432 Class 9 Slides

github.com/THOMASELOVE/2020-432

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Setup

```
library(janitor); library(magrittr); library(here)
library(skimr)
library(broom)
library(rms)
library(patchwork)
library(GGally)
library(tidyverse)
theme_set(theme_bw())
```

Today's Materials

- The maleptsd data
- Using ols to fit a linear model
 - ANOVA in ols
 - Plot Effects with summary and Predict
 - Validating summary statistics like R²
 - Nomogram
 - Evaluating Calibration
- Spending Degrees of Freedom on Non-Linearity
 - The Spearman ρ^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 1 . 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.

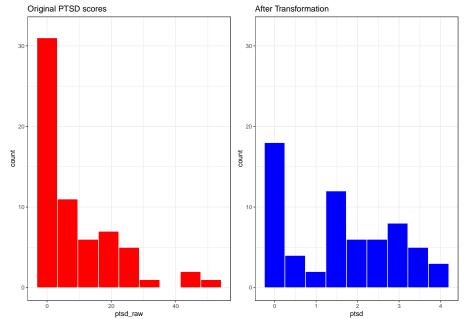
```
maleptsd <- read_csv(here("data/maleptsd.csv")) %>%
    clean_names() %>%
    mutate(ptsd = log(ptsd_raw + 1))
```

¹Source: 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.

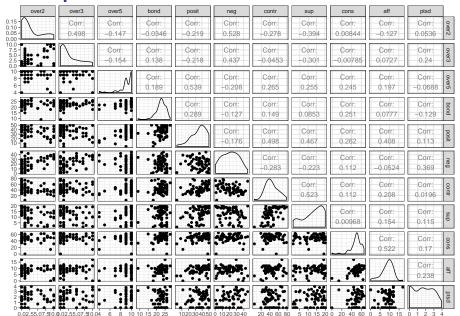
Skimming the maleptsd data

```
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 13
                                       5.87 1.2
                                                 9.28 14.25 18.3
      sup
                         64
                                                                   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.

Contents of mod_first?

```
> mod_first
Linear Regression Model
```

ols(formula = ptsd ~ over2 + over3, data = maleptsd)

		Model Likelihood		Discrimination	
		Ratio Test		Indexes	
0bs	64	LR chi2	4.18	R2	0.063
sigma1.2500		d.f.	2	R2 adj	0.033
d.f.	61	Pr(> chi2)	0.1235	a	0.345

Residuals

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)

```
Analysis of Variance Response: ptsd

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
```

summary for mod_first fit by ols

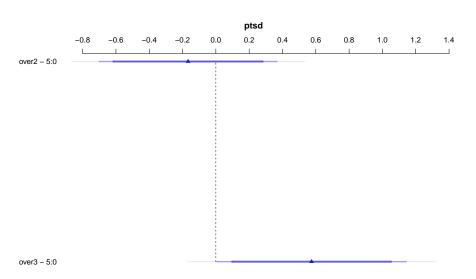
```
summary(mod_first)
```

```
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
```

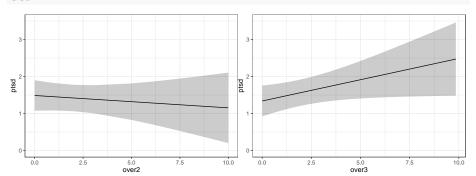
Plot the summary to see effect sizes

plot(summary(mod_first))



What do the individual effects look like?

ggplot(Predict(mod_first))



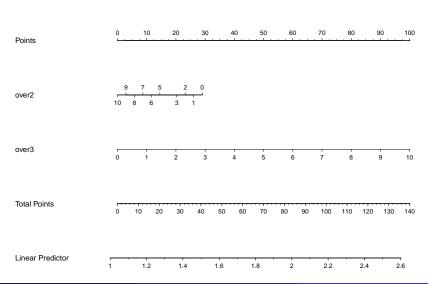
Validate the summary statistics of an ols fit

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

```
index.orig training test optimism
             0.0633 0.0812 0.0309
R-square
                                    0.0503
             1.4893 1.4426 1.5408 -0.0982
MSF.
           0.3450 0.3607 0.3055 0.0552
g
         0.0000 0.0000 0.2893 -0.2893
Intercept
         1.0000 1.0000 0.8371
                                    0.1629
Slope
         index.corrected n
R-square
                  0.0130 40
                  1.5874 40
MSE.
                  0.2899 40
g
                 0.2893 40
Intercept
Slope
                 0.8371 40
```

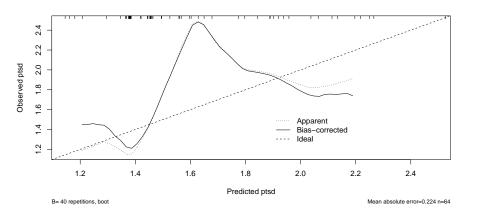
Build a nomogram for the ols fit

plot(nomogram(mod_first))



Is this model well-calibrated?

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



n = 64Mean absolute error=0.224 Mean squared error=0.1048

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?

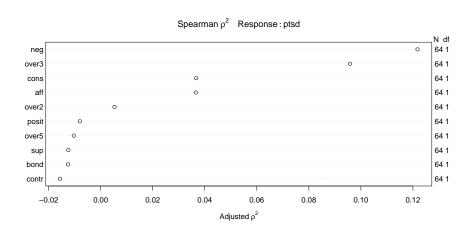
Spearman's ρ^2 plot: A smart first step?

Spearman's ρ^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 ρ^2 **Plot**

plot(spear_ptsd)



Conclusions from Spearman ρ^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 relatively tiny numbers of regression inputs.

 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

and even that would be tough to justify with this small sample size.

Contents of spear_ptsd

spear_ptsd

```
Spearman rho^2 Response variable: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
over5 0.006 0.36
                1 62 0.5527
                                 -0.01064
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
                  62 0.8602
                                 -0.01664
sup 0.004 0.23
                1 62 0.6357
                                 -0.01264
cons 0.052 3.40
                1 62 0.0699
                                  0.037 64
aff 0.052 3.39
                   62 0.0704
                                  0.037 64
```

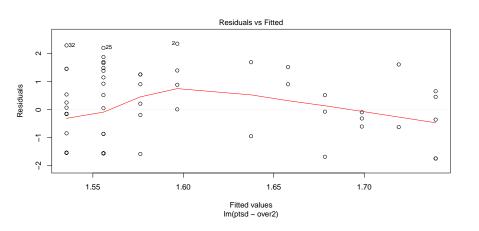
Actually Building Non-Linear Models

Predicting ptsd from over2

Linear and Loess Smooths of ptsd vs. over2 0.0 2.5 5.0 7.5 10.0 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>
```

```
Call:
```

```
lm(formula = ptsd ~ over2 + I(over2^2), data = maleptsd)
```

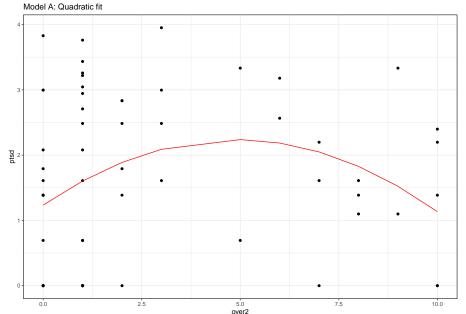
Coefficients:

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

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

```
modA2 <- lm(ptsd ~ pol(over2, degree = 2, raw = TRUE),</pre>
              data = maleptsd)
Coefficients:
                                      pol(over2, degree = 2, raw = TRUE)over2
                          (Intercept)
                             1.23412
                                                                  0.41128
pol(over2, degree = 2, raw = TRUE)over2^2
                             -0.04213
Do models give same fitted values?
temp <- fitted(modA2) - fitted(modA)
sum(temp != 0)
Γ1 0
```

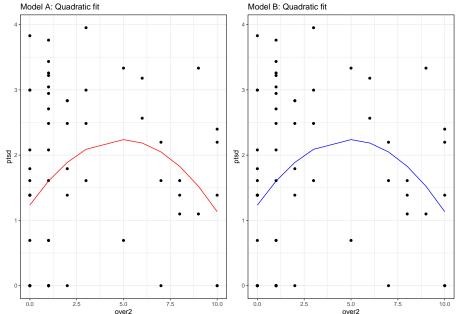
Orthogonal Polynomials

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

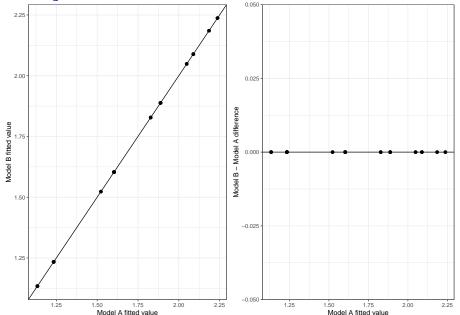
```
modB <- lm(ptsd ~ poly(over2, 2), data = maleptsd)</pre>
```

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 10 Median 30 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
```

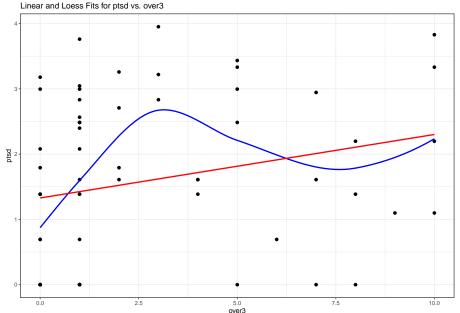
F-statistic: 1.588 on 3 and 60 DF, p-value: 0.2016 432 Class 9 Slides

37 / 66

Comparing Quadratic (red) and Cubic (blue) Models

Quadratic (red) vs. Cubic (blue) Polynomial Fits pstd 2 2.5 5.0 7.5 10.0 over2

What if we look instead at over3 as a predictor?



What if we predict using over3?

modD1 <- lm(ptsd ~ over3, data = maleptsd)</pre>

Plotting the Fitted Models

Linear, Quadratic and Cubic Fits for ptsd using over3 Cubic Fit Quadratic Fit ptg 2 Linear Fit 2.5 5.0 7.5 10.0 0.0

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,

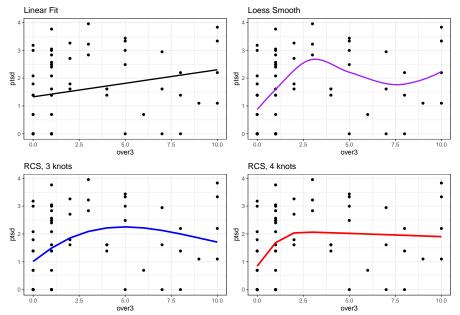
```
modE3 <- lm(ptsd ~ rcs(over3, 3), data = maleptsd)
modE4 <- lm(ptsd ~ rcs(over3, 4), data = maleptsd)</pre>
```

Summarizing the 4-knot model coefficients

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

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

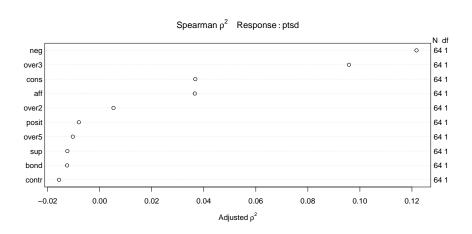
Does the fit improve markedly from 3 to 4 knots?

In-Sample comparisons of information criteria, etc.

```
glance(modE3) %>% select(r.squared, adj.r.squared, AIC, BIC)
# A tibble: 1 x 4
 r.squared adj.r.squared AIC BIC
     <dbl> <dbl> <dbl> <dbl> <dbl> <
     0.119 0.0906 211. 220.
glance(modE4) %>% select(r.squared, adj.r.squared, AIC, BIC)
# A tibble: 1 \times 4
 r.squared adj.r.squared AIC
                                BIC
     <dbl> <dbl> <dbl> <dbl> <dbl> <
 0.139 0.0963 212. 222.
```

Back to Spearman's ρ^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

```
modelF \leftarrow lm(ptsd \sim rcs(neg, 4) + rcs(over3, 3) +
              cons + aff, data = maleptsd)
> 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
rcs(neg, 4)neg'' 0.492
                             0.537 0.916
                                           0.363
rcs(over3, 3)over3 0.458
                             0.201 2.283
                                           0.026
rcs(over3, 3)over3' -2.125
                             0.943 - 2.252
                                           0.028
cons
                   -0.012
                             0.016 - 0.724
                                           0.472
```

0.145

aff

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
    1 0.636 0.6365 0.4885 0.48751
cons
           1 7.657 7.6566 5.8760 0.01860 *
aff
Residuals 56 72.969 1.3030
Signif. codes:
0 '***' 0.001 '**' 0.01 '*' 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 \sim rcs(neg, 4) + rcs(over3, 3) + cons + aff
Model 2: ptsd ~ rcs(over3, 3)
 Res.Df RSS Df Sum of Sq F Pr(>F)
     56 72.969
2 61 89.598 -5 -16.629 2.5524 0.03769 *
Signif. codes:
0 '***' 0.001 '**' 0.01 '*' 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 R², 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.

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	0.0660	0.0603	1.10	0.2780
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
                     0.3771 0.1484
                                    0.2287
             1.1401 0.9700 1.3539 -0.3838
MSE
           0.7630 0.8665 0.6393 0.2272
g
         0.0000 0.0000 0.4268 -0.4268
Intercept
          1.0000 1.0000 0.7228
                                    0.2772
Slope
         index.corrected n
R-square
                  0.0542 40
                  1.5240 40
MSE.
                  0.5358 40
g
                 0.4268 40
Intercept
Slope
                  0.7228 40
```

anova results for modF_ols

anova(modF_ols)

	Analy	analysis of Variance			Response: p		
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

Effects

summary(modF_ols)

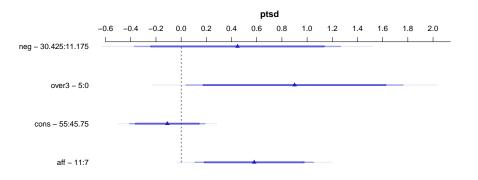
```
Factor Low High Diff. Effect S.E. Lower 0.95 neg 11.175 30.425 19.25 0.44727 0.41704 -0.388160 over3 0.000 5.000 5.00 0.90059 0.43913 0.020902 cons 45.750 55.000 9.25 -0.10997 0.15192 -0.414310 aff 7.000 11.000 4.00 0.57998 0.23926 0.100680 Upper 0.95 1.28270 1.78030
```

Response : ptsd

0.19437

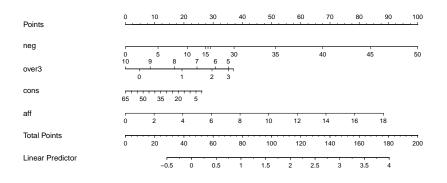
Plot of summary results for modF_ols

plot(summary(modF_ols))

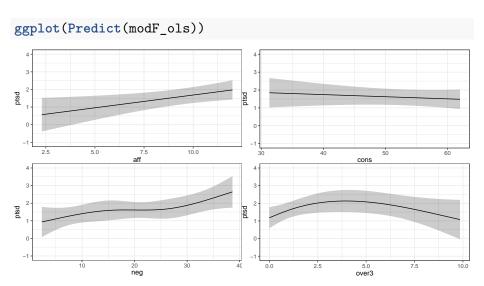


Nomogram for modF_ols

plot(nomogram(modF_ols))

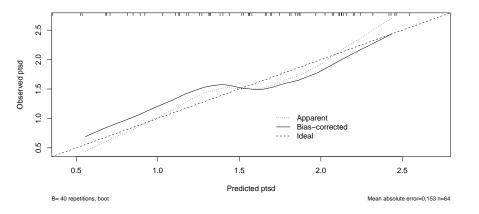


Seeing the impact of the modeling another way



Checking the model's calibration

set.seed(43220191); plot(calibrate(modF ols))



Mean absolute error=0.153 n=64Mean squared error=0.02813

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