

BIFX 553 - Complex Interactions

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Modeling and testing complex interactions

As a reminder, let's write out our model from a few weeks back:

$$nodes_i = \beta_0 + \beta_1 age_i + \beta_2 size_i + \beta_3 grade_i + \varepsilon_i$$

- ▶ $nodes_i$ is our outcome variable
- ▶ β_0, β_1, \dots are our regression coefficients
- ▶ $age_i, size_i, \dots$ are our predictors
- ▶ ε_i are the error terms for the model (i.e. how far off is the model prediction from what we observed)

Fitting categorical predictors

For variables that are categorical (e.g. sex, race), we normally include dummy variables for them in the model.

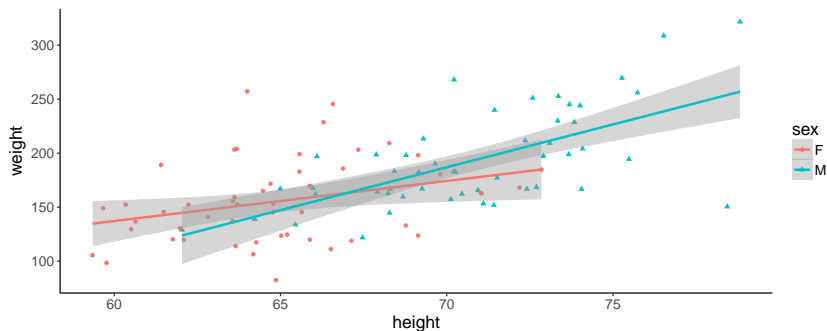
$$weight_i = \beta_0 + \beta_1 height_i + \beta_2 (sex_i = M) + \varepsilon_i$$

Fitting categorical predictors

```
set.seed(293847)
# data for our categorical predictor example
bmi <- data_frame(
  sex = c(rep(c('M', 'F'), each = 50)),
  # average US height
  height = rnorm(100, mean = ifelse(sex == 'M', 70, 65),
    sd = ifelse(sex == 'M', 4, 3.5)),
    # ave BMI - men
  bmi = ifelse(sex == 'M', 2^rnorm(100, 4.7004, 0.2305),
    # ave BMI - women
    2^rnorm(100, 4.6439, 0.3086)),
  # calculate weight
  weight = ((height / 12 / 3.28)^2 * bmi) * 2.2)
```

Fitting categorical predictors

```
# graphical view of relationship between height and weight  
ggplot(bmi, aes(x = height, y = weight, group = sex)) +  
  geom_point(aes(color = sex, shape = sex)) +  
  geom_smooth(method = 'lm', aes(color = sex))
```



Fitting categorical predictors

```
# and now for a statistical look
```

```
lm(weight ~ height + sex, data = bmi) %>%  
  tidy()
```

##	term	estimate	std.error	statistic	p.value
## 1	(Intercept)	-236.278051	69.799873	-3.3850785	1.028381e-03
## 2	height	6.032593	1.071821	5.6283572	1.764689e-07
## 3	sexM	2.437032	9.625050	0.2531969	8.006519e-01

Fitting categorical predictors

In the background R is doing the following:

```
# create a dummy variable for "sex == 'M'"  
bmi$male <- as.integer(bmi$sex == 'M')  
  
# this model is exactly the same as the model above  
lm(weight ~ height + male, data = bmi) %>%  
  tidy()
```

	term	estimate	std.error	statistic	p.value
## 1	(Intercept)	-236.278051	69.799873	-3.3850785	1.028381e-03
## 2	height	6.032593	1.071821	5.6283572	1.764689e-07
## 3	male	2.437032	9.625050	0.2531969	8.006519e-01

Fitting categorical predictors

When we write this out in a formula, we get

$$\begin{aligned} \text{weight}_i &= \beta_0 + \beta_1 \text{height}_i + \beta_2 (\text{sex}_i = M) + \varepsilon_i \\ &= \beta_0 + \beta_1 \text{height}_i + \beta_2 (1) + \varepsilon_i \\ &= \beta_0 + \beta_1 \text{height}_i + \beta_2 + \varepsilon_i \end{aligned}$$

when sex_i is 'M'

$$\begin{aligned} \text{weight}_i &= \beta_0 + \beta_1 \text{height}_i + \cancel{\beta_2 (0)} + \varepsilon_i \\ &= \beta_0 + \beta_1 \text{height}_i + \varepsilon_i \end{aligned}$$

when sex_i is 'F'

Fitting categorical predictors

So, exactly what does β_2 represent? It is interpreted as the difference in height between a male and a female who are otherwise similar (i.e. in our case, they are the same height).

$$\begin{aligned} E(\text{weight}_i - \text{weight}_j | \text{height}_i = \text{height}_j) &= \beta_0 + \beta_1 \text{height}_i + \beta_2 (\text{sex}_i = M) \\ &\quad - (\beta_0 + \beta_1 \text{height}_j + \beta_2 (\text{sex}_j = M)) \\ &= \cancel{\beta_0} + \cancel{\beta_1 \text{height}_i} + \beta_2 (1) \\ &\quad - (\cancel{\beta_0} + \cancel{\beta_1 \text{height}_j} + \cancel{\beta_2 (0)}) \\ &= \beta_2 \\ &= 2.4 \text{ in} \end{aligned}$$

An aside on the interpretation of the intercept

What does the intercept (β_0) really mean? In the model above, β_0 is what we get when $sex_i = 'F'$ and $height_i = 0$. So, the predicted weight of a Female who is 0 inches tall would be

$$\begin{aligned} E(weight_i) &= \beta_0 + \beta_1 height_i + \beta_2 (sex_i = M) \\ &= \beta_0 + \cancel{\beta_1(0)} + \cancel{\beta_2(0)} \\ &= \beta_0 \\ &= -236 \text{ lbs} \end{aligned}$$

This, of course, makes no sense, neither the height nor the weight. For this reason, the intercept is often ignored.

An aside on the interpretation of the intercept

If we wanted the intercept to make sense, we could recenter *height*; like so:

```
# lets center height at the sample median (or thereabouts)
median(bmi$height)
```

```
## [1] 67.89892
```

```
bmi <- mutate(bmi,
               ht_med = height - 67) # call it an even 5'7"

lm(weight ~ ht_med + sex, data = bmi) %>%
  tidy()
```

##	term	estimate	std.error	statistic	p.value
## 1	(Intercept)	167.905685	5.608466	29.9378991	8.506954e-51
## 2	ht_med	6.032593	1.071821	5.6283572	1.764689e-07
## 3	sexM	2.437032	9.625050	0.2531969	8.006519e-01

An aside on the interpretation of the intercept

Now, the intercept has a more useful meaning. It represents the expected weight of a 5'7" female:

$$\begin{aligned} E(\text{weight}_i) &= \beta_0 + \beta_1(\text{height}_i - 67) + \beta_2(\text{sex}_i = M) \\ &= \beta_0 + \cancel{\beta_1(67 - 67)} + \cancel{\beta_2(0)} \\ &= \beta_0 \\ &= 168 \text{ lbs} \end{aligned}$$

Dealing with Non-linearity

Simple non-linear terms

We saw in Discussion 3 that the number of nodes in the gbsg data set was more log-normally than normally distributed. Also, we looked at an example where the relationship between a predictor was a quadratic relationship, rather than a linear relationship. What do we do in these cases?

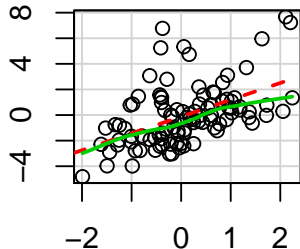
Simple non-linear terms: Example 1

```
# quadratic relationship between predictor and outcome
set.seed(293847)
tmp <- data_frame(x1 = rnorm(100),
                  x2 = rnorm(100),
                  y = x1 + x2^2 + rnorm(100))

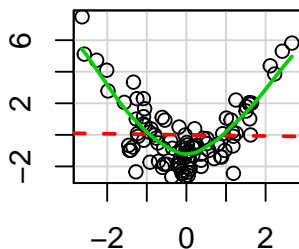
# wrong model... y ~ x2 is a quadratic relationship
lm(y ~ x1 + x2, data = tmp) %>%
  crPlots()
```

Component + Residual Plots

Component+Residual



Component+Residual

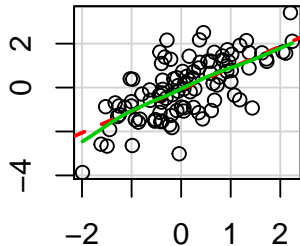


Simple non-linear terms: Example 1

```
# create a new variable and try this  
mutate(tmp, x2_sqrd = x2^2) %>%  
  lm(formula = y ~ x1 + x2_sqrd) %>%  
  crPlots() # looks much better!
```

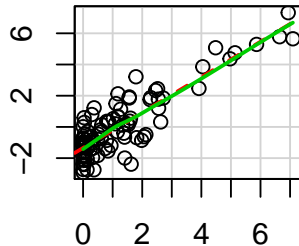
Component + Residual Plots

Component+Residual



x1

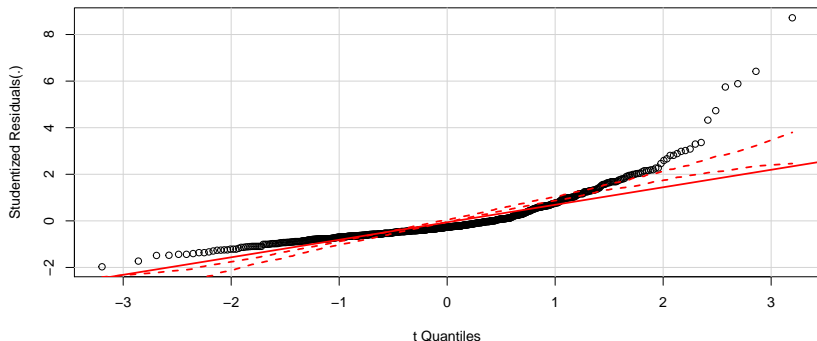
Component+Residual



x2_sqrd

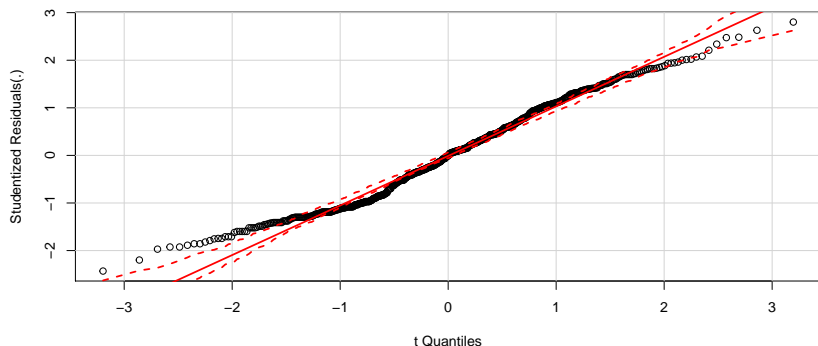
Simple non-linear terms: Example 2

```
# log-normally distributed outcome variable  
load('../1-26/gbgs.RData')  
  
# wrong model... nodes is log-normally distributed  
lm(nodes ~ size + grade, data = gbgs) %>%  
  qqPlot()
```



Simple non-linear terms: Example 2

```
# lets try with log(nodes) ... still not perfect
mutate(gbgs, lnodes = log(nodes)) %>%
  lm(formula = lnodes ~ size + grade) %>%
  # a lot better -- we will revisit this in a future discussion
  qqPlot()
```



Splines

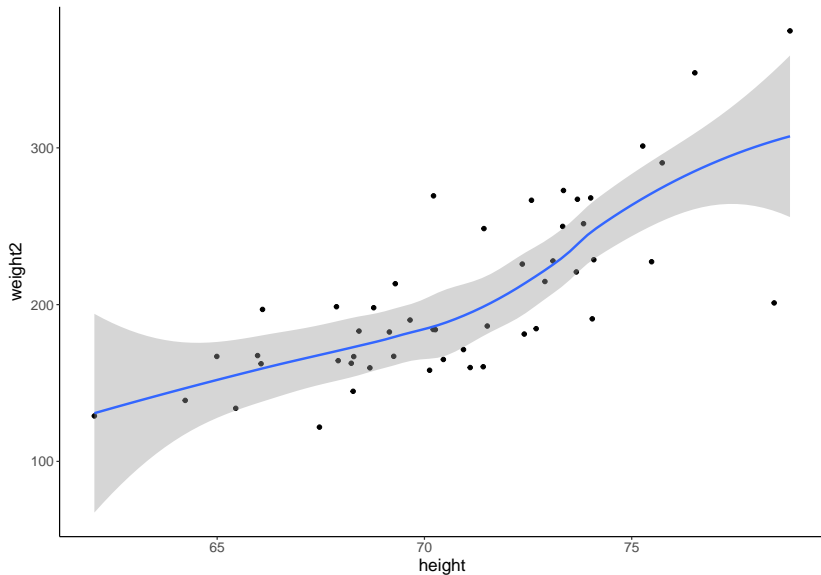
Sometimes, the relationship between a predictor and the outcome is neither linear, nor does it conform to a nice function that we can use for a simple transformation. In such a case, splines can help.

```
# add some additional weight for people over 70 inches tall
bmi <- mutate(bmi,
               weight2 = ifelse(height < 70, weight,
                                weight + 6*(height - 70)))

# what does this look like?
g <- filter(bmi, sex == 'M') %>%
  ggplot(aes(x = height, y = weight2)) +
  geom_point() +
  geom_smooth(se = FALSE)
```

Splines

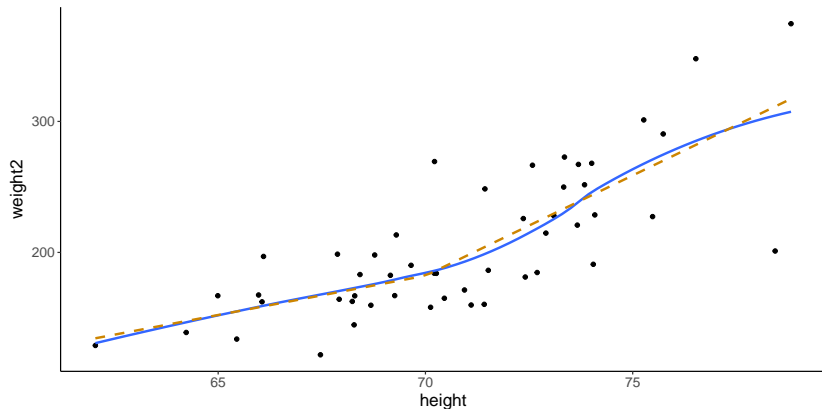
```
## `geom_smooth()` using method = 'loess'
```



Splines

```
# we can include a 1st degree spline with a knot at height = 70  
g + geom_smooth(method = 'lm', se = FALSE, color = 'orange3',  
               linetype = 2, formula = y ~ bs(x, knots = 70,  
                                             degree = 1))
```

```
## `geom_smooth()` using method = 'loess'
```



Splines

the linear regression model(s) would look like this:

```
mdl1 <- lm(weight2 ~ bs(height, knots = 70, degree = 1),  
           data = subset(bmi, sex == 'M'))
```

```
mdl2 <- lm(weight2 ~ bs(height, knots = 70, degree = 1) + sex,  
           data = bmi)
```

Splines: Interpretation/Prediction

Interpreting the regression coefficients directly is beyond the scope of this class, but there is an easy way to use this model to predict. This should work with any of the models we will be generating in this class. All you need is the model output from `lm` and a data frame with the values needed to predict.

```
# for the male-only model  
data_frame(height = 70) %>%  
  predict(object = mdl1)
```

```
##           1  
## 182.2475
```

Splines: Interpretation/Prediction

In mdl1, we only needed to include height, but we also need to include sex for mdl2.

```
# for the full model  
data_frame(height = c(70, 67),  
            sex = c('M', 'F')) %>%  
  predict(object = mdl2)
```

```
##           1           2  
## 179.8799 163.0864
```


Splines: Higher order splines

You can also use the `bs` function to fit higher order polynomial splines (the default is a cubic spline).

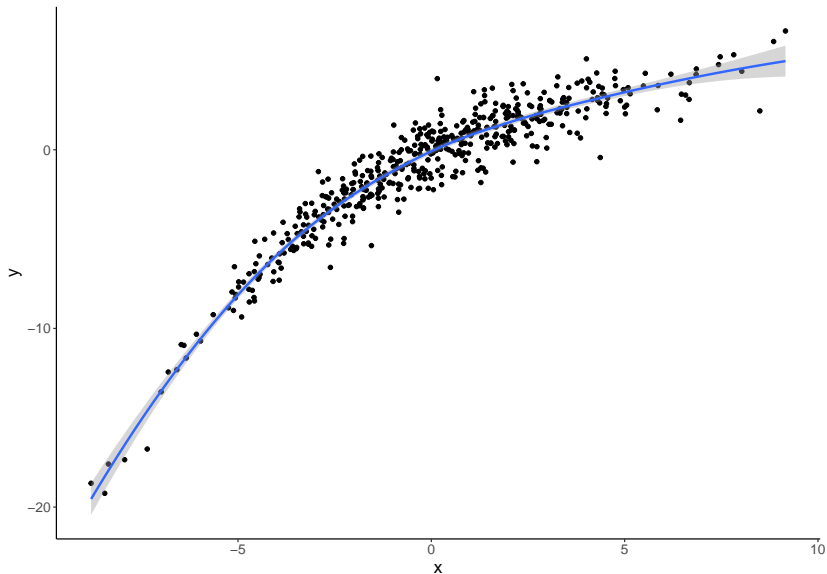
Non-parametric regression

You may have noticed that the default output of `geom_smooth()` is a smooth function that looks sort of like a moving average. The default smoother used for data sets with less than 1000 observations is called `loess`, and a generalized additive model is used with larger data sets. You won't get p-values from this, but it can be a valuable tool to graphically see what is going on.

```
# make up some data and plot the smoothing line  
g <- data_frame(x = rnorm(500, 0, 3),  
                 y = x - .1*x^2 + .005*x^3 + rnorm(500)) %>%  
  ggplot(aes(x = x, y = y)) +  
  geom_point() +  
  geom_smooth()
```

Non-parametric regression

```
## `geom_smooth()` using method = 'loess'
```



Homework

Three datasets will be provided for analysis. Pick an appropriate model for each data set, checking assumptions. Submit appropriately commented R code only. No write-up is required.