Lecture 2

Basic functions for building regression models: splines; indicator variables; interactions

Review of key concepts from Lecture 1

- Statistics: Methodology for the scientific method using quantitative evidence

- Statistical model:
  - a mathematical approximation that describes the mechanism by which the observed data might have been generated
  - Provides a precise statement of a set of hypotheses
  - Are models correct? True? Right?
  - Models can be useful by helping you operationalize the scientific method

- Regression:
  - (Y,X) have a joint distribution, note X may be a series of columns of information.
  - The regression of Y on X is E(Y|X)

Two key uses / purposes for regression

1. Study the etiology of a process; how Y is caused by or associated with a set of Xs
   - Let X=(R,C); Study how risk factors R affect the outcome Y while controlling for potential confounders C
   - Let X=(R,C,E); Study how the effects of risk factors R are modified by variables E while controlling for confounders C

2. Predict Y using X

Regression fundamentals are the same for both!

Features of the regression model fit of most interest and strategy for model building can differ depending on your purpose.

Types of regression discussed in 140.653-654

- General: ave(Y|X)
- Linear model: ave(Y|X) = B_0 + sum(j=1,p) B_jX_j
- Additive models: ave(Y|X) = sum(j=1,p) $s_j(X_j)$
- Generalized linear models (GLMs): g(ave(Y|X)) = B_0 + sum(j=1,p) B_jX_j ; g- "link" function
  - Linear: g(u) = u
  - Logistic: g(u) = log(u/(1-u)) = "logit"(u)
  - Log-linear: g(u) = log(u)
  - Probit, tobit, complementary log-log,…
- Generalized additive models (GAMs): g(ave(Y|X)) = B_0 + sum(j=1,p) $s_j(X_j)$
- Classification and regression trees (CART): E(Y|X) is a "step function" in higher dimensional X-space
- Random forests: E(Y|X) is an average of a large number of "bootstrapped" trees

Key datasets

Nepali Children's Anthropometry (NCA) Data

- Cross-sectional nutrition survey of 4,000+ pre-school children
- Height, weight, arm-circumference and age on each
- Questions:

1. How does height vary with age. What is the average "growth rate" over the first 5 years of life?

2. How does shorter-term nutritional status vary by age; are younger children in better or worse status as measured by weight or arm-circumference controlled for height?

3. How well can you predict a child's weight given his height and age?

Key datasets

National Medical Expenditure Survey – Medical costs and smoking-caused diseases

- Now known as Medical Expenditure Panel Survey, conducted by AHRQ
- ~~NEMS~~ NMES 1987 – national survey of 20,000 non-institutionalized adults, included supplemental survey on smoking behaviors
- Key variables: total medical expenditures, presence of smoking-caused disease (Lung cancer, COPD, CHD, Stroke,…), age, gender, SES, smoking status
- Questions:

1. How much more is spent per year on persons with smoking-caused diseases (SCDs) than on otherwise similar persons without SCDs?
2. Does this SCD-attributable expenditure differ by current smoking status or access to health care?
3. How does the risk of LC or COPD depend on the total pack-years of smoking and age?
4. How does the risk of CHD/Stroke change for former smokers as a function of the time since they quit?

Today's main topic

- Classical Multiple Linear Regression Model
- Basic tools for building regression models:
  - Step functions
  - Linear splines
  - Cubic splines
- Interactions

Classical multiple linear regression (mlr) model

Population of interest (Y, X) $\xrightarrow{\text{sample}}$ n observations (Y_i, X_i), $i = 1, \ldots, n$

MLR model

$Y_i = \mu_i + \varepsilon_i$, ε_i = residual $\sim N(0, \sigma^2)$, $Cor(\varepsilon_i, \varepsilon_j) = 0$

Constant variance

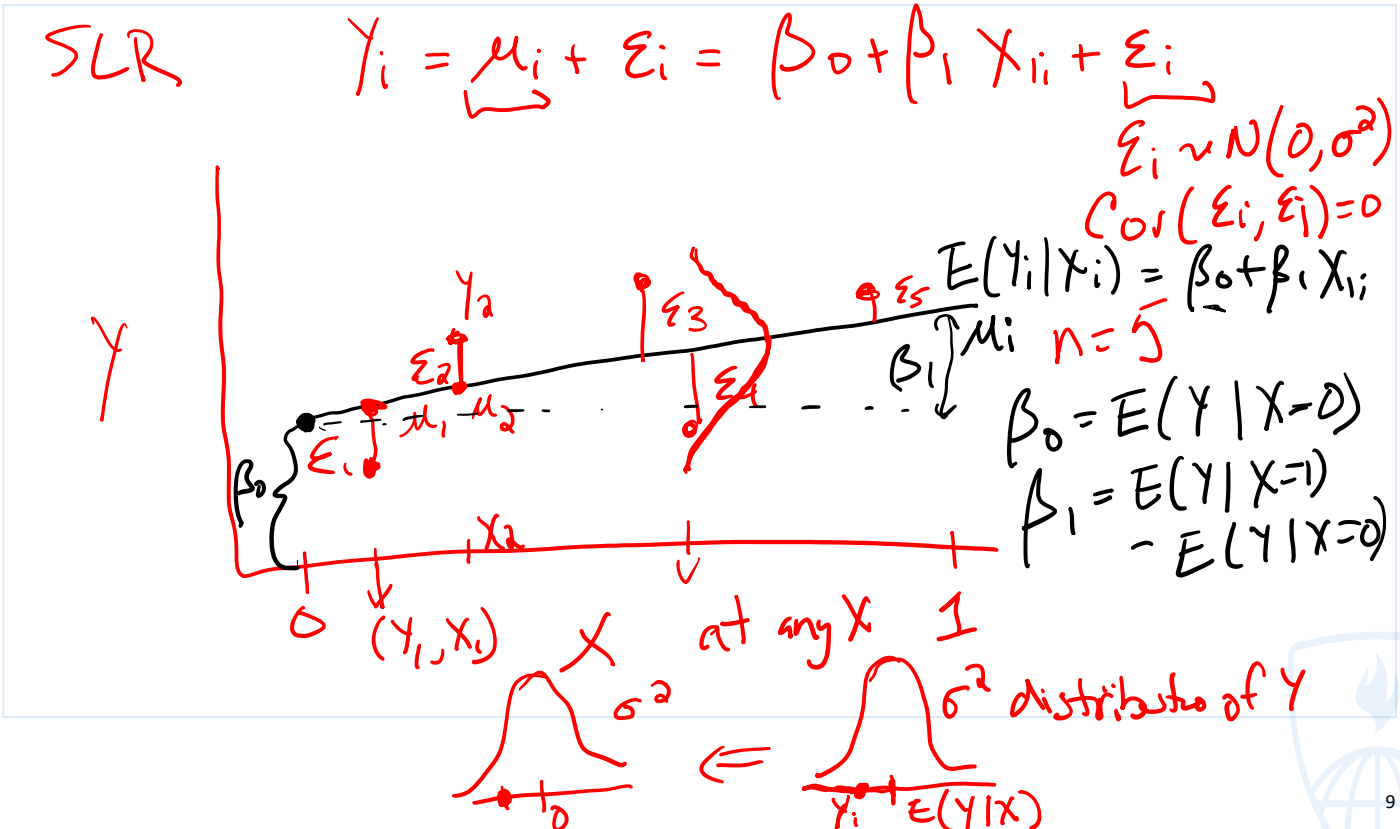
independent observations

Systematic component

$$\mu_i = E(Y_i | X_i) = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_p X_{pi}$$

→ systematic component is correctly specified

Picture of p = 1 case



What is linear about a MLR?

Linear model

$$E(Y|X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$$

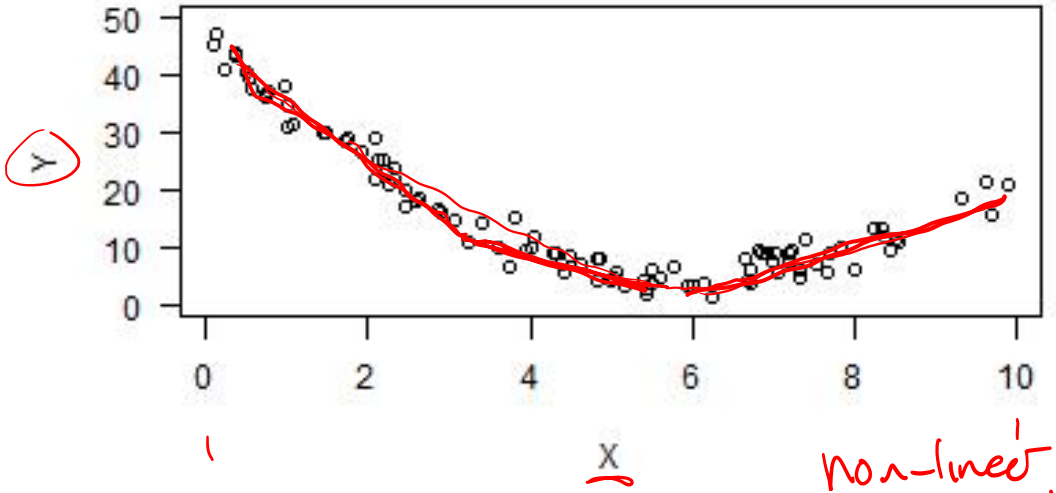
$$E(Y|X) = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2$$

Non-linear model

Fourier model $= \beta_0 + \cos(\beta_1 - \beta_2) + \sin(\beta_1 - \beta_3)$

Weibull growth

Toy example for today's lecture



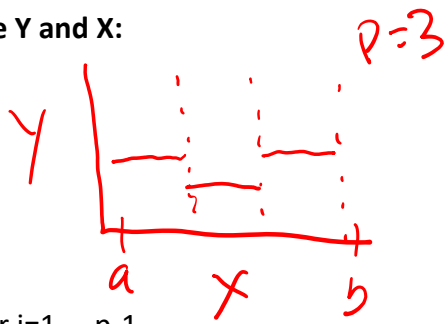
non-linear relationship between Y and X

Y and X are negatively correlated when $X \in (0, 6)$

Y and X are positively correlated when $X > 6$

Step functions

Creating a step function to describe the relationship between average Y and X:



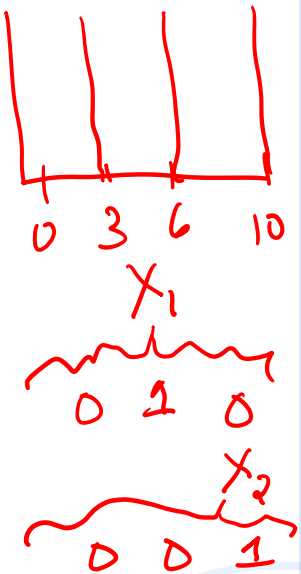
- X in range (a,b)
- Partition the range into p intervals: $(a=c_0,c_1,c_2,\ldots,c_p=b)$
  - e.g. p=4 for quartiles or p=10 for deciles of X
- Define (p-1) indicator variables: $X_j = 1$ if $c_j <= X < c_{j+1}$; 0 otherwise for j=1,…,p-1
- One less indicator variable than interval!
- Fit MLR with intercept: $Yi = B_0 + B_1 X_{i1} + \ldots + B_{p-1} X_{ip-1} + e_i$

Indicators for whether X is in each of the partitions

Step functions

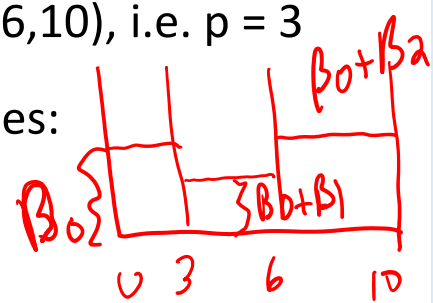
- Consider a step function with partition (0,3,6,10), i.e. p = 3
- We will need to define two indicator variables:
  - X_1 = 1 if 3 <= X < 6; 0 otherwise
  - X_2 = 1 if 6 <= X < 10; 0 otherwise
- The model is: $Y_i = B_0 + B_1 X_{1i} + B_2 X_{2i} + e_i$
- Interpret the following:
  - B_0
  - $B_0 + B_1$
  - B_1

Consider the model when X <



Step functions

- Consider a step function with partition (0,3,6,10), i.e. p = 3
- We will need to define two indicator variables:
  - X_1 = 1 if 3 <= X < 6; 0 otherwise
  - X_2 = 1 if 6 <= X < 10; 0 otherwise
- The model is: $Y_i = B_0 + B_1 X_{1i} + B_2 X_{2i} + e_i$
- Interpret the following:
  - $B_0 = E(Y \mid X < 3)$
  - $B_0 + B_1 = E(Y \mid 3 \leq X < 6)$
  - B_2



Consider the model when $X < 3$: $Y_i = B_0 + e_i$

Consider the model when $3 \leq X < 6$: $Y_i = B_0 + B_1 + e_i$

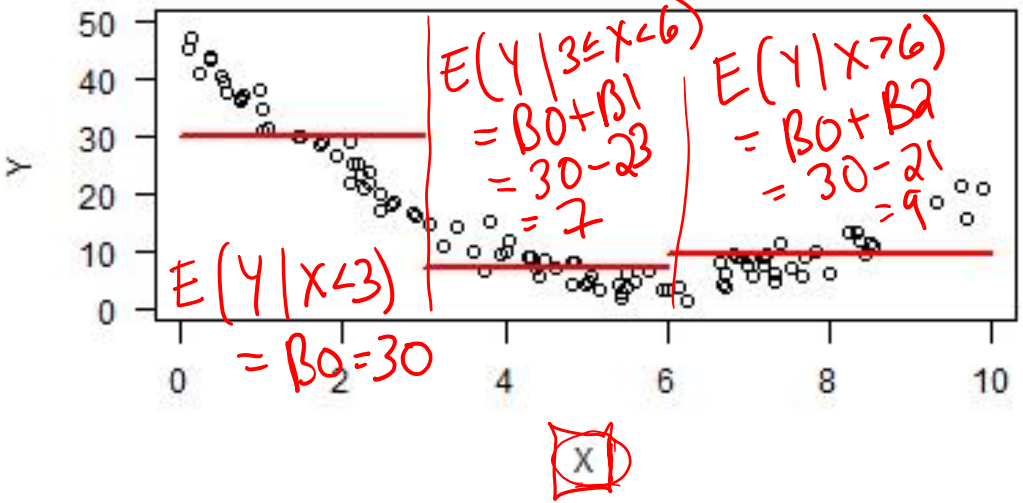
X_1: 0 1 0

X_2: 0 0 1 ($X < 3$)

difference in average Y comparing mean when 2nd bin minus mean in 1st bin

Step functions

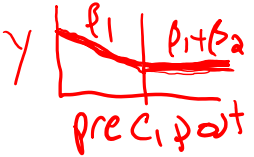
In our toy example, the estimated values for B_0, B_1 and B_2 are 30, -23 and -21, respectively.



Creating step functions is common; what do you think about this practice?

Linear splines

- Idea: linear spline (aka "broken arrow", "hockey stick"; "intervention" model) assumes that there is a linear relationship between Y and X with slope that can change at pre-specified locations called "knots"



- Formula: $E(Y|X) = B_0 + B_1 X + B_2 (X-c_1)^+ + B_3(X-c_2)^+ + \ldots B_{k+1} (X-c_K)^+$

linear trend in the 1st range of X

where $u^+ = u$ if $u > 0$ and 0 otherwise

- Interpretation of coefficients:
  - B_0, B_1 intercept and slope in the left-most interval
  - B_j, for j>=2: change in slope from before to after associated knot

Linear splines

- Back to our toy example, consider the multiple linear regression of Y on:

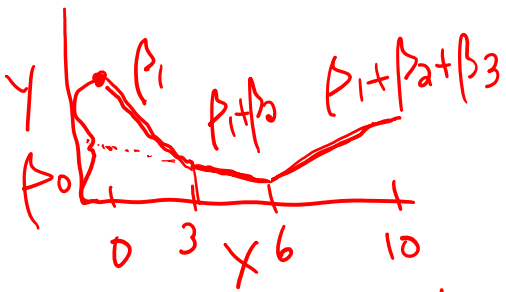
$X1 = X$, $X2 = (X-3)^+$; $X3 = (X-6)^+$

$X_1 = X$

$X_2 = 0$ if $X \le 3$
$= X-3$ if $X > 3$

$X_3 = 0$ if $X \le 6$
$= X-6$ if $X > 6$

$E(Y|X) = \beta_0 + \beta X_1 + \beta_2 X_2 + \beta_3 X_3$



Consider the model when $X \le 3$: $E(Y|X \le 3) = \beta_0 + \beta_1 X$

$3 < X \le 6$ $E(Y|3 < X \le 6) = \beta_0 + \beta_1 X + \beta_2 (X-3)$
$= (\beta_0 - 3\beta_2) + (\beta_1 + \beta_2) X$

$X > 6$ $E(Y|X > 6) = \beta_0 + \beta_1 X + \beta_2 (X-3) + \beta_3 (X-6)$
$= (\beta_0 - 3\beta_2 - 6\beta_3) + (\beta_1 + \beta_2 + \beta_3) X$

Linear splines

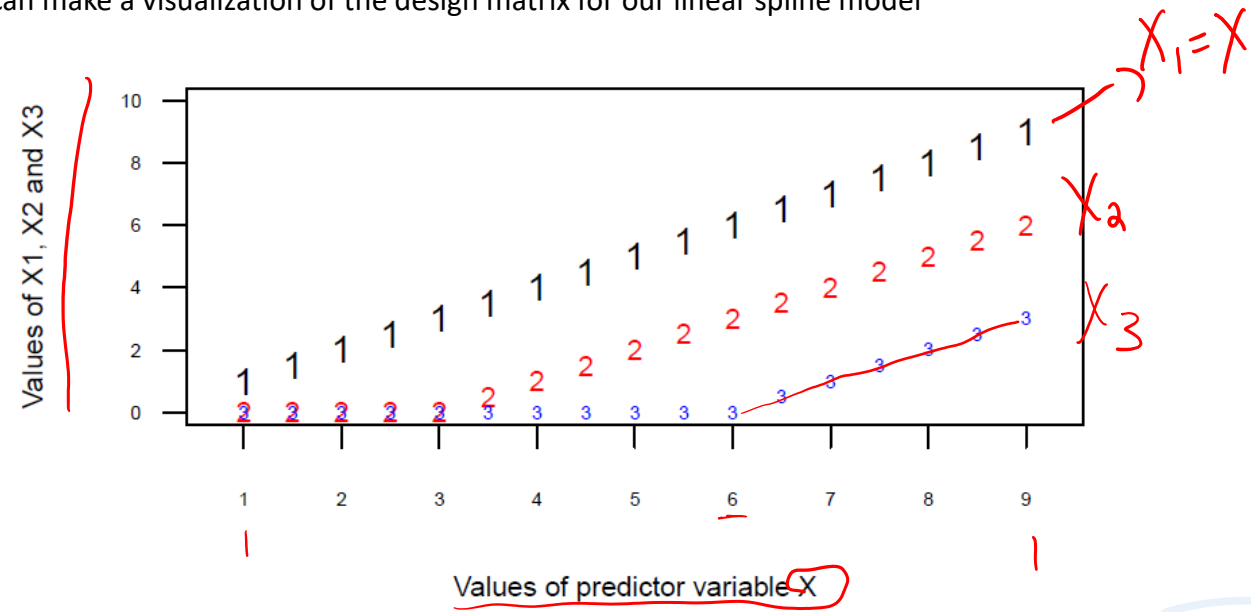
$E(Y|X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3$

- The design matrix contains information about predictor/covariate values for each observation in the data
  - The columns of the matrix define each predictor variable
  - The rows of the matrix provide the values of the predictor variable for the corresponding observation

Intercept	$X_1=X$	$X_2=(X-3)^+$	$X_3=(X-6)^+$
1	1	0	0
1	2	0	0
1	3	0	0
1	4	1	0
1	5	2	0
1	6	3	0
1	7	4	1
1	8	5	2
1	9	6	3

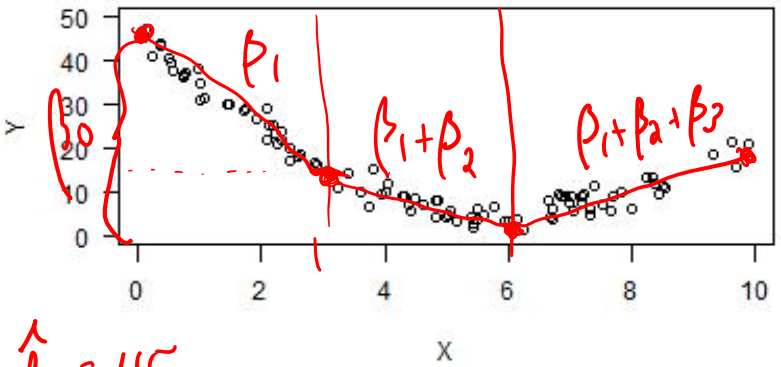
Linear splines

- We can make a visualization of the design matrix for our linear spline model



Linear splines

- Estimate the values of B_0, B_1, B_2, and B_3



$X \le 3: E(Y|X \le 3) = \beta_0 + \beta_1 X$

$3 < X \le 6: E(Y|3 < X \le 6) = \beta_0 - 3\beta_2 + (\beta_1 + \beta_2)X$

$X > 6: E(Y|X > 6) = \beta_0 - 3\beta_2 - 6\beta_3 + (\beta_1 + \beta_2 + \beta_3)X$

$\hat{\beta}_0 = 45$

$\hat{\beta}_1 = \frac{(15-45)}{3} = \frac{-30}{3} = -10$

$\hat{\beta}_1 + \hat{\beta}_2 = \frac{(5-15)}{3} = \frac{-10}{3} \approx -3.3$

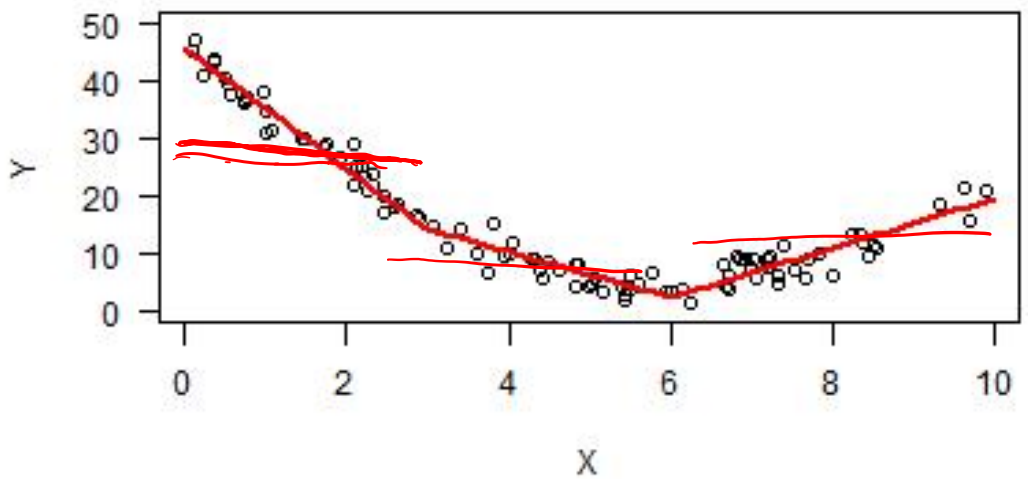
$\hat{\beta}_2 = -3.3 + 10 \approx 6.7$

$\hat{\beta}_1 + \hat{\beta}_2 + \hat{\beta}_3 = \frac{(20-5)}{4} = \frac{15}{4}$

$\hat{\beta}_3 = \frac{15}{4} - (-6.7)$

Linear splines

- I estimated the linear spline model parameters (we will discuss how later) and plotted the estimated mean of Y for each value of X.
- Do you prefer the linear spline model to the step function approach? Why?



Cubic splines

- Idea: linear splines are nice, but they have ugly elbows (discontinuities in their first derivative); make the functions join together smoothly at the boundaries and allow some more bend in each interval
- Express E(Y|X) as a "locally cubic" function of X that is continuous and has continuous first and second derivatives, with jumps in its third derivative at selected "knots"
- Formula: $E(Y|X) = B_0 + B_1 X + B_2 X^2 + B_3 X^3 + \text{Sum}(k=4,p)\ \{ B_k [(X-c_{k-3})^+]^3 \}$

Where $u^+ = u$ if $u > 0$ and 0 otherwise

Cubic Splines

- Formula:

$$E(Y|X) = B_0 + B_1 X + B_2 X^2 + B_3 X^3 + \text{Sum}(k=4,p)\ \{ B_k [(X-c_{k-3})^+]^3 \}$$

Where $u^+ = u$ if $u > 0$ and 0 otherwise

- Interpretation of coefficients:
  - B_0, B_1, B_2, B_3 – coefficients of a cubic function for left most interval
  - B_j, $j>3$ – change in cubic coefficient slope from j-3rd to j-2nd interval (not very useful on its own)

Cubic splines

- Within the toy example with knots of $c_1 = 3$; $c_2 = 6$, list (with definitions) the variables that will define your "Design Matrix". HINT: you need to define 5 variables.

$$X_1 = X$$

$$X_2 = X^2$$

$$X_3 = X^3$$

$$X_4 = [(X-3)^+]^3 = \begin{cases} 0 \text{ if } X \leq 3 \\ (X-3)^3 \text{ if } X > 3 \end{cases}$$

$$X_5 = [(X-6)^+]^3 = \begin{cases} 0 \text{ if } X \leq 6 \\ (X-6)^3 \text{ if } X > 6 \end{cases}$$

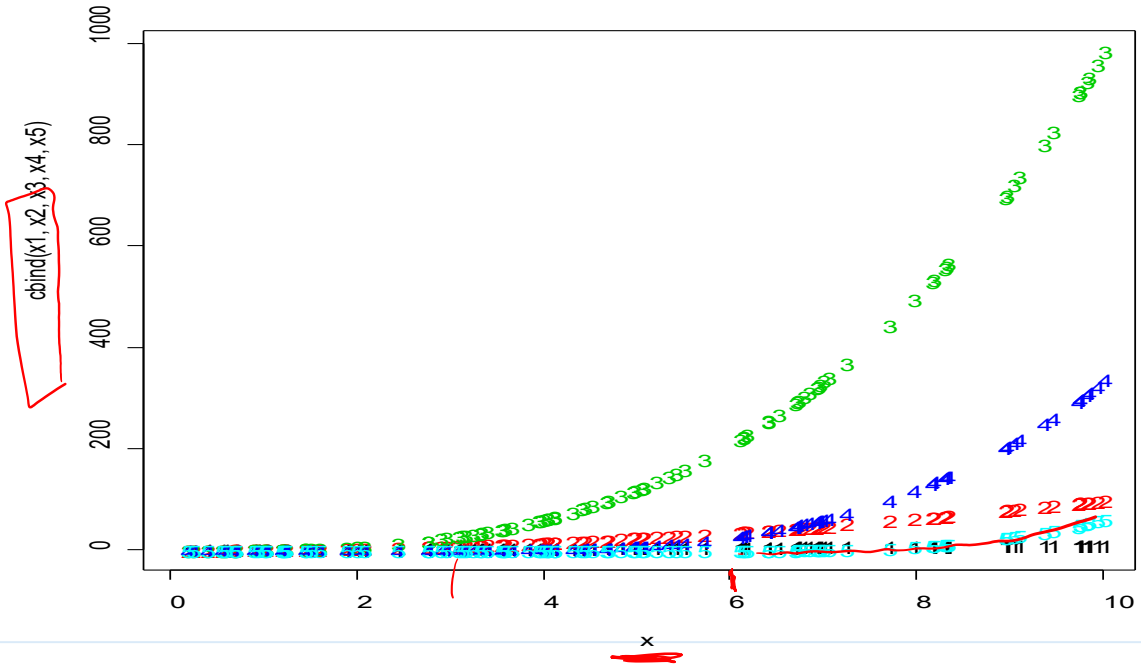
Cubic splines

- Example of rows of the design matrix for the cubic spline model for values of X = 1, 2, …, 9

Intercept	$X_1=X$	$X_2=X^2$	$X_3=X^3$	$X_4=[(X-3)^+]^3$	$X_5=[(X-6)^+]^3$
1	1	1	1	0	0
1	2	4	8	0	0
1	3	9	27	0	0
1	4	16	64	1	0
1	5	25	125	8	0
1	6	36	216	27	0
1	7	49	343	64	1
1	8	64	512	125	8
1	9	81	729	216	27

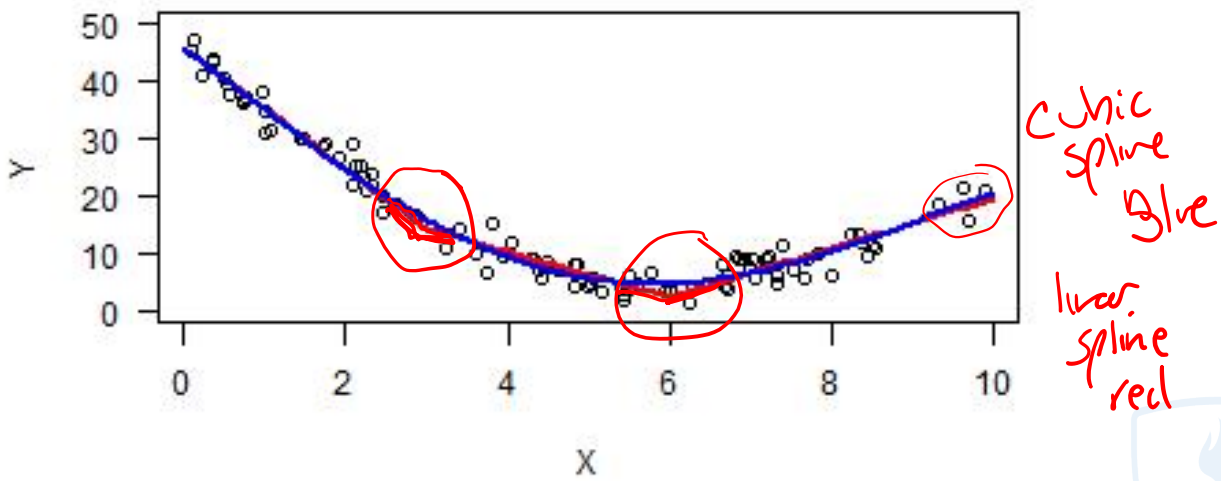
Cubic splines

- Visualization of the design matrix



Cubic splines

- I fit the cubic spline model and overlayed the estimated average Y vs. X based on the cubic spline model and the linear spline model.
- Which model do you prefer?



Evaluation of model fit

- You will review this idea in Lab 2
- Idea:
  - Which of these models “fits” the data best?
  - Which of the models minimizes the error or residual, i.e. the distance between the observed y and the average y given x.
- If you evaluate the model fit using the same data that you used to fit the model, you will be overly optimistic in your assessment
- Cross-validation!

Interactions of simple functions

- Interactions allow for $E(Y|X) = f(x)$ to vary across subsets of the population of interest
- Effect modification
- During the first year of life, is the average "growth rate" in weight for male infants the same as for female infants?

Interactions of simple functions

- During the first year of life, is the average “growth curve” in weight for male infants the same as for female infants?

Interactions of simple functions

- Is the effect on average medical expenditures of being both poor and older greater than would be expected given the independent effects of poverty and old age alone

In the next class session….

- We will work together to apply the concepts we learned in this lecture to the Nepal dataset