Linear Regression Models
P8111

Lecture 07

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February 11, 2016

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OF PUBLIC HEALTH

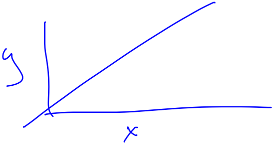
Today's lecture

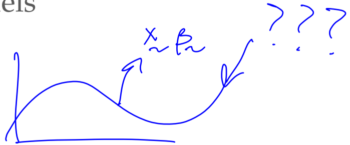
- Multiple Linear Regression
  - "Non-linear" models
  - MLR Estimation
  - LSE Properties

Non-linear relationships

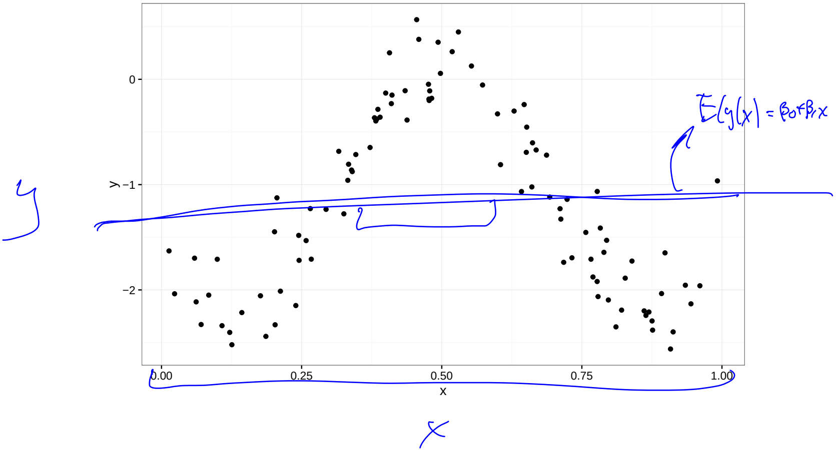
What do we mean by "linear models"? $\begin{bmatrix} 1 & x_1 & x_2 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$

- Linearity in the coeffcients
- Conditional expectations are a linear combination of scalar values and regression coefficients
  - $E(y|\boldsymbol{x}) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$ is linear; $E(y|\boldsymbol{x}) = \beta_0 + x_1^{\beta_1} + \log(\beta_2) x_2$ is not
- A non-linear relationship between y and x can still be addressed using linear models





Non-linear relationships



Non-linear relationships

Some ways to address this sort of thing

- Polynomials ✓
- Piece-wise linear models ✓
- Splines ✓

Polynomial models

$y_i = \underset{\sim}{x_i} \underset{\sim}{\beta} + \epsilon_i$

- Model of the form

$$\underline{y_i} = \underline{\beta_0} + \underline{\beta_1 x_i} + \underline{\beta_2 x_i^2} + \underline{\ldots} + \underline{\beta_p x_i^p} + \epsilon_i;\ \epsilon_i \overset{iid}{\sim} (0, \sigma^2)$$

- p is the polynomial order
- More polynomial terms can lead to a better approximation of $E(y|x)$, but also higher variability in the fit
- Conversely, smaller p can lead to inability to capture $E(y|x)$, but is often more stable
- Quadratic fits are pretty okay. I don't trust cubic and beyond.

Polynomial models

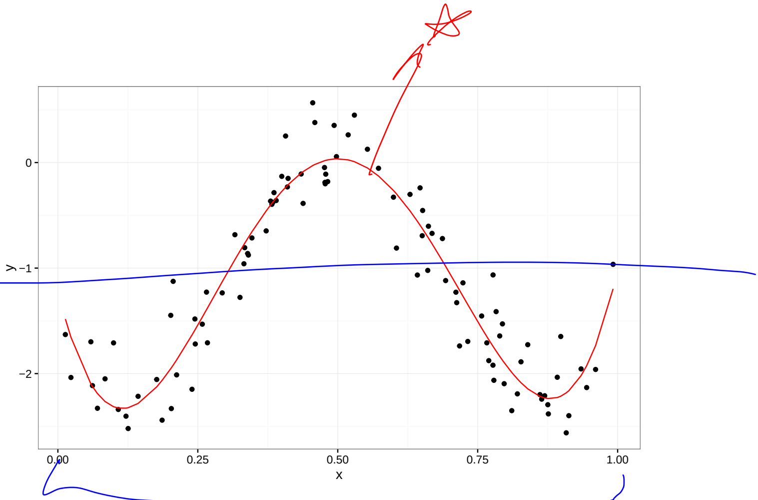
$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \beta_4 x_i^4 + \epsilon_i$

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

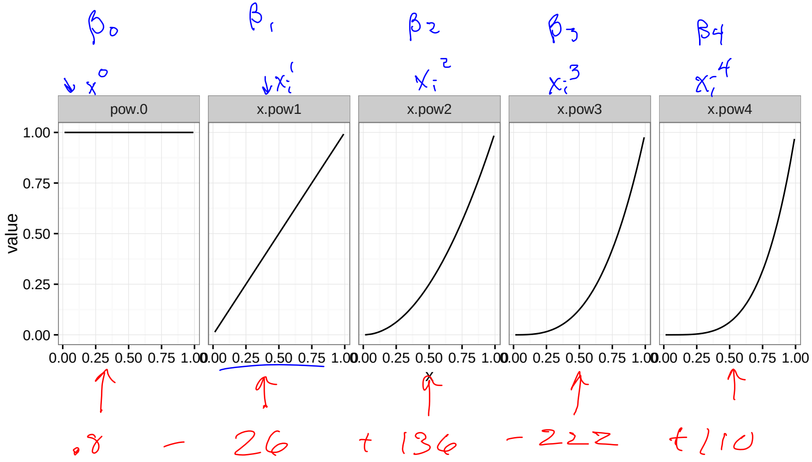
$$\begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 & x_1^4 \\ 1 & x_2 & & & \\ 1 & x_3 & & & \\ \vdots & \vdots & & & \\ 1 & x_n & x_n^2 & x_n^3 & x_n^4 \end{bmatrix}$$

```
> data.nonlin = mutate(data.nonlin,
+                      x.pow2 = x^2, x.pow3 = x^3, x.pow4 = x^4)
>
> quartfit = lm(y ~ x + x.pow2 + x.pow3 + x.pow4, data = data.nonlin)
> tidy(quartfit)
         term     estimate  std.error  statistic      p.value
1 (Intercept)   -0.8288032  0.2743086  -3.021426 3.232778e-03
2           x  -24.8618532  3.2948666  -7.545633 2.696508e-11
3      x.pow2  136.8666639 11.9951053  11.410209 1.671996e-19
4      x.pow3 -222.8346094 16.6191581 -13.408297 1.234857e-23
5      x.pow4  110.5772065  7.7358391  14.294145 2.079862e-25
```

Polynomial models



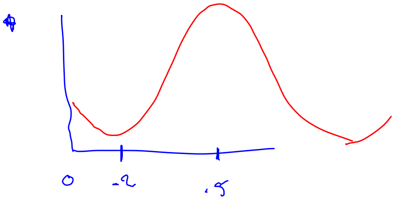
Polynomial models



Polynomial models

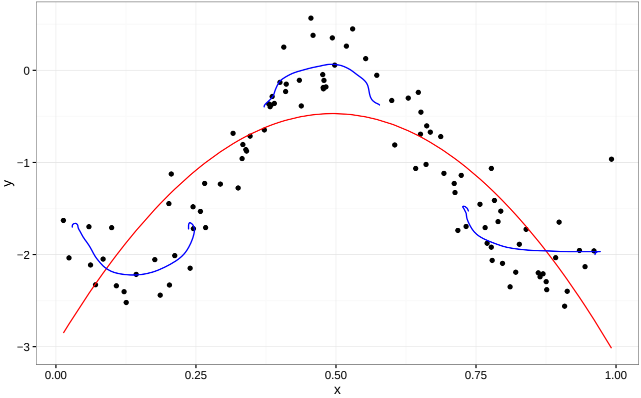
- Interpretation of β_1:

"Keeping everything else fixed" ??



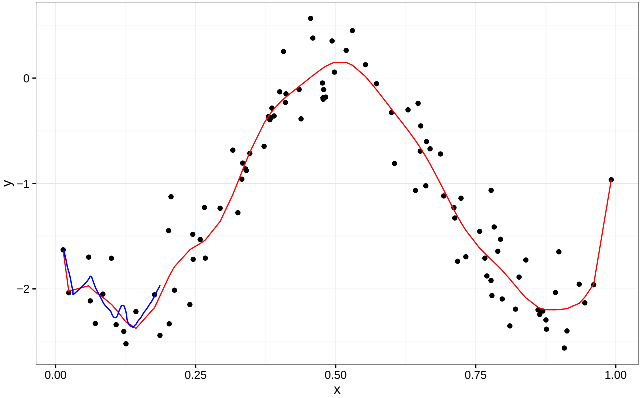
Not enough polynomial terms

$\beta_0 + \beta_1 x_i + \beta_2 x_i^2$

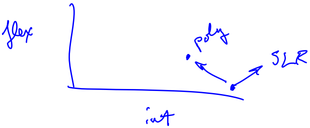


Too many polynomial terms

$\beta_0 + \beta_1 x_i + \ldots + \beta_{20} x_i^{20}$



Final thoughts on polynomial models

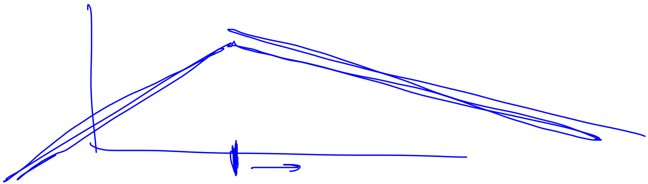


- Always include lower-order terms with higher-order terms
- You have to choose p, which isn't always easy
- Interpretation can be hard
- Raising continuous predictors for powers can lead to very large entries in your design matrix
- x is almost always correlated with x^2.

Piecewise linear models

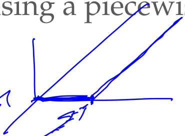
A piecewise linear model (also called a change point model or broken stick model) contains a few linear components

- Outcome is linear over full domain, but with a different slope at different points
- Points where relationship changes are referred to as "change points" or "knots"
- Often there's one (or a few) potential change points



Piecewise linear models

Suppose we want to estimate $E(y|x) = f(x)$ using a piecewise linear model.



- For one knot we can write this as

$$E(y|x) = \beta_0 + \beta_1 x + \beta_2 (x - \kappa)_+$$

where κ is the location of the change point

Interpretation of regression coefficients

$y_i = \beta_0 + \beta_1 x_i + \beta_2 (x_i - k)_+ + \epsilon_i$

$x < k$

$$E(y|x+1) - E(y|x)$$
$$= \beta_0 + \beta_1(x+1) - \beta_0 - \beta_1 x$$
$$= \cancel{\beta_0 - \beta_0} + \cancel{\beta_1 x - \beta_1 x} + \underbrace{\beta_1}$$

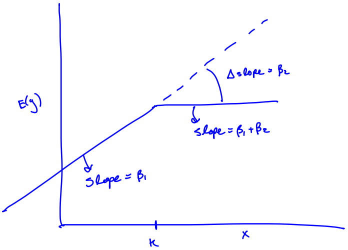
$\beta_1 = E\Delta y$ for a 1 unit Δx, $x < k$

$x > k$

$$E(y|x+1) - E(y|x)$$
$$= \beta_0 + \beta_1(x+1) + \beta_2(x+1-k) - \beta_0 - \beta_1 x - \beta_2(x-k)$$
$$= \cancel{\beta_0 - \beta_0} + \cancel{\beta_1 x - \beta_1 x} + \underbrace{\beta_1} + \cancel{\beta_2 x - \beta_2 x} + \cancel{\beta_2 k - \beta_2 k} + \underbrace{\beta_2}$$

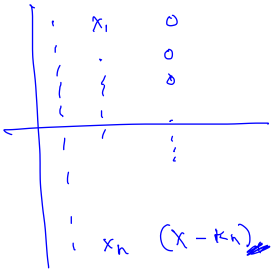
$\beta_1 + \beta_2 = E\Delta y$ for a 1 unit Δx, $x > k$

β_2 = change in slope, comparing $x > k$ to $x < k$



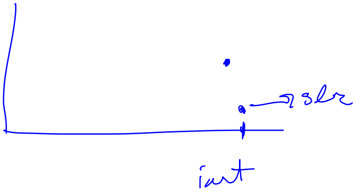
Estimation

- Piecewise linear models are low-dimensional ~~(no need for penalization)~~
- Parameters are estimated via OLS
- The design matrix is ...



$X > k$

flex



Multiple knots

Suppose we want to estimate $\mathrm{E}(y|x) = f(x)$ using a piecewise linear model.

- For multiple knots we can write this as

$$\mathrm{E}(y|x) = \beta_0 + \beta_1 x + \sum_{k=1}^{K} \beta_{k+1}(x - \kappa_k)_+$$

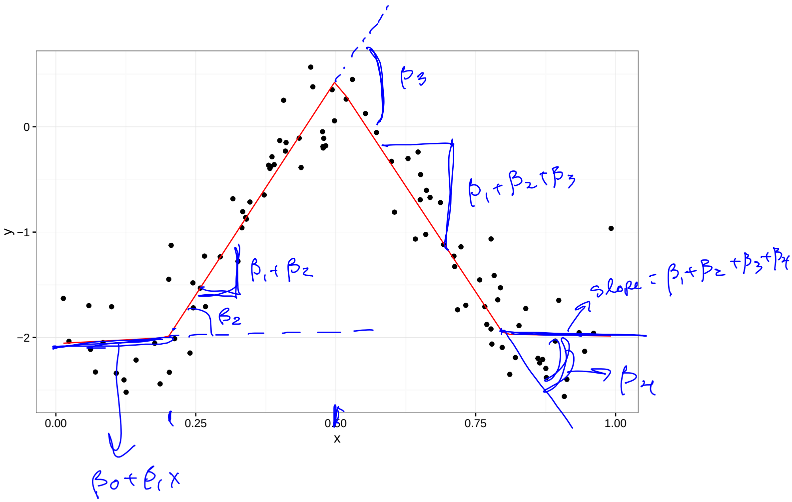
  where $\{\kappa_k\}_{k=1}^{K}$ are the locations of the change points
- Note that knot locations are defined before estimating regression coefficients
- Also, regression coefficients are interpreted conditional on the knots.

Example

$(X - .2)_+$

```
> data.nonlin = mutate(data.nonlin,
+                      spline_2 = (x - .2) * (x >= .2),
+                      spline_5 = (x - .5) * (x >= .5),
+                      spline_8 = (x - .8) * (x >= .8))
>
> piecewise.fit = lm(y ~ x + spline_2 + spline_5 + spline_8, data = data.nonlin)
> tidy(piecewise.fit)
         term   estimate std.error  statistic      p.value
1 (Intercept)  -2.266553 0.2098863 -10.798953 3.280465e-18
2           x   1.655019 1.3456918   1.229865 2.217847e-01
3    spline_2   6.071173 1.6974614   3.576619 5.497482e-04
4    spline_5 -15.917475 0.8574252 -18.564273 2.283994e-33
5    spline_8  10.891211 1.1754422   9.265629 6.136562e-15
```

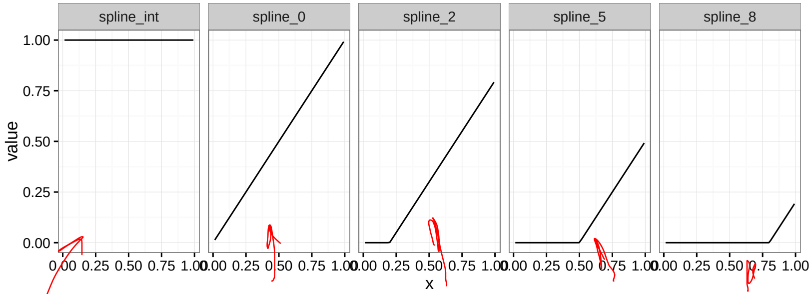
Example



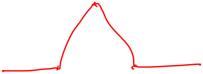
0
−1
−2
y
0.00
0.25
0.50
0.75
1.00
x
β_3
$\beta_1+\beta_2+\beta_3$
$\beta_1+\beta_2$
β_2
slope $=\beta_1+\beta_2+\beta_3+\beta_4$
β_4
$\beta_0+\beta_1 x$

Example

1 $\quad x \quad (x-.2)_+ \quad (x-.4)_+ \quad (x-.8)_+$



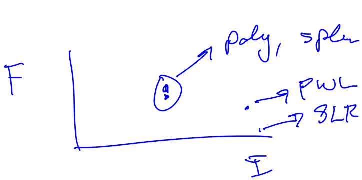
$-2 + 1 + 6 - 15 + 10$

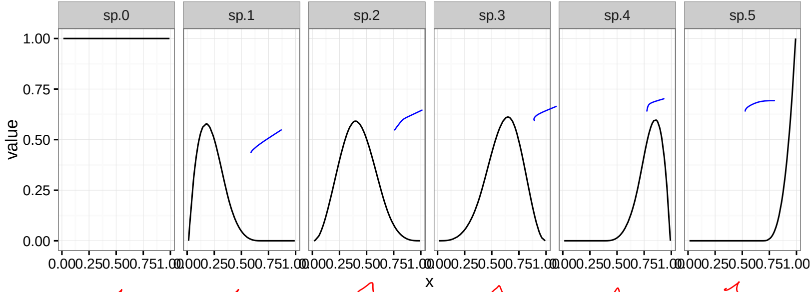


Final thoughts on piecewise linear models

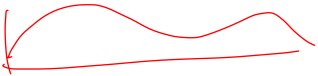
- Just like you can have too many polynomial terms, you can have too many knots
- You also have to choose where the knots go
- Interpretation is more straightforward than for polynomial models
- Can also have piecewise quadratic, piecewise cubic ...

Spline models





$$\hat{\beta}_0 + \hat{\beta}_1 + \hat{\beta}_2 + \hat{\beta}_3 + \hat{\beta}_4 + \hat{\beta}_5$$



Spline models

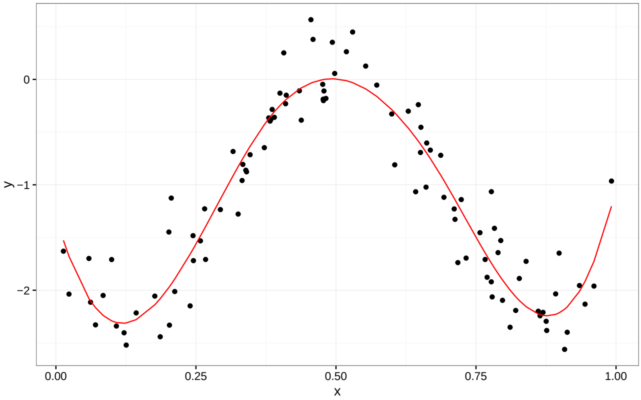
bs(x)

b

```
> data.nonlin = data.nonlin %>% bind_cols(., data.frame(ns(.[['x']], df = 5))) %>%
+   rename(sp.1 = X1, sp.2 = X2, sp.3 = X3, sp.4 = X4, sp.5 = X5)
>
> bspline.fit = lm(y ~ sp.1 + sp.2 + sp.3 + sp.4 + sp.5, data = data.nonlin)
> tidy(bspline.fit)
         term   estimate std.error  statistic      p.value
1 (Intercept) -1.9529246 0.1420332 -13.749775 3.152280e-24
2        sp.1  2.5173253 0.1629991  15.443796 1.573047e-27
3        sp.2  1.9125629 0.2212551   8.644151 1.398240e-13
4        sp.3 -0.3654431 0.1575141  -2.320066 2.250136e-02
5        sp.4 -0.4146350 0.3533596  -1.173408 2.435969e-01
6        sp.5  0.4320127 0.1742734   2.478937 1.495979e-02
```

β

Spline models



Final thoughts on spline models

- Splines are constructed as numerically-stable versions of piecewise polynomials
- Cubic B-splines are popular (default of `splines::bs()`)
- Still have to choose ~~knot location~~ and number of knots
- Interpretation is roughly equivalent to that of polynomials

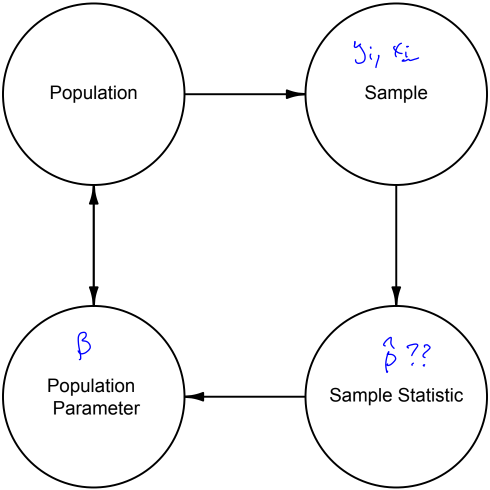
Bringing it all together

- MLR covers a lot of stuff
- Models can be easy or very complex
- All depends on your design matrix ...

SLR
Cat
inter a
Var

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

Circle of Life



Multiple linear regression

- Let

$$\boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \quad \boldsymbol{X} = \begin{bmatrix} 1 & x_{11} & \dots & x_{1p} \\ \vdots & \vdots & x_{ij} & \vdots \\ 1 & x_{n1} & \dots & x_{np} \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \vdots \\ \beta_p \end{bmatrix}, \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

- Then we can write the model in a more compact form:

$$\boldsymbol{y}_{n\times 1} = \boldsymbol{X}_{n\times(p+1)}\boldsymbol{\beta}_{(p+1)\times 1} + \boldsymbol{\epsilon}_{n\times 1}$$

- $\boldsymbol{X}$ is called the *design matrix*

$y = X\beta + \epsilon$

Matrix notation

$$\boldsymbol{y} = \boldsymbol{X\beta} + \boldsymbol{\epsilon}$$

- ϵ is a random vector rather than a random variable
- $E(\boldsymbol{\epsilon}) = 0$ and $Var(\boldsymbol{\epsilon}) = \sigma^2 I$
- Note that *Var* is potentially confusing; in the present context it means the "variance-covariance matrix"

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

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

Vector differentiation

- For two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ and a matrix $\boldsymbol{C}$, the following rules hold:
  - $\frac{d}{d\boldsymbol{a}}(\boldsymbol{a}^T\boldsymbol{b}) = \boldsymbol{b}$
  - $\frac{d}{d\boldsymbol{a}}(\boldsymbol{a}^T\boldsymbol{C}\boldsymbol{a}) = (\boldsymbol{C} + \boldsymbol{C}^T)\boldsymbol{a}$
  - In the special case when the matrix $\boldsymbol{C}$ is symmetric (i.e. $\boldsymbol{C} = \boldsymbol{C}^T$), we have $\frac{d}{d\boldsymbol{a}}(\boldsymbol{a}^T\boldsymbol{C}\boldsymbol{a}) = 2\boldsymbol{C}\boldsymbol{a}$

Least squares

As in simple linear regression, we want to find the $\boldsymbol{\beta}$ that minimizes the residual sum of squares.

$RSS(\boldsymbol{\beta}) = \sum_i \epsilon_i^2 = \begin{bmatrix} \epsilon_1 & \epsilon_2 & \epsilon_3 & \dots & \epsilon_n \end{bmatrix} \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$

$\epsilon^T \epsilon$

$\uparrow$

$(y - X\beta)^T (y - X\beta)$

Least squares

$$\frac{\partial\, RSS(\beta)}{\partial \beta} = \Bigg\|$$

$$(y - X\beta)^T (y - X\beta) =$$

$$(y^T - \beta^T X^T)(y - X\beta)$$

$$\beta^T X^T X \beta - \beta^T X^T y - y^T X \beta + y^T y$$

$$\underbrace{\left(\beta^T X^T X \beta - 2\beta^T X^T y + y^T y \right)}_{RSS(\beta)}$$

$$\underbrace{(X^T X + (X^T X)^T)}\beta - 2X^T y$$

$$2X^T X \beta - 2X^T y = 0$$

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

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

Unbiasedness of LSEs

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

Variance of LSEs

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

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

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

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

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

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

Definitions

- *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*: $n - p - 1$

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 $\hat{\epsilon} = (\boldsymbol{I} - \boldsymbol{H})\boldsymbol{y}$
- 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 $\boldsymbol{X}$.

Today's big ideas

- Non-linear models; least squares estimates and properties; definitions, hat matrix and vector space interpretation

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- Suggested reading: Faraway Ch 2.2 - 2.7; ISLR 3.2