

Linear Regression Models

P8111

Lecture 07

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BIostatISTICS



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**MAILMAN SCHOOL
OF PUBLIC HEALTH**

Today's lecture

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

Non-linear relationships

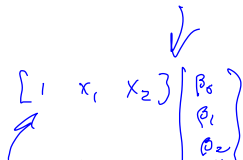
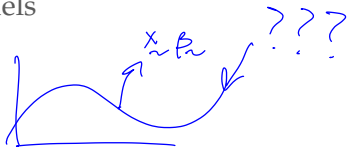
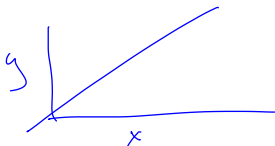
What do we mean by “linear models”?

- Linearity in the coefficients
- Conditional expectations are a linear combination of scalar values and regression coefficients

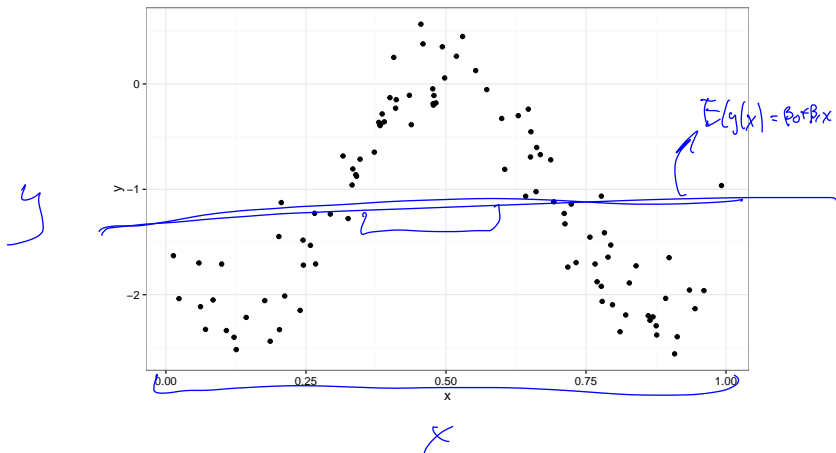
▶ $E(y|x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$ is linear;

$E(y|x) = \beta_0 + x_1^{\beta_1} + \log(\beta_2)x_2$ 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

$$y_i = x_i \beta + \epsilon_i$$

- Model of the form

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

- 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

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

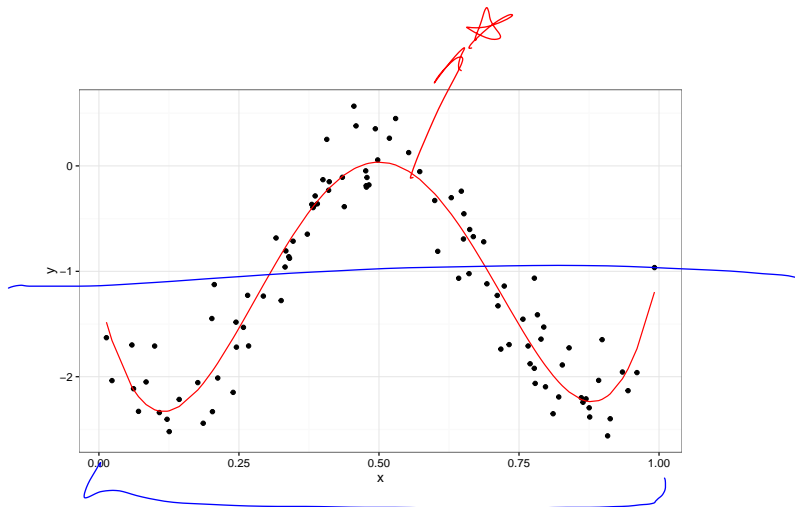
$$\hookrightarrow y = X\beta + \epsilon$$

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

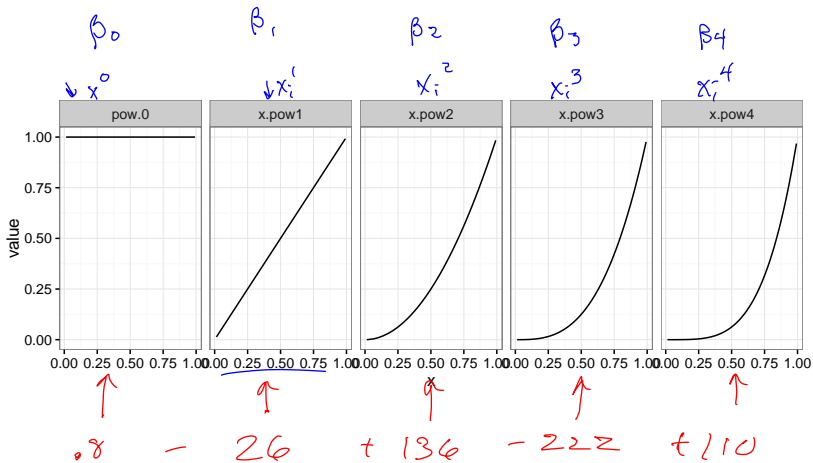
```
> data.nonlin = mutate(data.nonlin,  
+   x.pow2 = x^2, x.pow3 = x^3, x.pow4 = x^4)  
>  
> quartfit = lm(y ~ x + x.pow2 + x.pow3 + x.pow4, data = data.nonlin)  
> tidy(quartfit)
```

| | 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



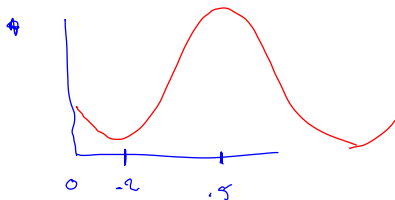
Polynomial models



Polynomial models

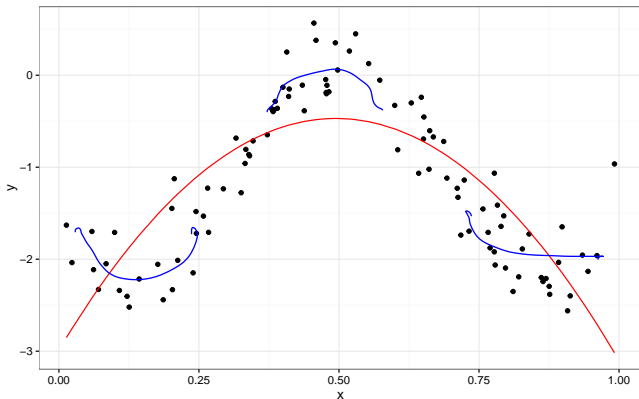
- Interpretation of β_1 :

"keeping everything else fixed" ??



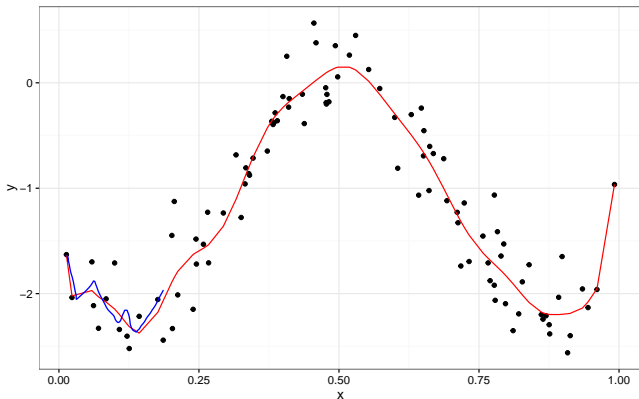
Not enough polynomial terms

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

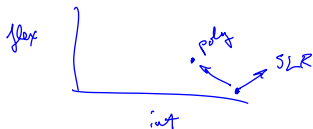


Too many polynomial terms

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



Final thoughts on polynomial models

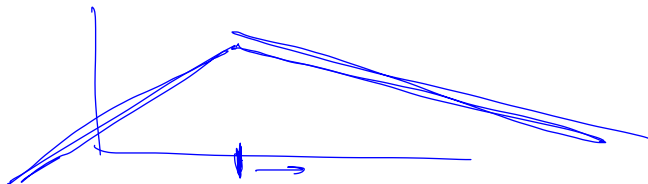


- Always include lower-order terms with higher-order terms
- You have to choose p , which isn't always easy
- Interpretation can be hard
- Raising continuous predictors for powers can lead to very large entries in your design matrix
- x is almost always correlated with x^2 .

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

$$\underline{E(y|x)} = \underline{\beta_0} + \underline{\beta_1 x} + \underline{\beta_2(x - \kappa)} \oplus$$

where κ is the location of the change point

Interpretation of regression coefficients

Estimation

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

Multiple knots

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

- For multiple knots we can write this as

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

where $\{\kappa_k\}_{k=1}^K$ are the locations of the change points

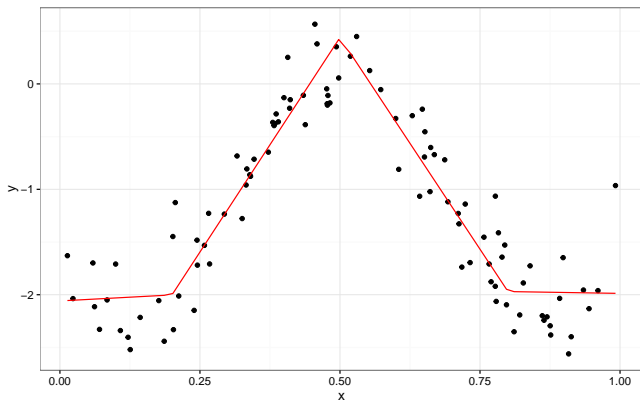
- Note that knot locations are defined before estimating regression coefficients
- Also, regression coefficients are interpreted conditional on the knots.

Example

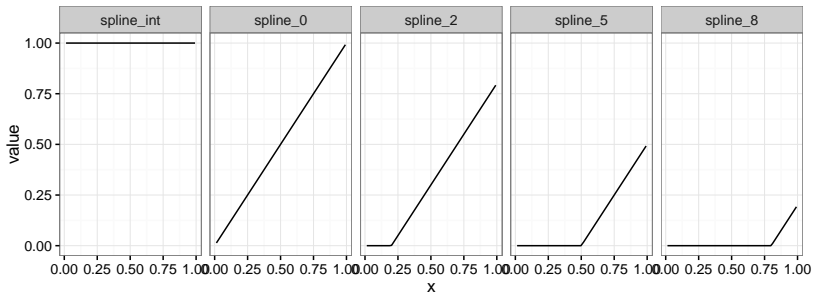
```
> data.nonlin = mutate(data.nonlin,  
+                       spline_2 = (x - .2) * (x >= .2),  
+                       spline_5 = (x - .5) * (x >= .5),  
+                       spline_8 = (x - .8) * (x >= .8))  
>  
> piecewise.fit = lm(y ~ x + spline_2 + spline_5 + spline_8, data = data.nonlin)  
> 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



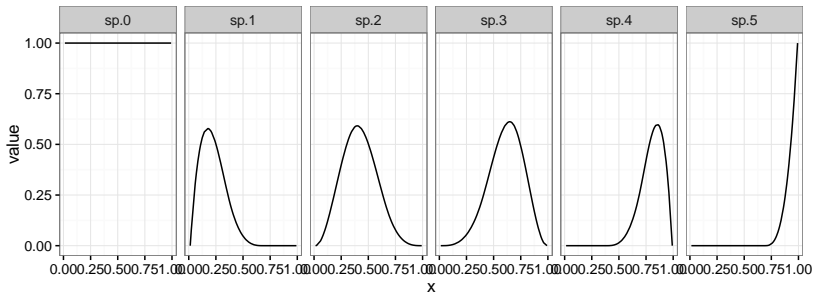
Example



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

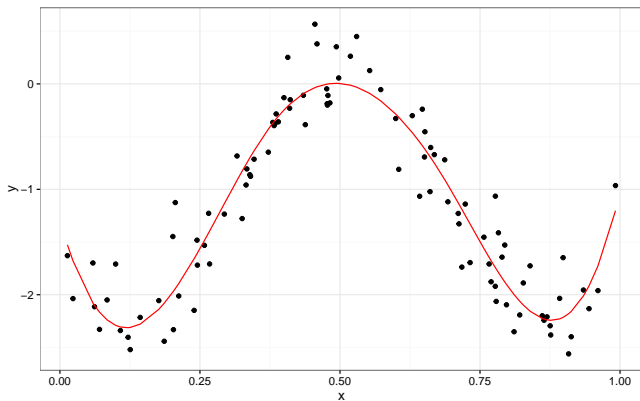


Spline models

```
> 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 |

Spline models



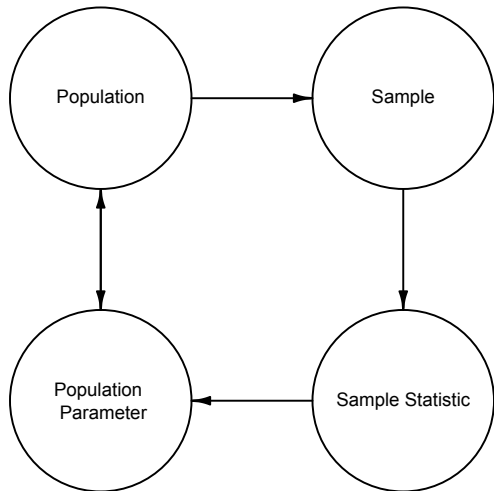
Final thoughts on spline models

- 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 ...

Circle of Life



Multiple linear regression

- Let

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

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

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

- \mathbf{X} is called the *design matrix*

Matrix notation

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

- ϵ is a random vector rather than a random variable
- $E(\epsilon) = 0$ and $Var(\epsilon) = \sigma^2 I$
- 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 $\mathbf{y}^T = [y_1, \dots, y_n]$ be an n -component random vector. Then its mean and variance are defined as

$$E(\mathbf{y})^T = [E(y_1), \dots, E(y_n)]$$

$$\text{Var}(\mathbf{y}) = E[(\mathbf{y} - E\mathbf{y})(\mathbf{y} - E\mathbf{y})^T] = E(\mathbf{y}\mathbf{y}^T) - (E\mathbf{y})(E\mathbf{y})^T$$

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

$$\text{Cov}(\mathbf{y}, \mathbf{z}) = E[(\mathbf{y} - E\mathbf{y})(\mathbf{z} - E\mathbf{z})^T]$$

Basics on random vectors

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

$$E(A\mathbf{y}) = AE\mathbf{y}$$

$$\text{Var}(A\mathbf{y}) = A\text{Var}(\mathbf{y})A^T$$

$$\text{Cov}(A\mathbf{y}, B\mathbf{z}) = A\text{Cov}(\mathbf{y}, \mathbf{z})B^T$$

Vector differentiation

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

Least squares

As in simple linear regression, we want to find the β that minimizes the residual sum of squares.

$$RSS(\beta) = \sum_i \epsilon_i^2 =$$

Least squares

Unbiasedness of LSEs

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

Variance of LSEs

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

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

Sampling distribution of $\hat{\beta}$

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

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

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

Definitions

- *Fitted values:* $\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \mathbf{H}\mathbf{y}$
- *Residuals / estimated errors:* $\hat{\boldsymbol{\epsilon}} = \mathbf{y} - \hat{\mathbf{y}}$
- *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: $\mathbf{H}\mathbf{H} = \mathbf{H}$
- It is symmetric: $\mathbf{H}^T = \mathbf{H}$
- The residuals are $\hat{\mathbf{e}} = (\mathbf{I} - \mathbf{H})\mathbf{y}$
- The inner product of $(\mathbf{I} - \mathbf{H})\mathbf{y}$ and $\mathbf{H}\mathbf{y}$ is zero (predicted values and residuals are uncorrelated).

Projection space interpretation

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