#### 432 Class 9 Slides

github.com/THOMASELOVE/2019-432

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## Setup

```
library(skimr); library(broom); library(janitor)
library(Hmisc); library(rms)
library(gridExtra); library(GGally)
library(tidyverse)
```

# Today's Materials (Chapters 9/10 in the Notes)

- The maleptsd data
- Using ols to fit a linear model
  - ANOVA in ols
  - Plot Effects with summary and Predict
  - Validating summary statistics like R<sup>2</sup>
  - Nomogram
  - Evaluating Calibration
- Spending Degrees of Freedom on Non-Linearity
  - The Spearman  $\rho^2$  (rho-squared) plot
- Building Non-Linear Predictors with
  - Polynomial Functions
  - Splines, including Restricted Cubic Splines

# The maleptsd data: Background and Exploration

# The maleptsd data

The maleptsd file on our web site contains information on PTSD (post traumatic stress disorder) symptoms following childbirth for 64 fathers<sup>1</sup>. There are ten predictors and the response is a measure of PTSD symptoms. The raw, untransformed values ( $ptsd_raw$ ) are right skewed and contain zeros, so we will work with a transformation, specifically,  $ptsd = log(ptsd_raw + 1)$  as our outcome, which also contains a lot of zeros.

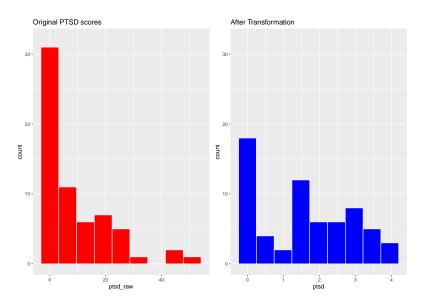
```
maleptsd <- read_csv("data/maleptsd.csv") %>%
    clean_names() %>%
    mutate(ptsd = log(ptsd_raw + 1))
```

<sup>&</sup>lt;sup>1</sup>Source: Ayers et al. 2007 *J Reproductive and Infant Psychology*. The data are described in more detail in Wright DB and London K (2009) *Modern Regression Techniques Using R* Sage Publications.

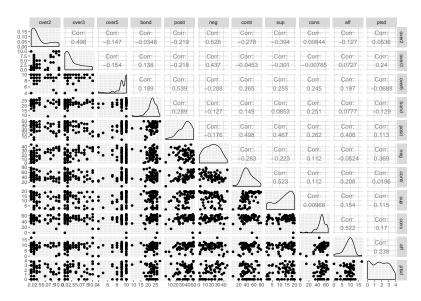
# Skimming the maleptsd data

```
maleptsd %>% select(-id, -ptsd_raw) %>% skim()
Skim summary statistics
n obs: 64
n variables: 11
-- Variable type:numeric
variable missing complete n mean
                                         sd p0
                                                 p25
                                                        p50
                                                               p75 p100
                                                                              hist
      aff
                         64 64
                                       3.08 0
                0
                                8 84
     bond
                0
                         64
                            64
                               22 52
                                       3.07 9
                                                             24.25 28
                                                             55
                                                                   65
     cons
    contr
                                                11.17
                                                      20 65 30 42 45 4
      nea
                0
                            64
                                2.8
                                       3.34 0
                                                                   10
    over2
                0
                            64
                                2.72
                                       3.13 0
                                                 0
                                                                   10
    over3
                0
                                                       9.5
                                                                   10
    over5
                                9.12
                                       1.34 4
                                                27.05 37
                                                             43.35 50.1
    posit
                               35 44
                                     11.02 2.5
                         64
                            64
                               1.59
                                      1.27 0
                                                       1.61 2.74
                                                                   3.95
     ptsd
                0
                         64 64 13
                                       5.87 1.2
                                                 9.28 14.25 18.3
      sup
                                                                   20
```

### **Transformation of Outcome**



## **Scatterplot Matrix**



## Using ols to fit a Two-Predictor Model

- ols is part of the rms package, by Frank Harrell and colleagues.
- A detailed discussion of ols is found in Chapter 10 of the Course Notes. We'll sketch out some key ideas now in a simple example, and add some more details later.

## Contents of mod\_first?

```
mod first
Linear Regression Model
ols(formula = ptsd ~ over2 + over3, data = maleptsd)
            Model Likelihood Discrimination
               Ratio Test
                               Indexes
    64 LR chi2 4.18 R2 0.063
Obs
sigma1.2500 d.f. 2 R2 adj 0.033
d.f. 61 Pr(> chi2) 0.1235
                             g 0.345
Residuals
     Min 10 Median 30
                                     Max
-2.259244 -1.337198 0.008866 1.140664 2.333183
        Coef S.E. t Pr(>|t|)
Intercept 1.3733 0.2202 6.24 < 0.0001
over2 -0.0333 0.0544 -0.61 0.5425
over3 0.1149 0.0579 1.98 0.0518
```

## ANOVA for mod\_first fit by ols

```
anova(mod_first)
```

```
Factor d.f. Partial SS MS F P
over2 1 0.5862441 0.5862441 0.38 0.5425
over3 1 6.1458656 6.1458656 3.93 0.0518
REGRESSION 2 6.4382526 3.2191263 2.06 0.1362
ERROR 61 95.3127887 1.5625047
```

Analysis of Variance

Response: ptsd

## summary for mod\_first fit by ols

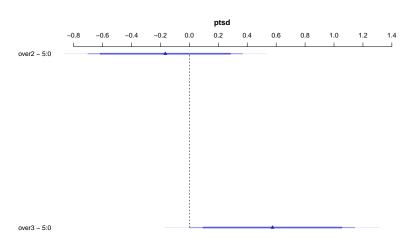
```
summary(mod_first)
```

```
Effects Response : ptsd
```

```
Factor Low High Diff. Effect S.E. Lower 0.95 over2 0 5 5 -0.16658 0.27195 -0.7103800 over3 0 5 5 0.57455 0.28970 -0.0047389 Upper 0.95 0.37722
```

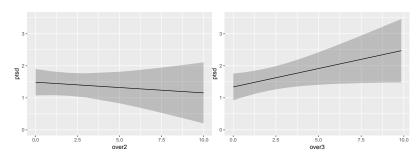
## Plot the summary to see effect sizes

plot(summary(mod\_first))



## What do the individual effects look like?

ggplot(Predict(mod\_first))



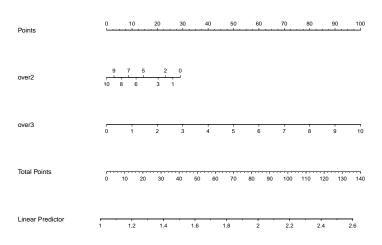
# Validate the summary statistics of an ols fit

```
set.seed(432010); validate(mod_first)
```

```
index.orig training test optimism
R-square
             0.0633 0.0940 0.0178 0.0762
MSF.
            1.4893 1.4185 1.5616 -0.1431
           0.3450 0.3792 0.2878 0.0914
g
Intercept 0.0000 0.0000 0.1656 -0.1656
Slope
         1.0000 1.0000 0.8854 0.1146
         index.corrected n
                -0.012940
R-square
MSE
                 1.6324 40
                 0.2536 40
g
                 0.1656 40
Intercept
                 0.8854 40
Slope
```

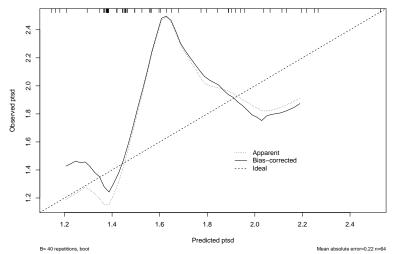
## Build a nomogram for the ols fit

plot(nomogram(mod\_first))



#### Is this model well-calibrated?

```
set.seed(432); plot(calibrate(mod_first))
```



# Spending degrees of freedom wisely

- Suppose we have a data set with many possible predictors, and minimal theory or subject matter knowledge to guide us.
- We might want our final inferences to be as unbiased as possible. To accomplish this, we have to pay a penalty (in terms of degrees of freedom) for any "peeks" we make at the data in advance of fitting a model.
- So that rules out a lot of decision-making about non-linearity based on looking at the data, if our sample size isn't much larger than 15 times the number of predictors we're considering including in our model.
- In our case, we have n = 64 observations on 10 predictors.
- In addition, adding non-linearity to our model costs additional degrees of freedom.
- What can we do?

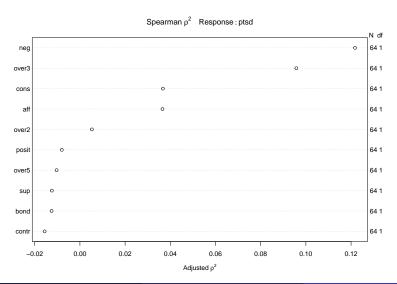
# Spearman's $\rho^2$ plot: A smart first step?

Spearman's  $\rho^2$  is an indicator (not a perfect one) of potential predictive punch, but doesn't give away the game.

• Idea: Perhaps we should focus our efforts re: non-linearity on predictors that score better on this measure.

# **Spearman's** $\rho^2$ **Plot**

#### plot(spear\_ptsd)



# Conclusions from Spearman $\rho^2$ Plot

- neg is the most attractive candidate for a non-linear term, as it packs
  the most potential predictive punch, so if it does turn out to need
  non-linear terms, our degrees of freedom will be well spent.
  - By no means is this suggesting that neg actually needs a non-linear term, or will show significant non-linearity. We'd have to fit a model with and without non-linearity in neg to know that.
  - Non-linearity will often take the form of a product term, a polynomial term, or a restricted cubic spline.
  - Since all of these predictors are quantitative, we'll think about polynomial or spline terms, soon.
- over3, also quantitative, has the next most potential predictive punch
- these are followed by cons and aff

# **Grim Reality**

With 64 observations (63 df) we should be thinking about models with at most 63/15 regression inputs, including the intercept, even if all were linear.

 Non-linear terms (polynomials, splines) just add to the problem, as they need additional df to be estimated.

In this case, we might choose between

- including non-linearity in one (or maybe 2) variables (and that's it),
- or a linear model including maybe 3-4 predictors, tops

in light of the small sample size.

# Contents of spear\_ptsd

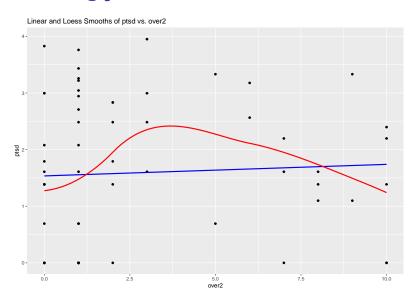
spear\_ptsd

```
rho2 F df1 df2
                         P Adjusted rho2 n
over2 0.021 1.34
                1 62 0.2522
                                  0.005 64
over3 0.110 7.67
                1 62 0.0074
                                  0.096 64
                1 62 0.5527
                                 -0.01064
over5 0.006 0.36
bond 0.004 0.22
                1 62 0.6405
                                 -0.01364
posit 0.008 0.50
                1 62 0.4825
                                 -0.00864
neg 0.136 9.73
                1 62 0.0027
                                0.122 64
contr 0.001 0.03
                1 62 0.8602
                                 -0.01664
sup 0.004 0.23
                1 62 0.6357
                                 -0.01264
cons 0.052 3.40
                  62 0.0699
                                  0.037 64
aff 0.052 3.39
                  62 0.0704
                                  0.037 64
```

Spearman rho^2 Response variable:ptsd

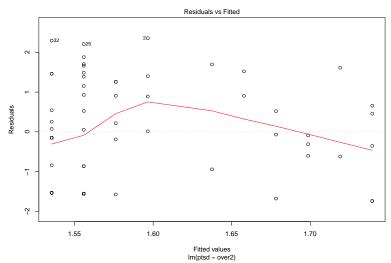
# **Actually Building Non-Linear Models**

# Predicting ptsd from over2



#### Linear Fit - does this work well?

```
plot(lm(ptsd ~ over2, data = maleptsd), which = 1)
```



# **Polynomial Regression**

A polynomial in the variable x of degree D is a linear combination of the powers of x up to D.

For example:

- Linear:  $y = \beta_0 + \beta_1 x$
- Quadratic:  $y = \beta_0 + \beta_1 x + \beta_2 x^2$
- Cubic:  $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$
- Quartic:  $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4$
- Quintic:  $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4 + \beta_5 x^5$

Fitting such a model creates a polynomial regression.

## Raw Quadratic Model for ptsd using over2

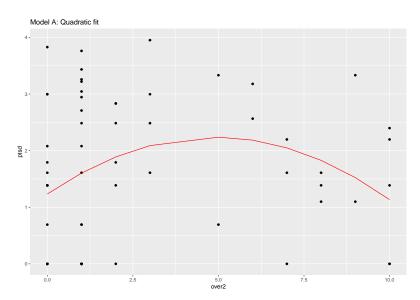
```
modA <- lm(ptsd ~ over2 + I(over2^2), data = maleptsd)
modA</pre>
```

$$ptsd = 1.234 + 0.411(over2) - 0.042(over2)^2$$

# **Summary of Quadratic Fit**

```
> summary(modA)
Call:
lm(formula = ptsd \sim over2 + I(over2^2), data = maleptsd)
Residuals:
   Min 10 Median 30 Max
-2.0487 -1.2341 0.1503 0.9570 2.5945
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 1.23412 0.24958 4.945 6.29e-06 ***
over2 0.41128 0.19271 2.134 0.0369 *
I(over2^2) -0.04213 0.02014 -2.092 0.0407 *
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Residual standard error: 1.246 on 61 degrees of freedom
Multiple R-squared: 0.0696, Adjusted R-squared: 0.03909
F-statistic: 2.281 on 2 and 61 DF, p-value: 0.1108
```

## Plot Fitted Values of Quadratic Fit



#### **Code for Previous Slide**

## Another Way to fit the Identical Model

#### Do models give same fitted values?

```
temp <- fitted(modA2) - fitted(modA)
sum(temp != 0)</pre>
```

[1] 0

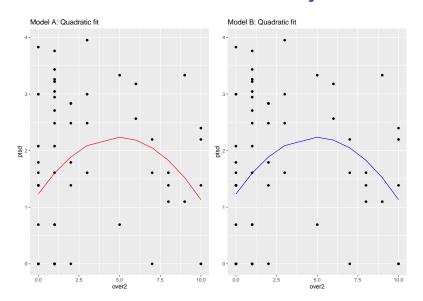
# **Orthogonal Polynomials**

Now, let's fit an orthogonal polynomial of degree 2 to predict ptsd using over2.

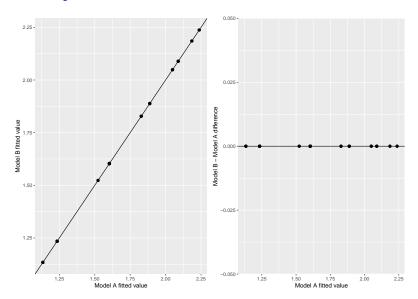
```
modB <- lm(ptsd ~ poly(over2, 2), data = maleptsd)</pre>
```

Looks very different ...

## But it fits the same model, exactly!



# Or, if you don't believe me...



# **Orthogonal Polynomial**

An orthogonal polynomial sets up a model design matrix using the coding we've seen previously: over2 and over2^2 in our case, and then scales those columns so that each column is **orthogonal** to the previous ones.

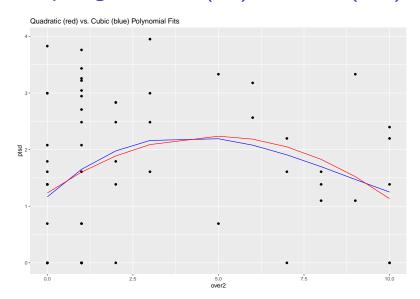
- Two columns are orthogonal if their correlation is zero.
- This eliminates the collinearity (correlation between predictors) and lets our t tests tell us whether the addition of any particular polynomial term improves the fit of the model over the lower orders.

# Would adding a cubic term help predict ptsd?

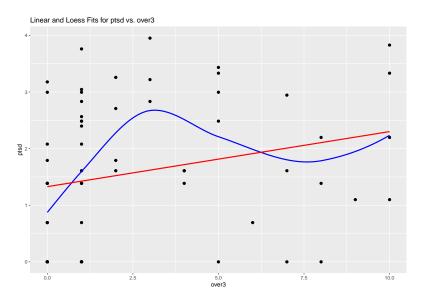
modC <- lm(ptsd ~ poly(over2, 3), data = maleptsd)</pre>

```
> summary(modC)
 Call:
 lm(formula = ptsd \sim poly(over2, 3), data = maleptsd)
 Residuals:
    Min 1Q Median 3Q Max
 -1.9770 -1.1658 0.1784 0.9220 2.6628
 Coefficients:
              Estimate Std. Error t value Pr(>|t|)
 (Intercept) 1.5925 0.1567 10.164 1.15e-14 ***
 poly(over2, 3)1 0.5407 1.2534 0.431 0.6677
 poly(over2, 3)2 -2.6056 1.2534 -2.079 0.0419 *
 poly(over2, 3)3 0.6363 1.2534 0.508 0.6135
 Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
 Residual standard error: 1.253 on 60 degrees of freedom
 Multiple R-squared: 0.07357, Adjusted R-squared: 0.02725
 F-statistic: 1.588 on 3 and 60 DF, p-value: 0.2016
github.com/THOMASELOVE/2019-432
                           432 Class 9 Slides
```

# Comparing Quadratic (red) and Cubic (blue) Models



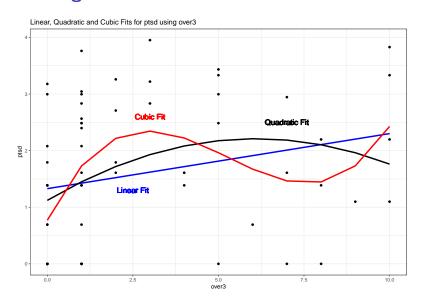
## What if we look instead at over3 as a predictor?



# What if we predict using over3?

```
modD1 <- lm(ptsd ~ over3, data = maleptsd)
modD2 <- lm(ptsd ~ poly(over3, degree = 2), data = maleptsd)
modD3 <- lm(ptsd ~ poly(over3, degree = 3), data = maleptsd)</pre>
```

## Plotting the Fitted Models



# Using Restricted Cubic Splines to Capture Non-Linearity

## **Splines**

- A linear spline is a continuous function formed by connecting points (called knots of the spline) by line segments.
- A restricted cubic spline is a way to build highly complicated curves into a regression equation in a fairly easily structured way.
- A restricted cubic spline is a series of polynomial functions joined together at the knots.
  - Such a spline gives us a way to flexibly account for non-linearity without over-fitting the model.
  - Restricted cubic splines can fit many different types of non-linearities.
  - Specifying the number of knots is all you need to do in R to get a reasonable result from a restricted cubic spline.

The most common choices are 3, 4, or 5 knots.

- 3 Knots, 2 degrees of freedom, allows the curve to "bend" once.
- 4 Knots, 3 degrees of freedom, lets the curve "bend" twice.
- 5 Knots, 4 degrees of freedom, lets the curve "bend" three times.

# Fitting Restricted Cubic Splines with 1m and rcs

For most applications, three to five knots strike a nice balance between complicating the model needlessly and fitting data pleasingly. Let's consider a restricted cubic spline model for ptsd based on over3 again, but now with:

- in modE3, 3 knots, and
- in modE4, 4 knots,

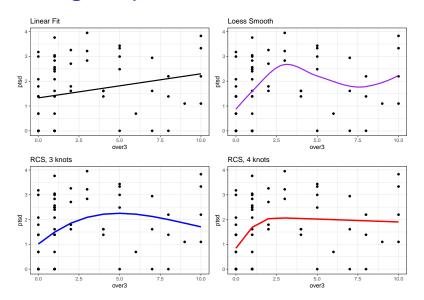
```
modE3 <- lm(ptsd ~ rcs(over3, 3), data = maleptsd)
modE4 <- lm(ptsd ~ rcs(over3, 4), data = maleptsd)</pre>
```

## Summarizing the 4-knot model coefficients

Values of the estimates, and where are the knots located?

```
> round(summary(modE4)$coef,3)
                  Estimate Std. Error t value Pr(>|t|)
                     0.843
                              0.290 2.908
(Intercept)
                                             0.005
rcs(over3, 4)over3 0.953
                              0.432 2.209
                                             0.031
rcs(over3, 4)over3' -8.914 5.982 -1.490
                                             0.141
rcs(over3, 4)over3'' 13.480
                              9.635 1.399
                                             0.167
> attributes(rcs(maleptsd$over3, 4))$parms
[1] 0.00 1.00 2.95 9.00
```

# Plotting the spline models



# Does the fit improve markedly from 3 to 4 knots?

In-sample comparison via ANOVA

```
anova(modE3, modE4)
```

```
Analysis of Variance Table
```

```
Model 1: ptsd ~ rcs(over3, 3)

Model 2: ptsd ~ rcs(over3, 4)

Res.Df RSS Df Sum of Sq F Pr(>F)

1 61 89.598

2 60 87.573 1 2.0246 1.3871 0.2435
```

# Does the fit improve markedly from 3 to 4 knots?

glance(modE3) %>% select(r.squared, adj.r.squared, AIC, BIC)

In-Sample comparisons of information criteria, etc.

r.squared adj.r.squared AIC

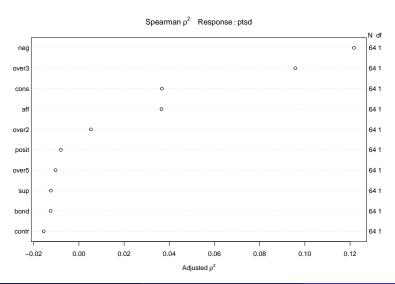
<dbl> <dbl> <dbl> <dbl> <dbl> 222.

BTC

Back to the Spearman's  $\rho^2$  Plot

# **Spearman's** $\rho^2$ **Plot**

#### plot(spear\_ptsd)



# **Proposed New Model F**

Fit a model to predict ptsd using:

- a 4-knot spline on neg
- a 3-knot spline on over3
- a linear term on cons
- a linear term on aff

Still more than we can reasonably do with 64 observations, but let's see how it looks.

#### Fit model F

```
> round(summary(modelf)$coef,3)
                Estimate Std. Error t value Pr(>|t|)
(Intercept)
          -0.425
                           0.749 -0.568 0.572
rcs(neg, 4)neg 0.066
                           0.060 1.095 0.278
rcs(neg, 4)neg' -0.126
                           0.164 -0.768 0.446
                           0.537 0.916 0.363
rcs(neg, 4)neg'' 0.492
rcs(over3, 3)over3 0.458
                           0.201 2.283
                                        0.026
rcs(over3, 3)over3' -2.125
                           0.943 - 2.252
                                         0.028
                 -0.012
                           0.016 - 0.724
                                         0.472
cons
aff
                  0.145
                           0.060 2.424
                                         0.019
```

#### **ANOVA for Model F**

#### anova(modelF)

Analysis of Variance Table

```
Response: ptsd

Df Sum Sq Mean Sq F value Pr(>F)

rcs(neg, 4) 3 14.597 4.8657 3.7342 0.01617 *

rcs(over3, 3) 2 5.892 2.9460 2.2609 0.11369

cons 1 0.636 0.6365 0.4885 0.48751

aff 1 7.657 7.6566 5.8760 0.01860 *

Residuals 56 72.969 1.3030

---

Signif. codes:
0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

Remember that this ANOVA testing is sequential.

#### Is Model F better than Model E3?

```
anova(modelF, modE3)
```

Analysis of Variance Table

```
Model 1: ptsd ~ rcs(neg, 4) + rcs(over3, 3) + cons + aff
Model 2: ptsd ~ rcs(over3, 3)

Res.Df RSS Df Sum of Sq F Pr(>F)

1 56 72.969

2 61 89.598 -5 -16.629 2.5524 0.03769 *

---

Signif. codes:
0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

# Limitations of 1m for fitting complex linear models

We can certainly assess this big, complex model using 1m in comparison to other models:

- with in-sample summary statistics like adjusted R<sup>2</sup>, AIC and BIC,
- we can assess its assumptions with residual plots, and
- we can also compare out-of-sample predictive quality through cross-validation,

But to really delve into the details of how well this complex model works, and to help plot what is actually being fit, we'll probably want to fit the model using ols, from the rms package.

 Again, a detailed discussion of ols is found in Chapter 10 of the Course Notes. We'll look at some key ideas now. Using ols to fit a complex linear model

## Model F, fitted using ols

## modF\_ols results (slide 1 of 2)

```
> modF_ols
Linear Regression Model
ols(formula = ptsd \sim rcs(neg, 4) + rcs(over3, 3) + cons + aff,
    data = maleptsd, x = TRUE, y = TRUE)
            Model Likelihood Discrimination
               Ratio Test
                                Indexes
Obs 64 LR chi2 21.28 R2 0.283
sigma1.1415 d.f. 7 R2 adj 0.193
d.f. 56 Pr(> chi2) 0.0034
                             q 0.763
Residuals
    Min 1Q Median 3Q Max
-2.06529 -0.81434 0.06745 0.81760 2.17200
```

# modF\_ols results (slide 2 of 2)

	Coef	S.E.	t	Pr(> t )
Intercept	-0.4255	0.7490	-0.57	0.5723
neg		0.0603		
neg'	-0.1261	0.1641	-0.77	0.4456
neg''	0.4924	0.5373	0.92	0.3634
over3	0.4582	0.2007	2.28	0.0263
over3'	-2.1247	0.9433	-2.25	0.0282
cons	-0.0119	0.0164	-0.72	0.4722
aff	0.1450	0.0598	2.42	0.0186

## **Validation of Summary Statistics**

```
set.seed(4322019); validate(modF_ols)
```

```
index.orig training test optimism
R-square
             0.2829
                     0.3747 0.1457
                                     0.2290
             1.1401 0.9753 1.3582 -0.3830
MSF.
           0.7630 0.8600 0.6520 0.2080
g
          0.0000 0.0000 0.4452 -0.4452
Intercept
Slope
          1.0000 1.0000 0.7327 0.2673
         index.corrected n
                  0.0538 40
R-square
MSE
                  1.5231 40
                  0.5550 40
g
                 0.4452 40
Intercept
                  0.7327 40
Slope
```

## anova results for modF\_ols

#### anova(modF\_ols)

1	Analysis of Variance			Response:		ptsd
Factor	d.f.	Partial SS	MS	F	P	
neg	3	11.4062336	3.8020779	2.92	0.0420	
Nonlinear	2	1.6536591	0.8268295	0.63	0.5339	
over3	2	6.8378486	3.4189243	2.62	0.0814	
Nonlinear	1	6.6106843	6.6106843	5.07	0.0282	
cons	1	0.6826901	0.6826901	0.52	0.4722	
aff	1	7.6565797	7.6565797	5.88	0.0186	
TOTAL NONLINEAR	3	7.8079300	2.6026433	2.00	0.1248	
REGRESSION	7	28.7821644	4.1117378	3.16	0.0070	
ERROR	56	72.9688769	1.3030157			

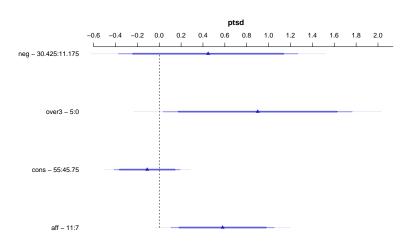
## summary results for modF\_ols

#### summary(modF\_ols)

```
Effects
                              Response: ptsd
Factor Low High Diff. Effect S.E. Lower 0.95
      11.175 30.425 19.25 0.44727 0.41704 -0.388160
neg
over3 0.000 5.000 5.00 0.90059 0.43913 0.020902
cons 45.750 55.000 9.25 -0.10997 0.15192 -0.414310
aff 7.000 11.000 4.00 0.57998 0.23926 0.100680
Upper 0.95
1.28270
1.78030
0.19437
1.05930
```

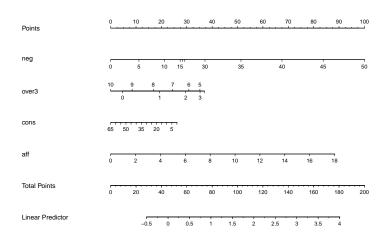
## Plot of summary results for modF\_ols

plot(summary(modF\_ols))



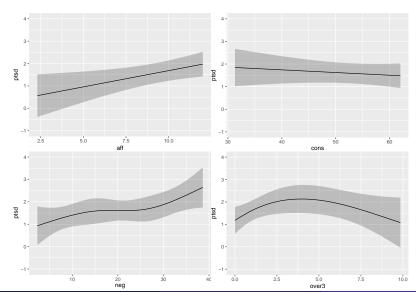
## Nomogram for modF\_ols

plot(nomogram(modF\_ols))



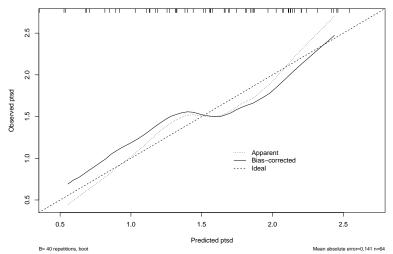
# Seeing the impact of the modeling another way

ggplot(Predict(modF\_ols))



# Checking the model's calibration

set.seed(43220191); plot(calibrate(modF\_ols))



#### **Next Time**

- The HERS data
- Fitting a more complex linear regression model
  - Dealing with categorical predictors
  - Dealing with interactions (another form of non-linearity)
  - Adding missing data into all of this, and running multiple imputation