Linear Regression Models
P8111

Lecture 08

Jeff Goldsmith
February 16, 2016

THE DEPARTMENT OF BIOSTATISTICS
Columbia University
MAILMAN SCHOOL
OF PUBLIC HEALTH

Today's Lecture

- LSE properties
- Identifiability in MLR
- Collinearity and near-collinearity
- MLR Example

Key points so far

$y_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip} + \epsilon_i$ ✓

- Our model is $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ with $\epsilon \sim (0, \sigma^2 \boldsymbol{I})$
- The design matrix $\boldsymbol{X}$ contains the terms included in the model
- We've derived least squares solutions under some conditions

$\hat{\beta}_{LSE} = (X^T X)^{-1} X^T y$ ✓✓✓

Mean, variance and covariance of a random vector

- Let $\boldsymbol{y}^T = [y_1, \ldots, y_n]$ be an n-component random vector. Then its mean and variance are defined as

$$
\begin{aligned}
E(\boldsymbol{y})^T &= [E(y_1), \ldots, E(y_n)] \\
Var(\boldsymbol{y}) &= E\left[(\boldsymbol{y} - E\boldsymbol{y})(\boldsymbol{y} - E\boldsymbol{y})^T\right] = E(\boldsymbol{y}\boldsymbol{y}^T) - (E\boldsymbol{y})(E\boldsymbol{y})^T
\end{aligned}
$$

- Let $\boldsymbol{y}$ and $\boldsymbol{z}$ be an n-component and an m-component random vector respectively. Then their covariance is an $n \times m$ matrix defined by

$$Cov(\boldsymbol{y}, \boldsymbol{z}) = E\left[(\boldsymbol{y} - E\boldsymbol{y})(\boldsymbol{z} - \boldsymbol{z})^T\right]$$

Basics on random vectors

Let $\boldsymbol{A}$ be a $t \times n$ non-random matrix and $\boldsymbol{B}$ be a $p \times m$ non-random matrix. Then

$$
\begin{aligned}
E(\boldsymbol{A}\boldsymbol{y}) &= \boldsymbol{A}E\boldsymbol{y} \\
Var(\boldsymbol{A}\boldsymbol{y}) &= \boldsymbol{A}Var(\boldsymbol{y})\boldsymbol{A}^T \\
Cov(\boldsymbol{A}\boldsymbol{y}, \boldsymbol{B}\boldsymbol{z}) &= \boldsymbol{A}Cov(\boldsymbol{y}, \boldsymbol{z})\boldsymbol{B}^T
\end{aligned}
$$

Unbiasedness of LSEs

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

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

$$y \sim (X\beta, \sigma^2 I)$$

$$E(\hat{\beta}) =$$

$$E\left(\underbrace{(X^T X)^{-1} X^T}\, y\right)$$

$$= (X^T X)^{-1} X^T E(y)$$

$$= \cancel{(X^T X)^{-1} X^T X}\, \beta$$

$$= \beta$$

Variance of LSEs

$Var(\hat{\beta}) =$

$Var\left((X^T X)^{-1} X^T y \right)$

$= (X^T X)^{-1} X^T \underbrace{Var(y)}_{\sigma^2 I} X (X^T X)^{-1}$

$= \sigma^2 (X^T X)^{-1} \cancel{(X^T X)(X^T X)^{-1}}$

$= \sigma^2 (X^T X)^{-1}$

$$\sigma^2 \begin{bmatrix} \square & & & \\ & \square & & \\ & & \ddots & \\ \bullet & & & \square \end{bmatrix}$$

$Cov(\beta_0, \beta_4)$

$\widehat{Var}(\hat{\beta}) = \hat{\sigma}^2 (X^T X)^{-1}$

$Var(c\hat{\beta}) =$

$c \, Var(\hat{\beta}) \, c^T$

$\sigma^2 c (X^T X)^{-1} c^T$

$\underbrace{\begin{bmatrix} 1 & x_{i1} & x_{i2} & x_{i3} \end{bmatrix}}_{\text{"}c\text{"}} \begin{pmatrix} \\ \\ \end{pmatrix} = \hat{y}_i$

Sampling distribution of $\hat{\boldsymbol{\beta}}$

$\hat{\beta} \sim (\beta, \sigma^2 (X^T X)^{-1})$

If our usual assumptions are satisfied and $\epsilon \sim \mathrm{N}\left[0, \sigma^2 I\right]$ then

$$\hat{\boldsymbol{\beta}} \sim \mathrm{N}\left[\boldsymbol{\beta}, \sigma^2 (\boldsymbol{X}^T \boldsymbol{X})^{-1}\right].$$

$y \sim N(X\beta, \sigma^2 I)$

- This will be used later for inference.
- Even without Normal errors, asymptotic Normality of LSEs is possible under reasonable assumptions.

Definitions

"Hat matrix"

- *Fitted values*: $\hat{\boldsymbol{y}} = \boldsymbol{X}\hat{\boldsymbol{\beta}} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{H}\boldsymbol{y}$
- *Residuals / estimated errors*: $\hat{\boldsymbol{\epsilon}} = \boldsymbol{y} - \hat{\boldsymbol{y}}$
- *Residual sum of squares*: $\sum_{i=1}^{n} \hat{\epsilon}_i^2 = \hat{\boldsymbol{\epsilon}}^T\hat{\boldsymbol{\epsilon}}$
- *Residual variance*: $\hat{\sigma}^2 = \frac{RSS}{n-p-1}$
- *Degrees of freedom*: $n - p - 1$

$y_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip} + \epsilon_i$

pred other than intercept

R^2 and sums of squares

- Regression sum of squares $SS_{reg} = \sum(\hat{y}_i - \bar{y})^2$
- Residual sum of squares $SS_{res} = \sum(y_i - \hat{y}_i)^2$
- Total sum of squares $SS_{tot} = \sum(y_i - \bar{y})^2$
- Coefficient of determination

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2} = \frac{\sum(\hat{y}_i - \bar{y})^2}{\sum(y_i - \bar{y})^2}$$

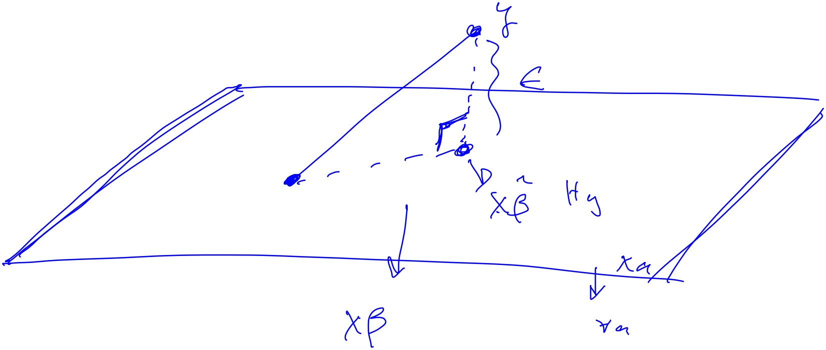
Hat matrix

Some properties of the hat matrix:

- It is a projection matrix: $\boldsymbol{H}\boldsymbol{H} = \boldsymbol{H}$
- It is symmetric: $\boldsymbol{H}^T = \boldsymbol{H}$
- The residuals are $\hat{\epsilon} = (\boldsymbol{I} - \boldsymbol{H})\boldsymbol{y}$ $y - Hy = y - \hat{y}$
- The inner product of $(\boldsymbol{I} - \boldsymbol{H})\boldsymbol{y}$ and $\boldsymbol{H}\boldsymbol{y}$ is zero (predicted values and residuals are uncorrelated).

Projection space interpretation

The hat matrix projects $\boldsymbol{y}$ onto the column space of $\boldsymbol{X}$. Alternatively, minimizing the $RSS(\boldsymbol{\beta})$ is equivalent to minimizing the Euclidean distance between $\boldsymbol{y}$ and the column space of $\boldsymbol{X}$.



MLR Example: Moneyball

- "Moneyball" used statistics to help identify key player features that contributed to winning baseball games
- We'll look at association between runs scored and team-level covariates
- First, load the data in R workspace and understand the variables:

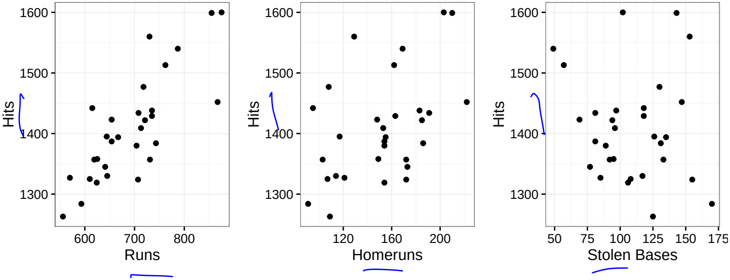
MLR Example: Moneyball

```
> setwd("~/Desktop")
> download.file("http://www.openintro.org/stat/data/mlb11.RData", destfile = "mlb11.RData")
> load("mlb11.RData")
>
> mlb11 %>% tbl_df
Source: local data frame [30 x 12]

                    team  runs at_bats  hits homeruns bat_avg strikeouts stolen_bases  wins new_
                  (fctr) (int)   (int) (int)    (int)   (dbl)      (int)        (int) (int)
1          Texas Rangers   855    5659  1599      210   0.283        930          143    96
2         Boston Red Sox   875    5710  1600      203   0.280       1108          102    90
3         Detroit Tigers   787    5563  1540      169   0.277       1143           49    95
4     Kansas City Royals   730    5672  1560      129   0.275       1006          153    71
5    St. Louis Cardinals   762    5532  1513      162   0.273        978           57    90
6          New York Mets   718    5600  1477      108   0.264       1085          130    77
7      New York Yankees    867    5518  1452      222   0.263       1138          147    97
8      Milwaukee Brewers   721    5447  1422      185   0.261       1083           94    96
9       Colorado Rockies   735    5544  1429      163   0.258       1201          118    73
10        Houston Astros   615    5598  1442       95   0.258       1164          118    56
..                   ...   ...     ...   ...      ...     ...        ...          ...   ...
Variables not shown: new_slug (dbl), new_obs (dbl)
```

y

Exploratory plots



MLB data

- team
- runs
- at_bats
- hits
- homeruns
- bat_avg
- strikeouts
- wins
- new_onbase
- new_slug
- new_obs

Multiple Linear Regression

```
> linmod = lm(runs ~ at_bats + hits + homeruns + stolen_bases, data = mlb11)
> tidy(linmod)
          term    estimate   std.error statistic      p.value
1  (Intercept) 581.2109940 526.4062575  1.104111 2.800591e-01
2      at_bats  -0.2023278   0.1173616 -1.723970 9.705991e-02
3         hits   0.6974143   0.1131428  6.164017 1.911117e-06
4     homeruns   1.2535062   0.1593185  7.867926 3.178626e-08
5 stolen_bases   0.5229741   0.1686315  3.101284 4.727771e-03
```

R does what we expect

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

```
> X = cbind(1, mlb11$at_bats, mlb11$hits, mlb11$homeruns, mlb11$stolen_bases)
> y = (mlb11$runs)
>
> betaHat = solve(t(X) %*% X) %*% t(X) %*% y
> betaHat
              [,1]
[1,] 581.2109940
[2,]  -0.2023278
[3,]   0.6974143
[4,]   1.2535062
[5,]   0.5229741
```

$(X^T \quad X)^{-1} \quad X^T \quad y$

$\hat{\beta}$

R does what we expect

```
> fitted = X %*% betaHat
> sigmaHat = sqrt(t(y - fitted) %*% (y - fitted) / (30-4-1))
> sigmaHat
         [,1]
[1,] 26.84777
```

RSS / (n - p - 1)

R does what we expect

$\hat{\text{var}}(\hat\beta) = \hat\sigma^2 (X^T X)^{-1}$

$\hat{\text{var}}(\hat\beta_2)$

```
> VarBeta = as.numeric(sigmaHat^2) * (solve(t(X) %*% X))
> VarBeta
              [,1]          [,2]          [,3]          [,4]          [,5]
[1,] 277103.547951 -6.092180e+01 42.6907437568 -1.1735722100 -5.003475e+00
[2,]    -60.921800  1.377374e-02 -0.0108596986  0.0008804808  8.390983e-05
[3,]     42.690744 -1.085970e-02  0.0128013011 -0.0054905039  8.247119e-04
[4,]     -1.173572  8.804808e-04 -0.0054905039  0.0253823891  1.779074e-03
[5,]     -5.003475  8.390983e-05  0.0008247119  0.0017790736  2.843658e-02
> sqrt(diag(VarBeta))
[1] 526.4062575   0.1173616   0.1131428   0.1593185   0.1686315
```

Least squares estimates

$$\boxed{(X^T X)\,\beta = X^T y}$$

- $\hat{\boldsymbol{\beta}} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}$
- A condition on $\left(\boldsymbol{X}^T\boldsymbol{X}\right)$:

invertible!!

- If $\left(\boldsymbol{X}^T\boldsymbol{X}\right)$ is singular, there are infinitely many least squares solutions, making $\hat{\boldsymbol{\beta}}$ non-identifiable (can't choose between different solutions)

Non-identifiability

- Can happen if $\boldsymbol{X}$ is not of full rank, i.e. the columns of $\boldsymbol{X}$ are linearly dependent (for example, including weight in Kg and lb as predictors)
- Can happen if there are fewer data points than terms in $\boldsymbol{X}$: $n < p$ (having 100 predictors and only 50 observations)

- Generally, the $p \times p$ matrix $\left(\boldsymbol{X}^T\boldsymbol{X}\right)$ is invertible if and only if it has rank p.

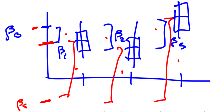
Infinite solutions

Suppose I fit a model $y_i = \beta_0 + \beta_1 x_{i1} + \epsilon_i$.

- I have estimates $\hat{\beta}_0 = 1, \hat{\beta}_1 = 2$
- I put in a new variable $x_2 = x_1$
- My new model is $y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i$
- Possible least squares estimates that are equivalent to my first model:
  - $\hat{\beta}_0 = 1, \hat{\beta}_1 = 2, \hat{\beta}_2 = 0$
  - $\hat{\beta}_0 = 1, \hat{\beta}_1 = 0, \hat{\beta}_2 = 2$
  - $\hat{\beta}_0 = 1, \hat{\beta}_1 = 1002, \hat{\beta}_2 = -1000$
  - $\ldots$

Non-identifiablity

$$y_i = \beta_0 + \beta_1 g_{R1} + \beta_2 g_{RP2} + \beta_3 g_{RP3} + \epsilon_i$$



- Often due to data coding errors (variable duplication, scale changes)
- Pretty easy to detect and resolve
- Certain kinds can be addressed using *penalties* (later topic)
- A bigger problem is near-unidentifiability (collinearity)

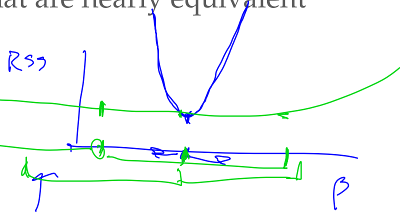
Causes of collinearity

- Arises when variables are highly correlated, but not exact duplicates
- Commonly arises in data (perfect correlation is usually there by mistake)
- Might exist between several variables, i.e. a linear combination of several variables exists in the data
- A variety of tools exist (correlation analyses, multiple R^2, eigen decompositions)

Effects of collinearity

Suppose I fit a model $y_i = \beta_0 + \beta_1 x_{i1} + \epsilon_i$.

- I have estimates $\hat{\beta}_0 = 1, \hat{\beta}_1 = 2$
- I put in a new variable $x_2 = x_1 + \mathit{error}$, where *error* is pretty small
- My new model is $y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i$
- Possible least squares estimates that are nearly equivalent to my first model:
  - $\hat{\beta}_0 = 1, \hat{\beta}_1 = 2, \hat{\beta}_2 = 0$
  - $\hat{\beta}_0 = 1, \hat{\beta}_1 = 0, \hat{\beta}_2 = 2$
  - $\hat{\beta}_0 = 1, \hat{\beta}_1 = 1002, \hat{\beta}_2 = -1000$
  - ...



- A unique solution exists, but it is hard to find

Effects of collinearity

- Collinearity results in a “flat” RSS
- Makes identifying a unique solution difficult
- Dramatically inflates the variance of LSEs

Example: mother and daughter heights

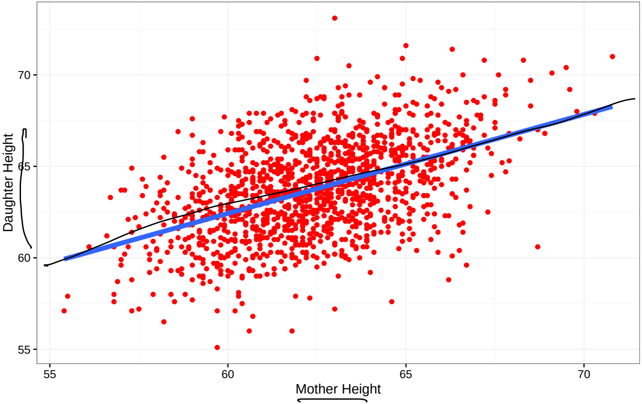
- 1375 mother/daughter pairs (see Lecture 1)
- Want to predict daughter height based on mother height
- Data originally comes in inches

Example: mother and daughter heights

Simple linear regression analysis

```
> linmod = lm(Dheight~Mheight, data = heights)
> tidy(linmod)
         term  estimate  std.error statistic      p.value
1 (Intercept) 29.917437 1.62246940  18.43945 5.211879e-68
2     Mheight  0.541747 0.02596069  20.86797 3.216915e-84
```

Example: mother and daughter heights

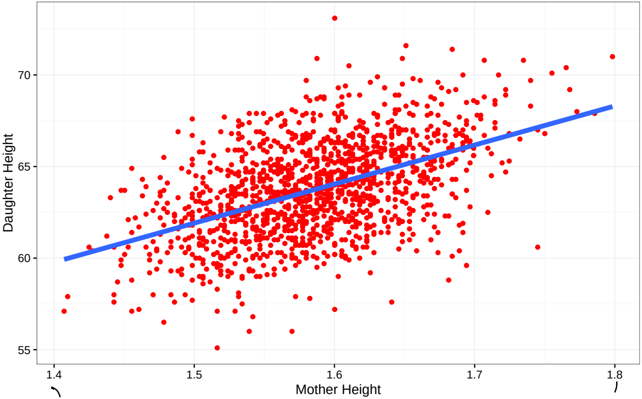


Example: change of variables

What happens if mother's height is expressed in meters?

```
> heights = mutate(heights, Mheight_m = Mheight * .0254)
>
> linmod = lm(Dheight~Mheight_m, data = heights)
> tidy(linmod)
         term estimate std.error statistic      p.value
1 (Intercept) 29.91744  1.622469  18.43945 5.211879e-68
2   Mheight_m 21.32862  1.022074  20.86797 3.216915e-84
```

Example: change in variables



Example: non-identifiability

What if we include mother's height in both inches and meters?

```
> linmod.col = lm(Dheight ~ Mheight + Mheight_m, data = heights)
> summary(linmod.col)

Call:
lm(formula = Dheight ~ Mheight + Mheight_m, data = heights)

Residuals:
   Min     1Q Median     3Q    Max 
-7.397 -1.529  0.036  1.492  9.053 

Coefficients: (1 not defined because of singularities)
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 29.91744    1.62247   18.44   <2e-16 ***
Mheight      0.54175    0.02596   20.87   <2e-16 ***
Mheight_m         NA         NA      NA       NA    
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 2.266 on 1373 degrees of freedom
Multiple R-squared:  0.2408,Adjusted R-squared:  0.2402 
F-statistic: 435.5 on 1 and 1373 DF,  p-value: < 2.2e-16
```

Example: non-identifiability

What if we include mother's height in both inches and meters?

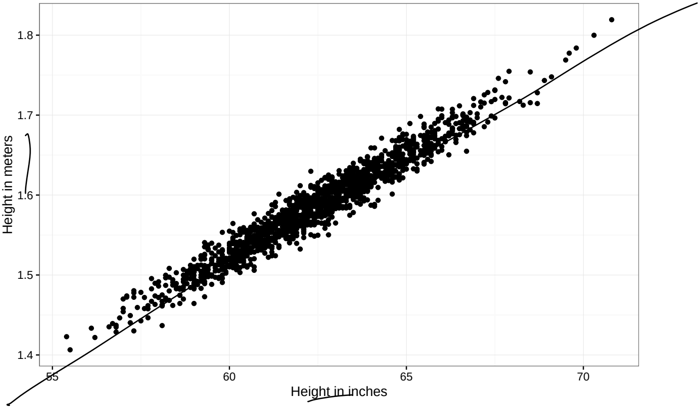
```
> X = as.matrix(cbind(1, select(heights, Mheight, Mheight_m)))
> solve(t(X) %*% X)
Error in solve.default(t(X) %*% X) :
  system is computationally singular: reciprocal condition number = 6.681e-18
```

Example: near-unidentifiability

Suppose height was measured twice: once in inches, once in meters. There's some measurement error comparing the two. What happens now?

```
> heights = mutate(heights, Mheight_m = Mheight_m + rnorm(1375, mean = 0, sd = .01))
> summarize(heights, cor = cor(Mheight, Mheight_m))
        cor
1 0.9716345
>
> X = as.matrix(cbind(1, select(heights, Mheight, Mheight_m)))
> solve(t(X) %*% X)
                      1      Mheight   Mheight_m
1           0.512809433 -0.007399262 -0.03150439
Mheight    -0.007399262  0.002346264 -0.08770449
Mheight_m  -0.031504393 -0.087704488  3.47264911
```

Example: near-unidentifiability



Example: near-unidentifiability

What if we include mother′s height in both inches and meters?

```
> linmod.me = lm(Dheight ~ Mheight + Mheight_m, data = heights)
> tidy(linmod.me)
         term   estimate std.error statistic      p.value
1 (Intercept) 29.9594863  1.622801 18.461592 3.796458e-68
2     Mheight  0.6588078  0.109768  6.001822 2.493306e-09
3   Mheight_m -4.6350101  4.222967 -1.097572 2.725840e-01
```

Some take away messages

- Collinearity can (and does) happen, so be careful
- Worst cases tend to be “pathological examples”, so don’t lose hope
- Often contributes to the problem of variable selection, which we’ll touch on later

Categorical predictor design matrix

Which of the following is a “correct” design matrix for a categorical predictor with 3 levels?

$$
X_1 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 1 \end{bmatrix}
\quad \text{or} \quad
X_2 = \begin{bmatrix} 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \end{bmatrix}
\quad \text{or} \quad
X_3 = \begin{array}{c} \begin{array}{ccc} \mu_{g_1} & \mu_{g_2} & \mu_{g_3} \end{array} \\ \begin{bmatrix} 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 1 \end{bmatrix} \end{array}
$$

Today's big ideas

- Identifiability, collinearity, categorical predictors

- Suggested reading: Faraway Ch 3.7 (pdf); ISLR 3.3.1