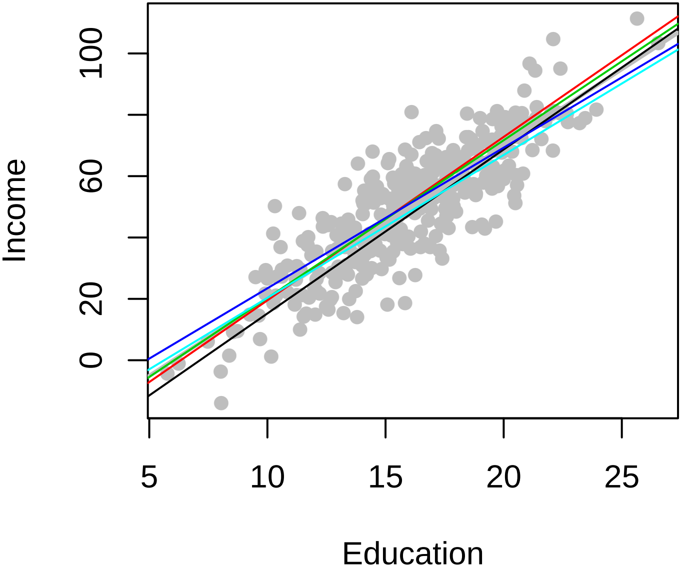
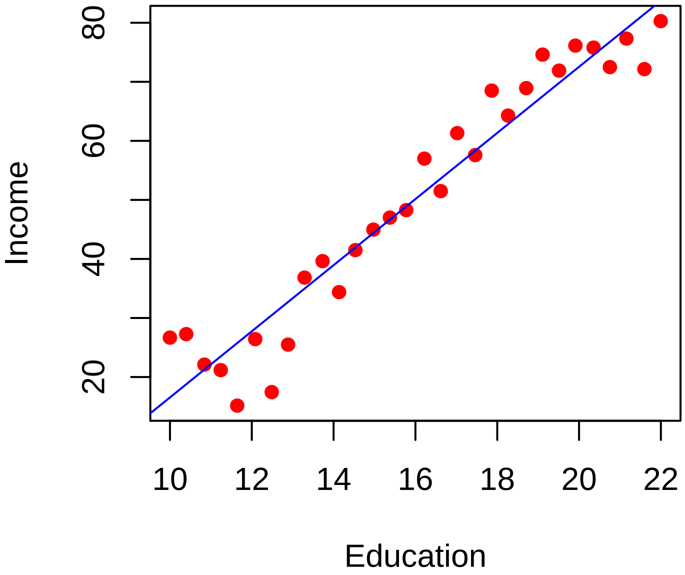


How to determine variability?



Inference for linear regression

Standard errors of the coefficients describe how the coefficients vary under repeated sampling:

$$SE(\widehat{\beta}_0) = \sqrt{\sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}\right]}$$

$$SE(\widehat{\beta}_1) = \sqrt{\frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}}$$

where $\sigma^2 = Var(\epsilon)$.

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where $\sigma^2 = Var(\epsilon)$. A 95% confidence interval for β_i is approximately:

$$\widehat{\beta}_i \pm 2 \cdot SE(\widehat{\beta}_i)$$

Inference for linear regression

```
##
## Call:
## lm(formula = Income ~ Education, data = x)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -13.046  -2.293   0.472   3.288  10.110
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -39.4463     4.7248  -8.349  4.4e-09 ***
## Education     5.5995     0.2882  19.431  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.653 on 28 degrees of freedom
## Multiple R-squared:  0.931,Adjusted R-squared:  0.9285
## F-statistic: 377.6 on 1 and 28 DF,  p-value: < 2.2e-16
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A 95% confidence interval for β_1 is approximately:

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For a one-year increase in an individual's education, the model predicts that the individual's income will rise by between 5.0 and 6.2 units.

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For a one-year increase in an individual's education, the model predicts that the individual's income will rise by between 5.0 and 6.2 units. Note: This statement is about the population slope β_1!

Sums of squares and R^2

Partitioning the sums of squares:

$$\underbrace{\sum (y_i - \bar{y})^2}_{\text{total sum of squares}(TSS)} = \underbrace{\sum (\widehat{y}_i - \bar{y})^2}_{\text{explained sum of squares}(ESS)} + \underbrace{\sum (y_i - \widehat{y}_i)^2}_{\text{residual sum of squares}(RSS)}$$

(need some algebra to show this)

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(need some algebra to show this)

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

We can interpret R^2 (**multiple R-squared**) as the proportion of variability in y explained by the model.

- Between 0 and 1
- Doesn't depend on the scale of Y.

Inference for linear regression

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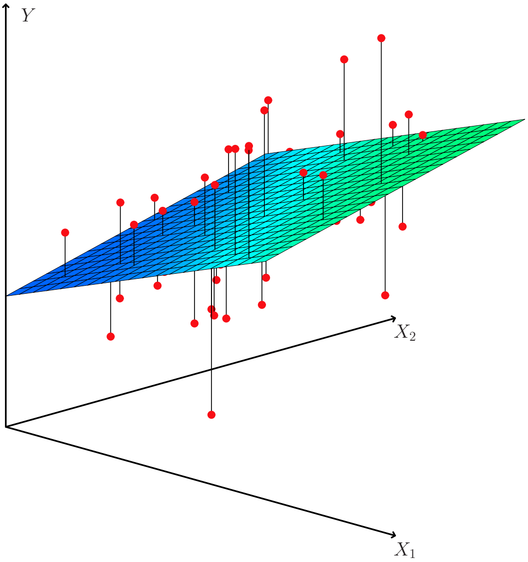
Multiple linear regression



General form

With p predictors $x_1, \ldots, x_p$,

$$y = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p + \epsilon,$$

where $\epsilon \sim N(0, \sigma^2)$.

In matrix notation,

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_{1,1} & x_{1,2} & \cdots & x_{1,p} \\ 1 & x_{2,1} & \ddots & & x_{2,p} \\ \vdots & & \ddots & \vdots & \\ 1 & x_{n,1} & x_{n,2} & \cdots & x_{n,p} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}$$

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where $\epsilon \sim N(0, \sigma^2)$.

In matrix notation,

$$y = X\beta + \epsilon$$

(where the intercept β_0 corresponds to a column of all 1s)

Residual sum of squares

Recall that

$$\widehat{\beta} = \arg\min_{\beta} RSS(\beta).$$

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$$\begin{aligned}
RSS(\beta) &= \|y - X\beta\|_2^2 \\
&= (y - X\beta)^T (y - X\beta) \\
&= (y^T - \beta^T X^T)(y - X\beta) \\
&= y^T y - y^T X\beta - \beta^T X^T y + \beta^T X^T X\beta \\
&= y^T y - 2y^T X\beta + \beta^T X^T X\beta
\end{aligned}$$

Residual sum of squares

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&= y^T y - 2y^T X\beta + \beta^T X^T X\beta
\end{aligned}$$

Hence,

$$\begin{aligned}
\widehat{\beta} &= \arg\min_{\beta} \left[-2y^T X\beta + \beta^T X^T X\beta\right] \\
&= \arg\min_{\beta} \left[-2\tfrac{1}{n} y^T X\beta + \beta^T \tfrac{1}{n} X^T X\beta\right].
\end{aligned}$$

Estimating β

Compute derivatives of $RSS(\beta)$ with respect to β_i and set equal to 0.

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The β that minimizes $RSS(\beta)$ satisfies the **normal equations**:

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Compute derivatives of $RSS(\beta)$ with respect to β_i and set equal to 0.

The β that minimizes $RSS(\beta)$ satisfies the **normal equations**:

$$X^T X\beta = X^T y.$$

If the matrix $X^T X$ is invertible, solve to get

$$\widehat{\beta} = (X^T X)^{-1} X^T y.$$

Interpretation

The coefficients are just the correlations between the variables X_j and the data Y—*after* the variables are "whitened" to become uncorrelated.

For the algebraically inclined

Let $\widetilde{X} = X\widehat{\Sigma}^{-1/2}$, where $\widehat{\Sigma} = \frac{1}{n}X^T X$ is the sample covariance.

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Then $\widetilde{X}$ is "whitened" (uncorrelated):

$$\begin{aligned}\frac{1}{n}\widetilde{X}^T\widetilde{X} &= \widehat{\Sigma}^{-1/2}\left(\frac{1}{n}X^T X\right)\widehat{\Sigma}^{-1/2} \\ &= \widehat{\Sigma}^{-1/2}\widehat{\Sigma}\widehat{\Sigma}^{-1/2} \\ &= \widehat{\Sigma}^{1/2}\widehat{\Sigma}^{-1/2} \\ &= I\end{aligned}$$

For the algebraically inclined

Let $\widetilde{X} = X\widehat{\Sigma}^{-1/2}$, where $\widehat{\Sigma} = \frac{1}{n}X^T X$ is the sample covariance.

Then $\widetilde{X}$ is "whitened" (uncorrelated):

$$\begin{aligned}
\frac{1}{n}\widetilde{X}^T\widetilde{X} &= \widehat{\Sigma}^{-1/2}\left(\frac{1}{n}X^T X\right)\widehat{\Sigma}^{-1/2} \\
&= \widehat{\Sigma}^{-1/2}\widehat{\Sigma}\widehat{\Sigma}^{-1/2} \\
&= \widehat{\Sigma}^{1/2}\widehat{\Sigma}^{-1/2} \\
&= I
\end{aligned}$$

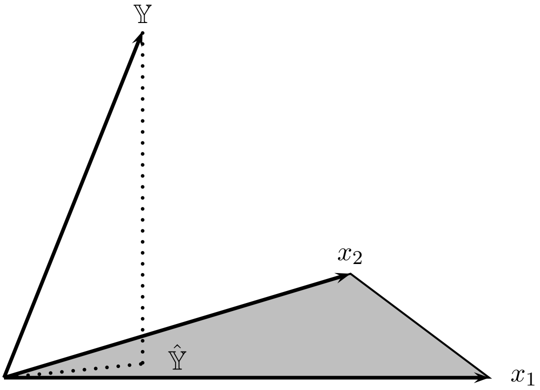
So the regression coefficients are

$$\widetilde{\beta} = \frac{1}{n}\widetilde{X}^T Y$$

which is (proportional to) correlation of $\widetilde{X}$ with Y. Transforming back gives $\widehat{\beta}$.

For the geometrically inclined

The **predicted values** (aka **fitted values**) $\widehat{Y} = X\widehat{\beta}$ are the orthogonal projection of the data $Y \in \mathbb{R}^n$ onto the column space of X (the span of columns $X_1, X_2, \ldots, X_p \in \mathbb{R}^n$)



Potential issues

$$\widehat{\beta} = (X^T X)^{-1} X^T y.$$

- $X^T X$ may not be invertible (if $n < p$)
- Inverting $X^T X$ can be computationally intensive, $O(p^3)$

Multiple linear regression

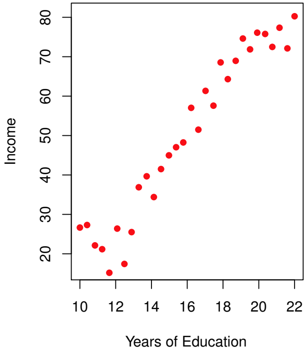
```
##
## Call:
## lm(formula = Income ~ ., data = x)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -9.113 -5.718 -1.095  3.134 17.235
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -50.08564    5.99878  -8.349 5.85e-09 ***
## Education     5.89556    0.35703  16.513 1.23e-15 ***
## Seniority     0.17286    0.02442   7.079 1.30e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 7.187 on 27 degrees of freedom
## Multiple R-squared:  0.9341,Adjusted R-squared:  0.9292
## F-statistic: 191.4 on 2 and 27 DF,  p-value: < 2.2e-16
```

Comparing methods

Let's now go over some of the discussion from last lecture

Regression example

Back to regression with $p = 1$:



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

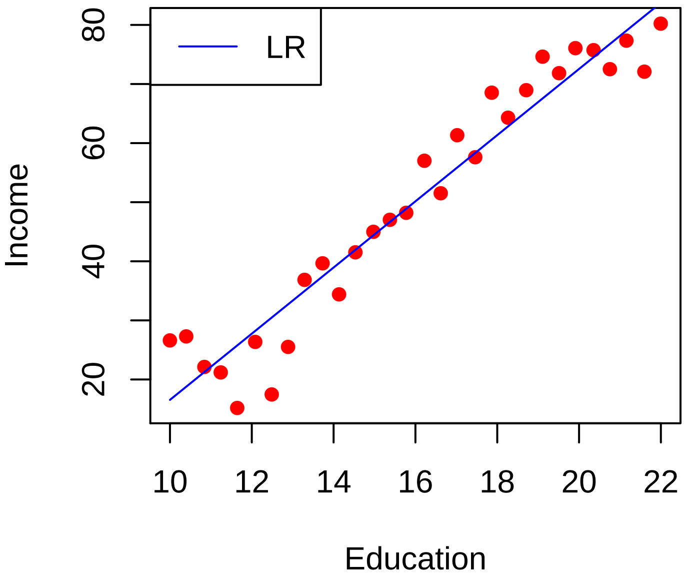
Modeling:

Use a procedure to get $\widehat{f}$. Derive estimates $\widehat{Y} = \widehat{f}(X)$.

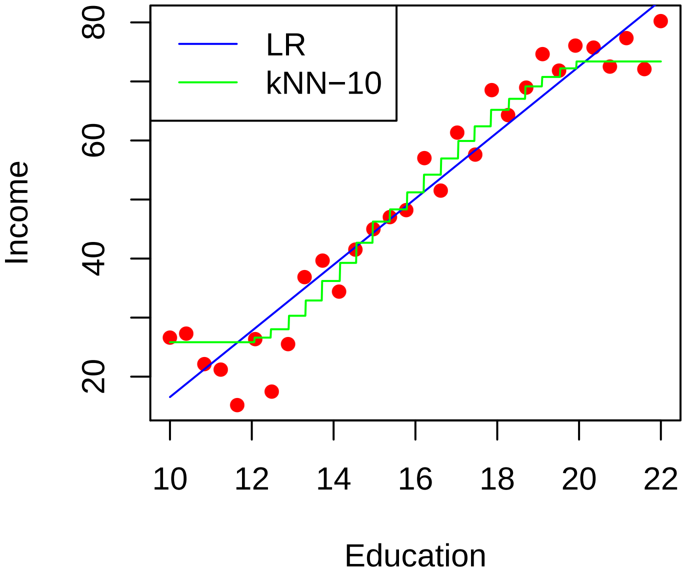
Possible regression approaches

- linear regression
  - Fitting a straight line through the data.
- *k*-nearest neighbors regression
  - Average together the y_i for x_i close to x

Possible regression approaches



Possible regression approaches



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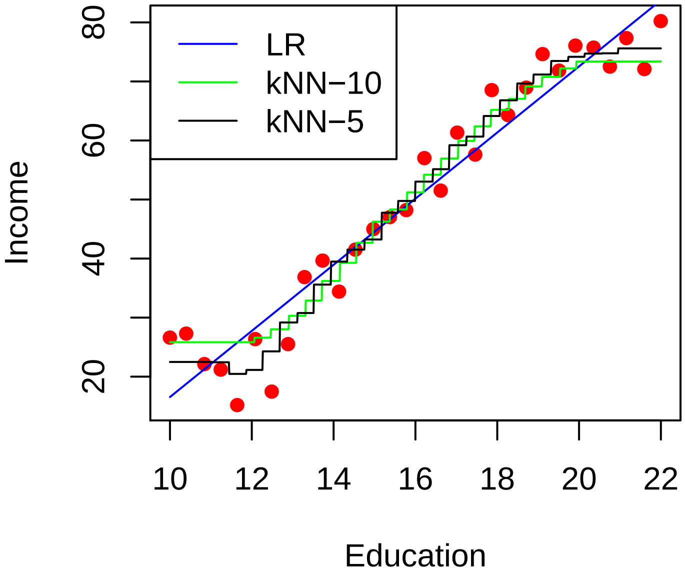
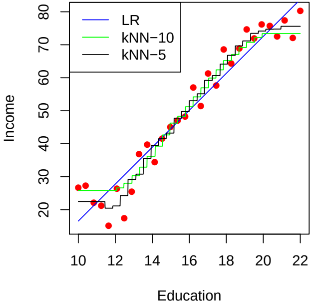


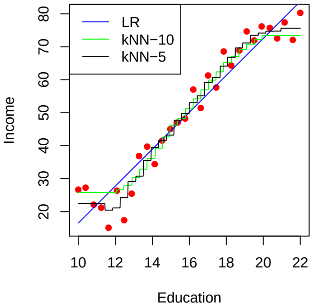
Possible regression approaches



Measuring performance via **Mean Squared Error**

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

Possible regression approaches



Measuring performance via **Mean Squared Error**

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

MSEs for three methods:

Linear Regression	29.829
k-Nearest Neighbors (k=10)	23.519
k-Nearest Neighbors (k=5)	16.21

A k-nearest neighbors model with $k = 5$ achieves lowest error. Is it the best?

Training MSE vs. Test MSE

MSE in the previous table, **training MSE**, was computed based on data used in fitting the model.

We are more interested in **test MSE** computed on *unseen data*.

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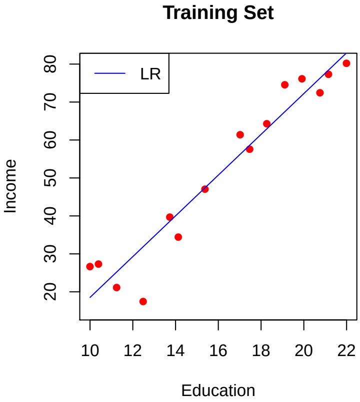
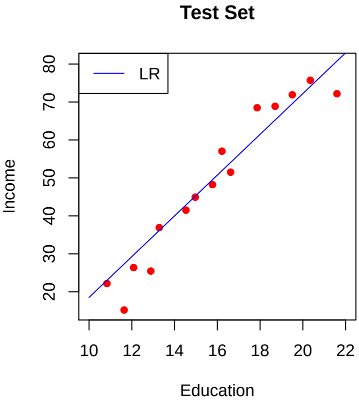
We are more interested in **test MSE** computed on *unseen data*.What if we don't have other data?

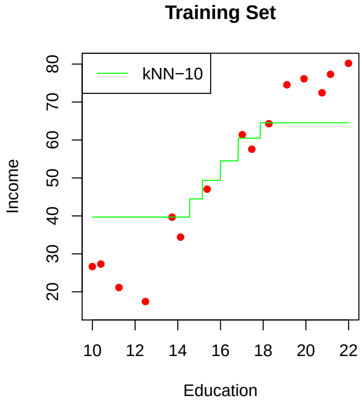
We can randomly split our data into a test set and a training set.

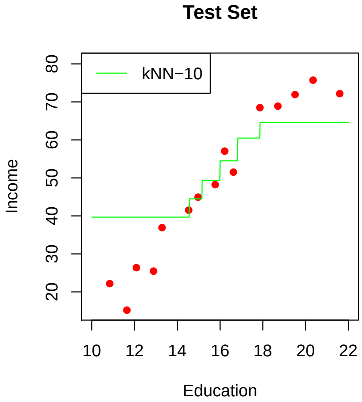
Regression approaches revisited





Regression approaches revisited





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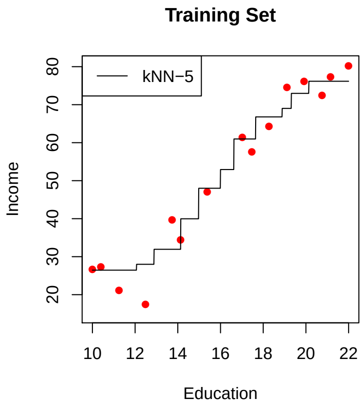

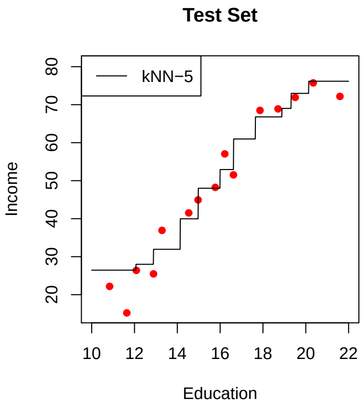

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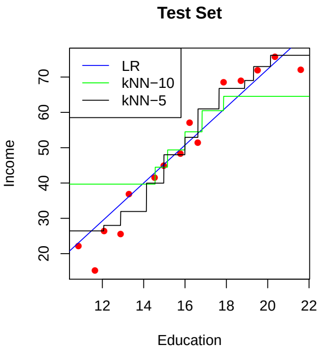
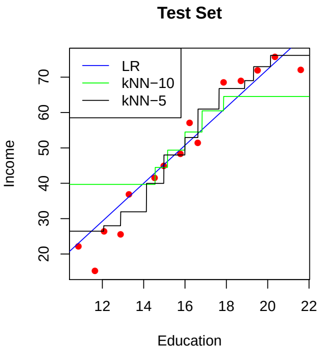


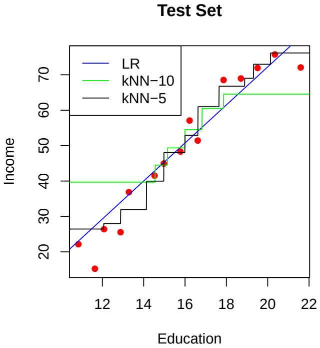
Regression approaches revisited

Compute MSE on the test set:

$$MSE = \frac{1}{n}\sum(y_i - \widehat{f}(x_i))^2$$



Regression approaches revisited

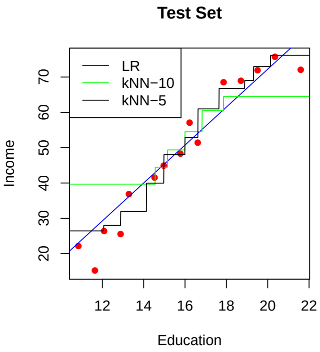


Compute MSE on the test set:

$$MSE = \frac{1}{n}\sum(y_i - \widehat{f}(x_i))^2$$

Linear Regression	28.502
k-Nearest Neighbors (k=10)	105.783
k-Nearest Neighbors (k=5)	24.898

Regression approaches revisited



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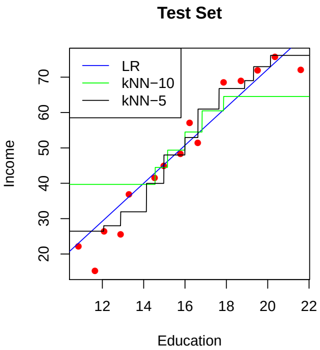
Regression approaches revisited



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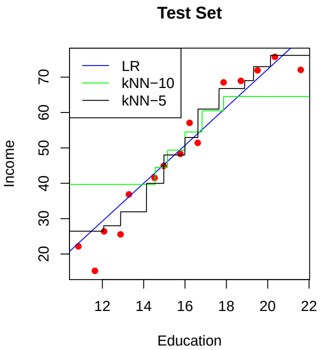

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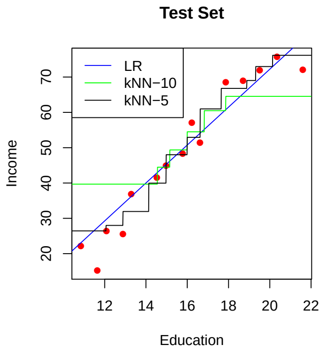

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With different random splits of test vs. training, we could have gotten different results.

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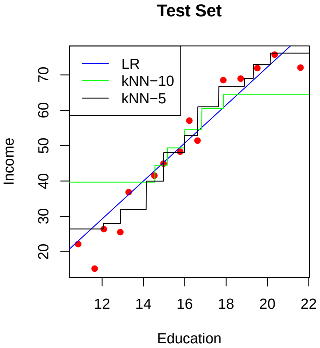

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So it appears that linear regression wins. Does it?

With different random splits of test vs. training, we could have gotten different results. We'll talk about ways around this later.

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A method is **overfitting** the data when it has a small training MSE but a large test MSE.

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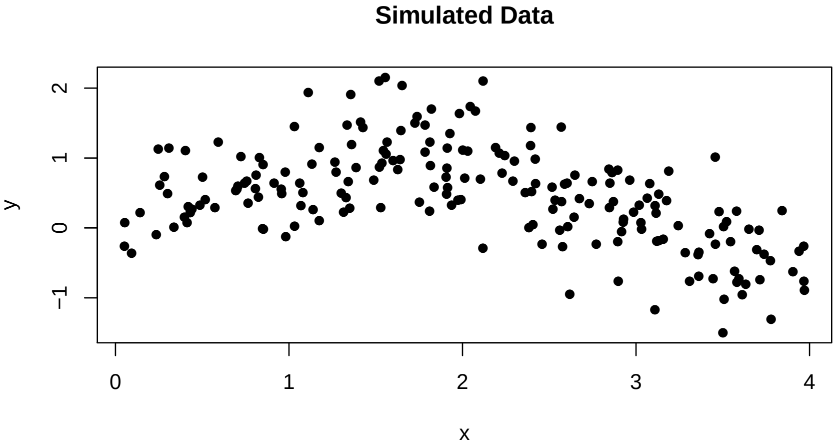

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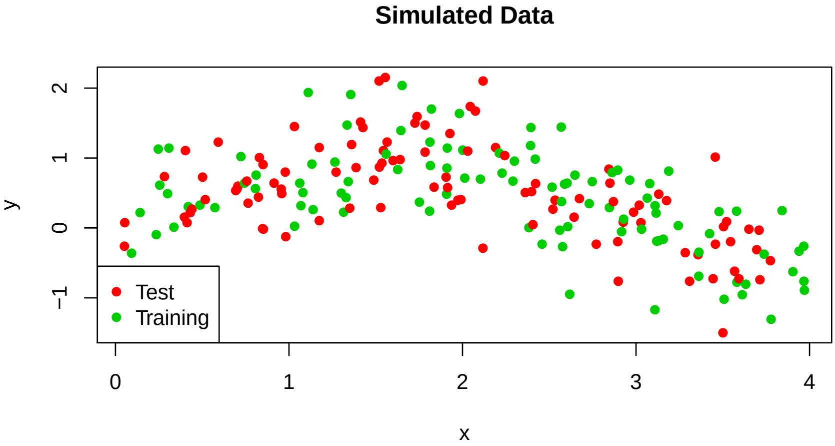

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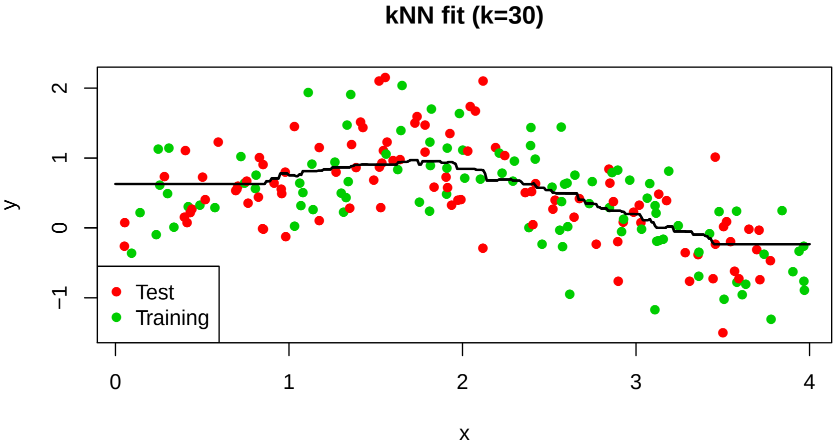

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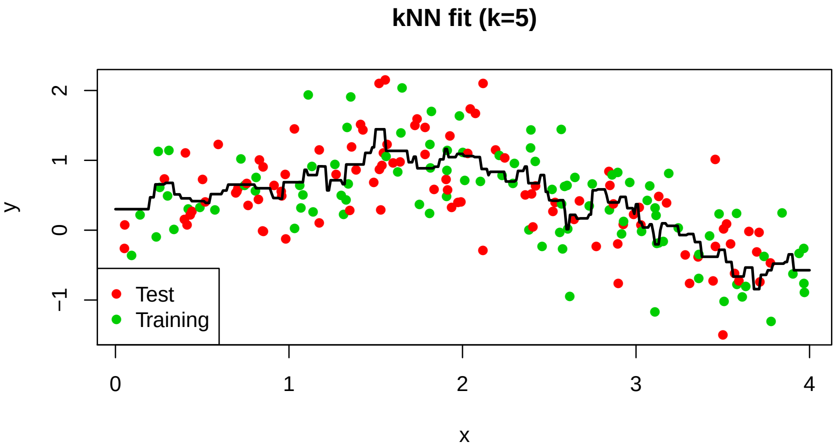
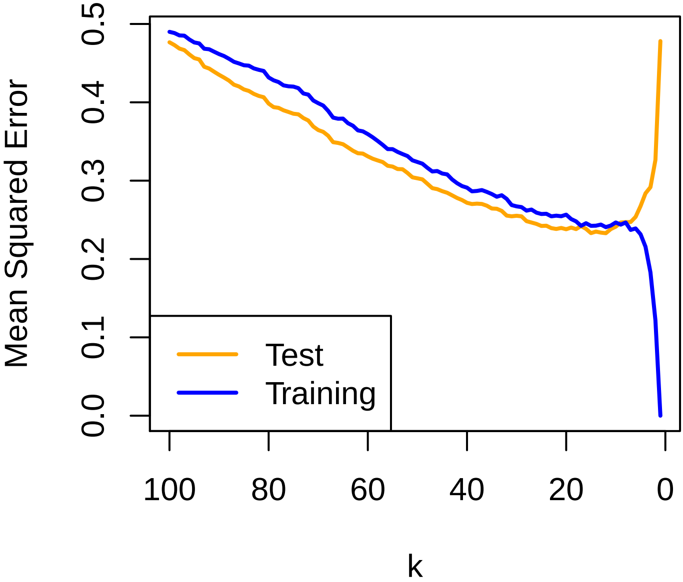


Overfitting via *k*-nearest neighbors



MSE decomposition

Given $Y = f(X) + \epsilon$, where $E(\epsilon) = 0$ and $Var(\epsilon) = \sigma^2$, consider a predictor $\widehat{f}$

Expected MSE for predicting new Y at $X = x$ decomposes as:

$$E[(Y - \widehat{f}(x))^2] = Var(\widehat{f}(x)) + [Bias(\widehat{f}(x))]^2 + \sigma^2$$

Bias-variance tradeoff

Interpretation:

- *Var*$(\widehat{f})$ is the amount of variability in our predictor with respect to the training data.
- *Bias*$(\widehat{f})$ is the systematic error introduced by model approximation.
- σ^2 is *irreducible error*, inherent in the error term ϵ.

Bias-variance tradeoff

Interpretation:

- $Var(\widehat{f})$ is the amount of variability in our predictor with respect to the training data. Increases with increasing model flexibility.
- $Bias(\widehat{f})$ is the systematic error introduced by model approximation. Decreases with increasing model flexibility.
- σ^2 is *irreducible error*, inherent in the error term ϵ. Cannot get rid of this!

If we have a family of flexible regression methods, we should try to balance squared bias and variance.

Summary from today

- Least squares coefficients correspond to minimum of a quadratic surface
- Confidence intervals computed using standard errors of coefficients
- R^2 is a scale-invariant accuracy measure — proportion of variance in Y explained by the model
- Multiple linear regression (many predictors) estimated by solving a linear system — normal equations

Readings in ISL

- Chapter 2 (mostly last lecture)
- Chapter 3 (today and Thursday)

Messing around with R

- R excerpts from slides
- Markdown and R Markdown
- knitr in a knutshell
(`http://kbroman.org/knitr_knutshell/`)