# 432 Class 07 Slides

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# Setup

```
library(mosaic)                ## auto-loads mosaicData
library(here)
library(janitor)
library(magrittr)
library(knitr)
library(broom)
library(patchwork)
library(GGally)                ## for scatterplot matrix
library(rms)                   ## auto-loads Hmisc
library(tidyverse)

theme_set(theme_bw())
```

# Today's Materials

- The HELP study (today's data) and preliminaries
- Using `ols` to fit a linear model
  - Obtaining coefficients and basic summaries
  - Validating summary statistics like $R^2$
  - ANOVA in `ols`
  - Plot Effects with `summary` and `Predict`
  - Building and using a nomogram
  - Evaluating Calibration
  - Influential points and `dfbeta`
- Spending Degrees of Freedom on Non-Linearity
  - The Spearman $\rho^2$ (rho-squared) plot
- Building Non-Linear Predictors in `ols`
  - Polynomial Functions
  - Restricted Cubic Splines
  - Resticting Interaction (Product) Terms

# Today's Data, from the HELP study

# Today's Data (`day7`, from the HELP study)

Today's data set comes from the Health Evaluation and Linkage to Primary Care trial, and is stored as `HELPrct` in the `mosaicData` package. HELP was a clinical trial of adult inpatients recruited from a detoxification unit. Patients with no primary care physician were randomized to receive a multidisciplinary assessment and a brief motivational intervention or usual care, with the goal of linking them to primary medical care. We will look at 453 subjects with complete data today.

```
day7 <- tibble(mosaicData::HELPrct) %>%
    select(id, cesd, age, sex, subst = substance,
           mcs, pcs, pss_fr)

dim(day7)
```

```
[1] 453   8
```

# Key Variables for Today

| Variable | Description |
|---|---|
| `id` | subject identifier |
| `cesd` | Center for Epidemiologic Studies Depression measure (higher scores indicate more depressive symptoms) |
| `age` | subject age (in years) |
| `sex` | female (n = 107) or male (n = 346) |
| `subst` | primary substance of abuse (alcohol, cocaine or heroin) |
| `mcs` | SF-36 Mental Component Score (lower = worse status) |
| `pcs` | SF-36 Physical Component Score (lower = worse status) |
| `pss_fr` | perceived social support by friends (higher = more support) |

- All measures from baseline during the subjects' detoxification stay.
- More data and details at https://nhorton.people.amherst.edu/help/.

# The day7 categorical data

```
day7 %>% tabyl(sex, subst) %>%
    adorn_totals(where = c("row", "col")) %>%
    adorn_percentages() %>%
    adorn_pct_formatting() %>%
    adorn_ns(position = "front") %>%
    adorn_title(placement = "combined") %>%
    kable(align = 'lrrrr')
```

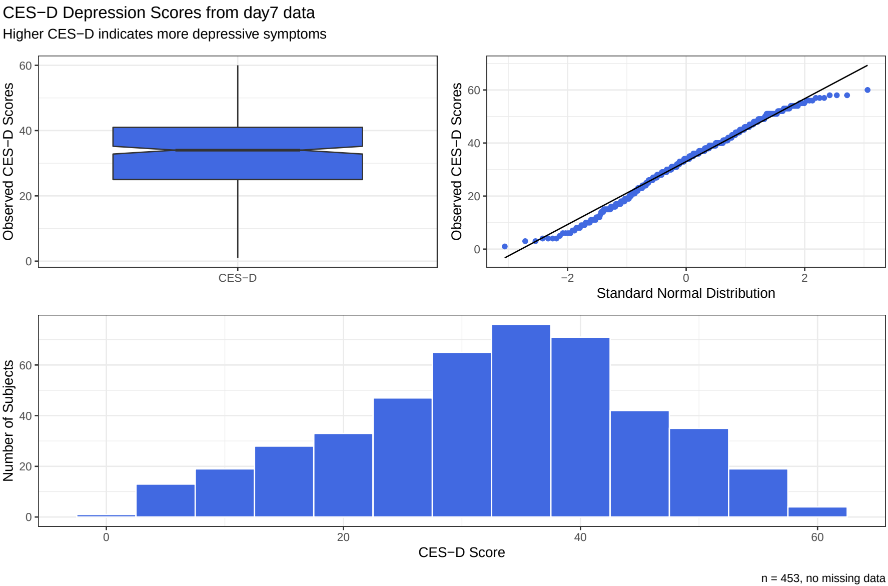
| sex/subst | alcohol | cocaine | heroin | Total |
|:---|---:|---:|---:|---:|
| female | 36 (33.6%) | 41 (38.3%) | 30 (28.0%) | 107 (100.0%) |
| male | 141 (40.8%) | 111 (32.1%) | 94 (27.2%) | 346 (100.0%) |
| Total | 177 (39.1%) | 152 (33.6%) | 124 (27.4%) | 453 (100.0%) |

# Summarizing the day7 quantitative data

```
day7 %>% select(cesd, age, mcs, pcs, pss_fr) %>%
    inspect(digits = 2)
```

```
quantitative variables:
       name   class  min Q1 median Q3 max mean   sd   n
...1   cesd integer  1.0 25     34 41  60 32.8 12.5 453
...2    age integer 19.0 30     35 40  60 35.7  7.7 453
...3    mcs numeric  6.8 22     29 41  62 31.7 12.8 453
...4    pcs numeric 14.1 40     49 57  75 48.0 10.8 453
...5 pss_fr integer  0.0  3      7 10  14  6.7  4.0 453
     missing
...1       0
...2       0
...3       0
...4       0
...5       0
```

# Our Outcome (CES-Depression score)



# Hmisc::describe() for our outcome CES-D

```
day7 %$% describe(cesd)
```

```
cesd : CESD at baseline
       n  missing distinct     Info     Mean      Gmd
     453        0       58    0.999    32.85    14.23
     .05      .10      .25      .50      .75      .90
    10.0     15.2     25.0     34.0     41.0     49.0
     .95
    52.4

lowest :  1  3  4  5  6, highest: 55 56 57 58 60
```

- `Info` measures the variable's information between 0 and 1: the higher the `Info`, the more continuous the variable is (the fewer ties there are.)
- `Gmd` = Gini's mean difference, a robust measure of variation. If you randomly selected two of the 453 subjects many times, the mean difference in `cesd` would be 14.23 points.

# We have some labels in our data

```
str(day7)
```

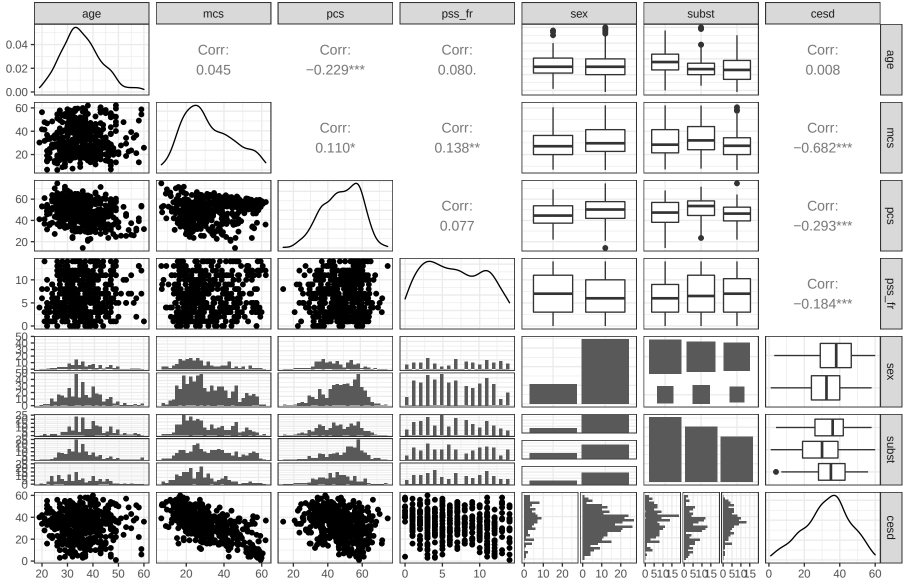
```
tibble [453 x 8] (S3: tbl_df/tbl/data.frame)
 $ id    : int [1:453] 1 2 3 4 5 6 7 8 9 10 ...
  ..- attr(*, "label")= chr "subject ID"
 $ cesd  : int [1:453] 49 30 39 15 39 6 52 32 50 46 ...
  ..- attr(*, "label")= chr "CESD at baseline"
 $ age   : int [1:453] 37 37 26 39 32 47 49 28 50 39 ...
  ..- attr(*, "label")= chr "age (years)"
 $ sex   : Factor w/ 2 levels "female","male": 2 2 2 1 2 1 1 2
  ..- attr(*, "label")= chr "sex"
 $ subst : Factor w/ 3 levels "alcohol","cocaine",..: 2 1 3 3
  ..- attr(*, "label")= chr "primary substance of abuse"
 $ mcs   : num [1:453] 25.11 26.67 6.76 43.97 21.68 ...
  ..- attr(*, "label")= chr "SF-36 Mental Component Score"
 $ pcs   : num [1:453] 58.4 36 74.8 61.9 37.3 ...
  ..- attr(*, "label")= chr "SF-36 Physical Component Score"
```

# Scatterplot Matrix (code)

```
temp <- day7 %>%
    select(age, mcs, pcs, pss_fr, sex, subst, cesd)

ggpairs(temp)  ## ggpairs from the GGally package
```

Note that we're placing the outcome (`cesd`) last, and we'll want to set message = FALSE in the code chunk when producing the result (next slide.)

# Scatterplot Matrix (result)



# Saving the Data Set

```r
saveRDS(day7, here("data", "day7.Rds"))
```

Could also have used

```r
saveRDS(day7, here("data/day7.Rds"))
```

# Using `ols` to fit a linear regression model

# Fitting using `ols`

The `ols` function stands for ordinary least squares and comes from the `rms` package, by Frank Harrell and colleagues. Any model fit with `lm` can also be fit with `ols`.

- To predict `var_y` using `var_x` from the `my_tibble` data, we would use the following syntax:

```
dd <- datadist(my_tibble)
options(datadist = "dd")

model_name <- ols(var_y ~ var_x, data = my_tibble,
                  x = TRUE, y = TRUE)
```

This leaves the following questions:

1. What's the `datadist` stuff doing?
2. Why use `x = TRUE, y = TRUE` in the fit?

# What is `datadist`?

Before we fit any `ols` model to data from `my_tibble`, we'll use:

```
dd <- datadist(my_tibble)
options(datadist = "dd")
```

> *Run (the datadist code above) once before any models are fitted, storing the distribution summaries for all potential variables. Adjustment values are 0 for binary variables, the most frequent category (or optionally the first category level) for categorical (factor) variables, the middle level for ordered factor variables, and medians for continuous variables.*

- excerpted from the `datadist` documentation

## Why use `x = TRUE, y = TRUE` in the fit?

Once we've set up the distribution summaries with the `datadist` code, we fit linear regression models using the same fitting routines as `lm` with `ols`:

```
model_name <- ols(var_y ~ var_x, data = my_tibble,
                  x = TRUE, y = TRUE)
```

- `ols` stores additional information beyond what `lm` does
- `x = TRUE` and `y = TRUE` save even more expanded information that we'll need in building plots and summaries of the fit.
- The defaults are `x = FALSE, y = FALSE`, but in this class, we'll always want to include these additional pieces.

# Using `ols` to fit a Two-Predictor Model

Now, we'll fit an `ols` model predicting our outcome (`cesd`) using two predictors (`mcs` and `subst`) using the `day7` tibble.

- Start with setting the `datadist` up
- Then fit the model, including `x = TRUE, y = TRUE`

```
dd <- datadist(day7)
options(datadist = "dd")

mod1 <- ols(cesd ~ mcs + subst, data = day7,
            x = TRUE, y = TRUE)
```

# Contents of `mod1`?

```
mod1
```

```
> mod1
Linear Regression Model

 ols(formula = cesd ~ mcs + subst, data = day7, x = TRUE, y = TRUE)

                 Model Likelihood    Discrimination
                       Ratio Test           Indexes
 Obs      453    LR chi2     295.10    R2         0.479
 sigma9.0657     d.f.             3    R2 adj     0.475
 d.f.     449    Pr(> chi2) 0.0000    g          9.827

 Residuals

       Min        1Q    Median        3Q       Max
 -25.43696  -6.74592   0.09334   6.16212  24.24842


               Coef    S.E.   t      Pr(>|t|)
 Intercept      55.3026 1.2724  43.46 <0.0001
 mcs            -0.6570 0.0337 -19.48 <0.0001
 subst=cocaine -3.4440 1.0055  -3.43 0.0007
 subst=heroin  -1.7791 1.0681  -1.67 0.0965
```

- Likelihood Ratio Test?
- What is the discrimination index g?

# New elements in `ols`

For our `mod1`,

- Model Likelihood Ratio test output includes `LR chi2 = 295.10, d.f. = 3, Pr(> chi2) = 0.0000`

The log of the likelihood ratio, multiplied by -2, yields a test against a $\chi^2$ distribution. Interpret this as a goodness-of-fit test that compares `mod_first` to a null model with only an intercept term. In `ols` this is similar to a global (ANOVA) F test.

- Under the $R^2$ values, we have `g = 9.827`.
- This is the $g$-index, based on Gini's mean difference. If you randomly selected two of the subjects in the model, the average difference in predicted `cesd` will be 9.827.
- This can be compared to the Gini's mean difference for the original `ptsd` values, from `Hmisc::describe`, which was `Gmd = 14.23`.

# Validate the summary statistics of an `ols` fit

- Can we validate summary statistics by resampling?

```
set.seed(4322022)
validate(mod1)
```

```
> validate(mod1)
          index.orig training    test optimism index.corrected  n
R-square      0.4787   0.4827  0.4741   0.0086          0.4701 40
MSE          81.4606  81.6585 82.1755  -0.5170         81.9776 40
g             9.8272   9.9173  9.8011   0.1162          9.7110 40
Intercept     0.0000   0.0000  0.2719  -0.2719          0.2719 40
Slope         1.0000   1.0000  0.9914   0.0086          0.9914 40
```

- The data used to fit the model provide an over-optimistic view of the quality of fit.
- We're interested here in assessing how well the model might work in new data, and to do so, we can use a resampling approach.
- Consider $R^2$ here...

# Interpreting the Resampling Validation Results

```
         index.orig training   test optimism index.corrected  n
R-square     0.4787   0.4827 0.4741   0.0086          0.4701 40
```

- `index.orig` for $R^2$ is 0.4787. That's what we get from the data we used to fit the model, and is what we see in our standard output.
- With `validate` we create 40 (by default) bootstrapped resamples of the data and then split each of those into training and test samples.
  - For each of the 40 splits, R refits the model (same predictors) in the `training` sample to obtain $R^2$: mean across 40 splits is 0.4827
  - Check each model in its `test` sample: average $R^2$ was 0.4741
- `optimism` = `training` result - `test` result = 0.0086
- `index.corrected` = `index.orig` - `optimism` = 0.4701

While our *nominal* $R^2$ is 0.4787 for this model, but correcting for optimism yields a *validated* $R^2$ of 0.4701.

- $R^2 = 0.4701$ better estimates how the model will perform in new data.

# ANOVA for `mod1` fit by `ols`

```
anova(mod1)
```

```
> anova(mod1)
                Analysis of Variance          Response: cesd

 Factor     d.f. Partial SS MS          F      P
 mcs          1  31182.7237 31182.72373 379.42 <.0001
 subst        2    968.7563   484.37816   5.89 0.003
 REGRESSION   3  33886.8359 11295.61195 137.44 <.0001
 ERROR      449  36901.6542    82.18631
```

- This adds a line for the complete regression model (both terms) which can be helpful, but is otherwise the same as `anova` after `lm`.
- As with `lm`, this is a sequential ANOVA table, so if we had included `subst` in the model first, we'd get a different SS, MS, F and p for `mcs` and `subst`, but the same `REGRESSION` and `ERROR` results.

# summary for `mod1` fit by `ols`

```r
summary(mod1)
```

```
> summary(mod1)
             Effects              Response : cesd

Factor                   Low    High   Diff.  Effect   S.E.    Lower 0.95 Upper 0.95
mcs                      21.676 40.941 19.266 -12.6580 0.64984 -13.9350   -11.38100
subst - cocaine:alcohol   1.000  2.000     NA  -3.4440 1.00550  -5.4200    -1.46790
subst - heroin:alcohol    1.000  3.000     NA  -1.7791 1.06810  -3.8782     0.31993
```

- How do we interpret the `subst` effects estimated by this model?
  - Effect of `subst` being `cocaine` instead of `alcohol` on `ces_d` is `-3.4440` assuming no change in `mcs`, with 95% CI (-5.42, -1.47).
  - Effect of `subst` being `heroin` instead of `alcohol` on `ces_d` is `-1.7791` assuming no change in `mcs`, with 95% CI (-3.88, +0.32).

But what about the `mcs` effect?

# summary for `mod1` fit by `ols`

```
summary(mod1)
```

```
> summary(mod1)
             Effects              Response : cesd

 Factor                      Low    High   Diff.  Effect   S.E.    Lower 0.95 Upper 0.95
 mcs                         21.676 40.941 19.266 -12.6580 0.64984 -13.9350   -11.38100
 subst - cocaine:alcohol      1.000  2.000     NA  -3.4440 1.00550  -5.4200    -1.46790
 subst - heroin:alcohol       1.000  3.000     NA  -1.7791 1.06810  -3.8782     0.31993
```

- Effect of `mcs`: `-12.6580` is the estimated change in `cesd` associated with a move from `mcs` = 21.676 (see `Low` value) to `mcs` = 40.941 (the `High` value) assuming no change in `subst`.
- `ols` chooses the `Low` and `High` values from the interquartile range.

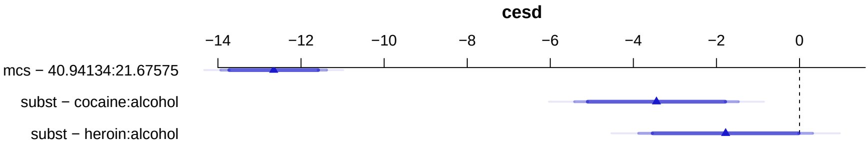
```
day7 %$% quantile(mcs, c(0.25, 0.75))
```

```
     25%      75% 
21.67575 40.94134 
```

# Plot the summary to see effect sizes

- Goal: plot effect sizes for similar moves within predictor distributions.

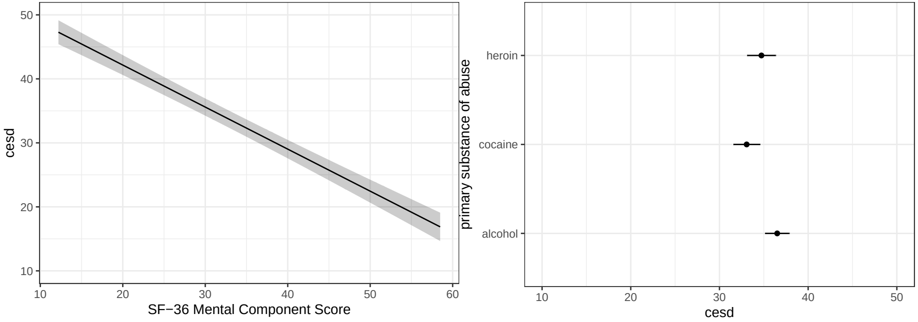
```
plot(summary(mod1))
```




- The triangles indicate the point estimate, augmented with confidence interval bars.
  - The 90% confidence intervals are plotted with the thickest bars.
  - The 95% CIs are then shown with thinner, more transparent bars.
  - Finally, the 99% CIs are shown as the longest, thinnest bars.

# What do the individual effects look like?

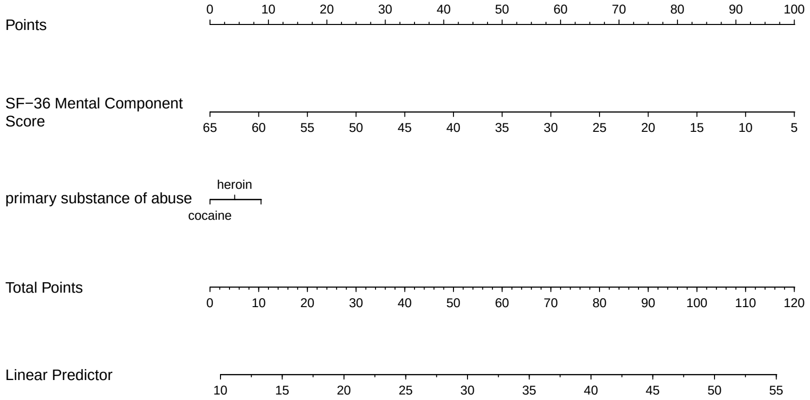
```
ggplot(Predict(mod1, conf.int = 0.95), layout = c(1,2))
```




- The left plot shows the impact of changing `mcs` on `cesd` holding `subst` at its baseline level (alcohol).
- The right plot shows the impact of changing `subst` on `cesd` holding `mcs` at its median value which is 28.602417.
- Defaults: add 95% CI bands and layout tries for a square.

# Build a nomogram for the `ols` fit

```
plot(nomogram(mod1))
```



# Nomograms

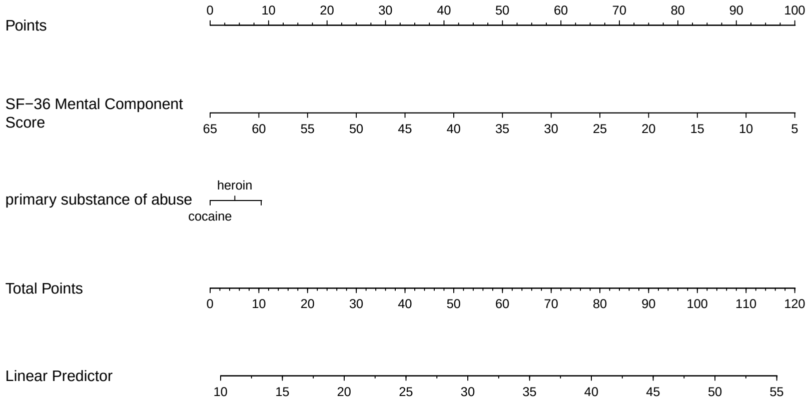
For complex models (this model isn't actually very complex) it can be helpful to have a tool that will help you see the modeled effects in terms of their impact on the predicted outcome.

A *nomogram* is an established graphical tool for doing this.

- Find the value of each predictor on its provided line, and identify the "points" for that predictor by drawing a vertical line up to the "Points".
- Then sum up the points over all predictors to obtain "Total Points".
- Draw a vertical line down from the "Total Points" to the "Linear Predictor" to get the predicted `cesd` for this subject.

# Using the nomogram for the `mod1` fit

Predicted `cesd` for a subject with `mcs` = 35 and `subst` = heroin?



# Actual Prediction for such a subject. . .

- The `predict` function for our `ols` fit provides fitted values.

```
predict(mod1,
          newdata = tibble(mcs = 35, subst = "heroin"))
```

```
       1
30.52766
```

- The `broom` package doesn't (really) support `rms` fits, and throws a warning (omitted here), but you could always refit the model with `lm`. . .

```
augment(mod1,
          newdata = tibble(mcs = 35, subst = "heroin"))
```

```
# A tibble: 1 x 3
    mcs subst  .fitted
  <dbl> <chr>    <dbl>
1    35 heroin    30.5
```

# Assessing the Calibration of `mod1`

We would like our model to be well-calibrated, in the following sense...

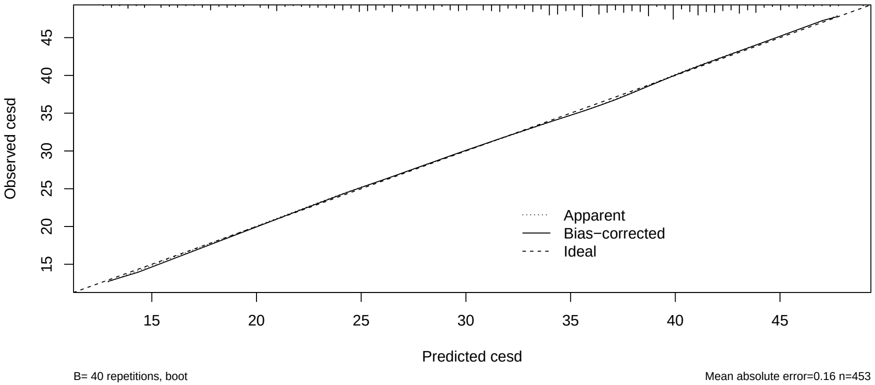
- Suppose our model assigns a predicted outcome of 6 to several subjects. If the model is well-calibrated, then we expect the mean of those subjects' actual outcomes to be very close to 6.

We'd like to look at the relationship between the observed `cesd` outcome and our predicted `cesd` from the model.

- The calibration plot we'll create provides two estimates (with and without bias-correction) of the predicted vs. observed values of our outcome, and compares these to the ideal scenario (predicted = observed).
- The plot uses resampling validation to produce bias-corrected estimates and uses lowess smooths to connect across predicted values.
- Calibration plots require `x = TRUE, y = TRUE` in the `ols` fit.

# Calibration Plot for `mod1`

```
set.seed(4320123); plot(calibrate(mod1))
```




```
n=453   Mean absolute error=0.16   Mean squared error=0.03522
0.9 Quantile of absolute error=0.32
```

# Influential Points for `mod1`?

The `dfbeta` value for a particular subject and coefficient $\beta$ is the change in the coefficient that happens when the subject is excluded from the model.

```
which.influence(mod1, cutoff = 0.2)
```

```
$Intercept
[1]   8 351 405 433

$mcs
[1] 351 402 450

$subst
[1] 351
```

- These are the subjects that have absolute values of `dfbetas` that exceed the specified cutoff (default is 0.2 but it's an arbitrary choice.)

# Show the influential points more directly?

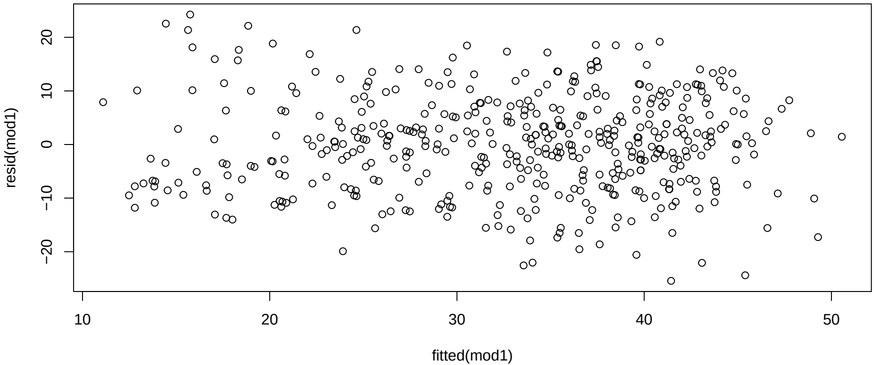
```
w <- which.influence(mod1, cutoff = 0.2)
d <- day7 %>% select(mcs, subst, cesd) %>% data.frame()
show.influence(w, d)
```

```
    Count       mcs   subst
8       1   9.16053  alcohol
351     3 *57.48944 *heroin
402     1 *55.47938  alcohol
405     1  15.07887  alcohol
433     1  18.59431  alcohol
450     1 *62.17550  alcohol
```

- Count = number of coefficients where this row appears influential.
- Use `day7 %>% slice(351)` to see row 351 in its entirety.
- Use residual plots (with an `lm` fit) to check Cook's distances.

# Residuals vs. Fitted Values is easy from `ols`

```
plot(resid(mod1) ~ fitted(mod1))
```



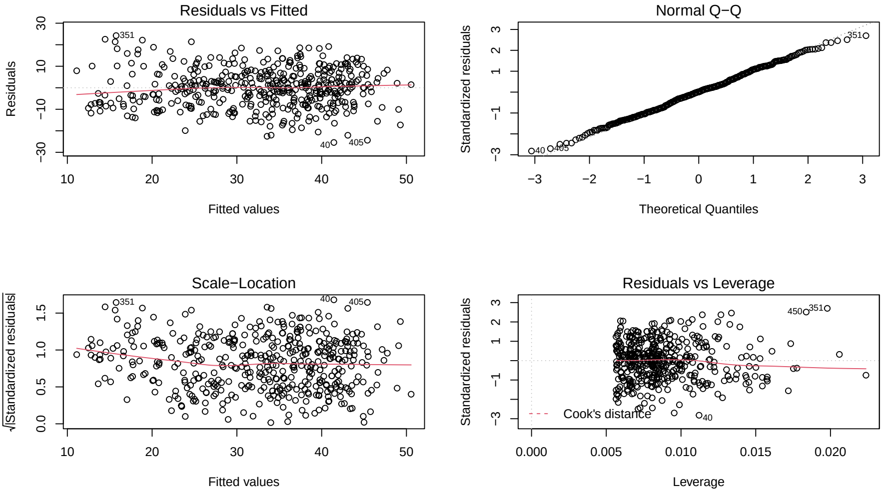
# Fitting all Residual Plots for `mod1`

To fit more complete residual plots (and to do other things) we will fit the `lm` version of this same model...

```
mod1_lm <- lm(cesd ~ mcs + subst, data = day7)

par(mfrow = c(2,2))
plot(mod1_lm)
par(mfrow = c(1,1))
```

- Plots are shown on the next slide. While the subject in row 351 is more influential than most other points, it doesn't reach the standard of a problematic Cook's distance.

# Residual Plots for `mod_first`



# Thinking about Non-Linear Terms?

# Non-Linear Terms

In building a linear regression model, we're most often going to be thinking about:

- for quantitative predictors, some curvature...
  - perhaps polynomial terms
  - but more often restricted cubic splines
- for any predictors, possible interactions
  - between categorical predictors
  - between categorical and quantitative predictors
  - between quantitative predictors

# Polynomial Regression

A polynomial in the variable `x` of degree D is a linear combination of the powers of `x` up to D. Fitting such a model creates a **polynomial regression**.

- 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: $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 x^4 + \beta_5 x^5$

An **orthogonal polynomial** sets up a model design matrix and then scales those columns so that each column is uncorrelated with the previous ones.

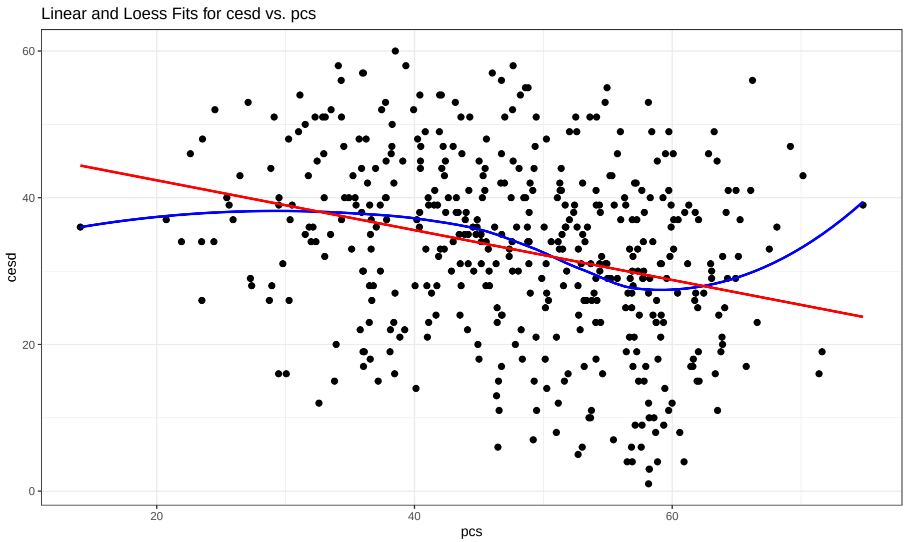
- This reduction in collinearity (correlation between predictors) lets us gauge whether the addition of any particular polynomial term improves model fit.

# A new predictor: use pcs to predict cesd?

- Let's look at both a linear fit and a loess smooth to see if they indicate meaningfully different things about the association between pcs and cesd

```
ggplot(day7, aes(x = pcs, y = cesd)) +
    geom_point(size = 2) +
    geom_smooth(method = "loess", formula = y ~ x,
                se = FALSE, col = "blue") +
    geom_smooth(method = "lm", formula = y ~ x,
                se = FALSE, col = "red") +
    labs(title = "Linear and Loess Fits for cesd vs. pcs")
```

# Linear and Loess Fits for `cesd` with `pcs`



# Fitting polynomial regressions with `ols`

```
dd <- datadist(day7)
options(datadist = "dd")

mod_B1 <- ols(cesd ~ pcs,
              data = day7, x = TRUE, y = TRUE)
mod_B2 <- ols(cesd ~ pol(pcs, 2),
              data = day7, x = TRUE, y = TRUE)
mod_B3 <- ols(cesd ~ pol(pcs, 3),
              data = day7, x = TRUE, y = TRUE)
```

- Note the use of `pol()` from the `rms` package here to fit orthogonal polynomials, rather than `poly()` which we used for an `lm` fit.

# Model B1 (linear in pcs)

```
mod_B1
```

```
> mod_B1
Linear Regression Model

 ols(formula = cesd ~ pcs, data = day7, x = TRUE, y = TRUE)

                   Model Likelihood     Discrimination
                      Ratio Test           Indexes
 Obs       453    LR chi2      40.57    R2       0.086
 sigma11.9796     d.f.             1    R2 adj   0.084
 d.f.      451    Pr(> chi2) 0.0000    g        4.177

 Residuals

      Min       1Q    Median       3Q      Max
 -28.4116  -7.8036   0.6846   8.7917  29.3281


           Coef    S.E.   t     Pr(>|t|)
 Intercept 49.1673 2.5728 19.11 <0.0001
 pcs       -0.3396 0.0522 -6.50 <0.0001
```

# Model B2 (quadratic polynomial in `pcs`)

```
mod_B2
```

```
> mod_B2
Linear Regression Model

 ols(formula = cesd ~ pol(pcs, 2), data = day7, x = TRUE, y = TRUE)

                  Model Likelihood    Discrimination
                        Ratio Test           Indexes
 Obs       453    LR chi2     40.68    R2        0.086
 sigma11.9915    d.f.            2    R2 adj    0.082
 d.f.      450    Pr(> chi2) 0.0000    g         4.199

 Residuals

     Min       1Q   Median       3Q      Max
 -28.387   -7.750    0.591    8.634   29.697


           Coef     S.E.    t      Pr(>|t|)
 Intercept 46.4007 8.7967  5.27 <0.0001
 pcs       -0.2136 0.3867 -0.55 0.5809
 pcs^2     -0.0014 0.0041 -0.33 0.7424
```

# Model B3 (cubic polynomial in pcs)

```
mod_B3
```

```
> mod_B3
Linear Regression Model

 ols(formula = cesd ~ pol(pcs, 3), data = day7, x = TRUE, y = TRUE)

                  Model Likelihood    Discrimination
                        Ratio Test           Indexes
 Obs       453    LR chi2      48.70    R2       0.102
 sigma11.8991    d.f.             3    R2 adj   0.096
 d.f.      449    Pr(> chi2) 0.0000    g        4.556

 Residuals

      Min       1Q   Median       3Q      Max
 -27.5245  -8.2651   0.7988   8.9004  27.4480


           Coef     S.E.    t     Pr(>|t|)
 Intercept -13.4076 22.8605 -0.59 0.5578
 pcs         4.1323  1.5825  2.61 0.0093
 pcs^2      -0.1010  0.0354 -2.85 0.0046
 pcs^3       0.0007  0.0003  2.83 0.0049
```

# Store the polynomial fits

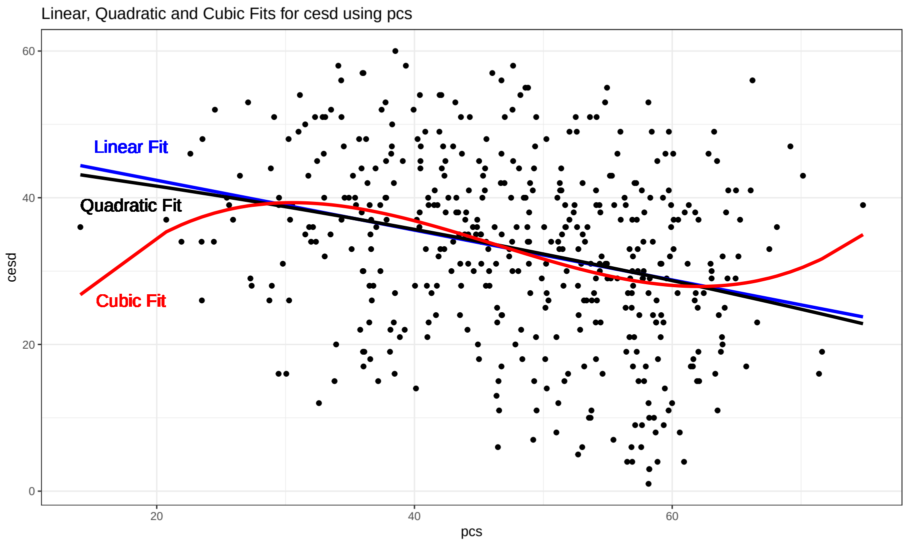
First, we need to store the values. Again broom doesn't play well with ols fits, so I'll just add the predictions as columns

```
cesd_fits <- day7 %>%
    mutate(fitB1 = predict(mod_B1),
           fitB2 = predict(mod_B2),
           fitB3 = predict(mod_B3))
```

# Code to plot polynomial fits

```
ggplot(cesd_fits, aes(x = pcs, y = cesd)) +
    geom_point() +
    geom_line(aes(x = pcs, y = fitB1),
              col = "blue", size = 1.25) +
    geom_line(aes(x = pcs, y = fitB2),
              col = "black", size = 1.25) +
    geom_line(aes(x = pcs, y = fitB3),
              col = "red", size = 1.25) +
    geom_text(x = 18, y = 47, label = "Linear Fit",
              size = 5, col = "blue") +
    geom_text(x = 18, y = 39, label = "Quadratic Fit",
              size = 5, col = "black") +
    geom_text(x = 18, y = 26, label = "Cubic Fit",
              size = 5, col = "red") +
    labs(title = "Linear, Quadratic and Cubic Fits for cesd us
```

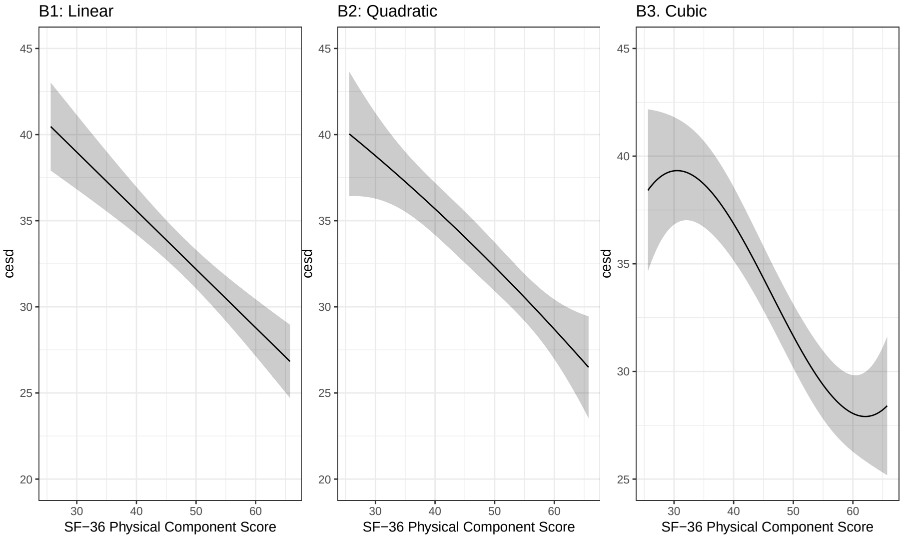
# The Polynomial Fits, plotted



# Code to plot polynomial fits with Predict

```
p1 <- ggplot(Predict(mod_B1)) + ggtitle("B1: Linear")
p2 <- ggplot(Predict(mod_B2)) + ggtitle("B2: Quadratic")
p3 <- ggplot(Predict(mod_B3)) + ggtitle("B3. Cubic")

p1 + p2 + p3
```

# Visualizing the polynomial fits with Predict



# 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 `ols`

Let's consider a restricted cubic spline model for `cesd` based on `pcs` with:

- 3 knots in `modC3`, 4 knots in `modC4`, and 5 knots in `modC5`

```
dd <- datadist(day7)
options(datadist = "dd")

mod_C3 <- ols(cesd ~ rcs(pcs, 3),
              data = day7, x = TRUE, y = TRUE)
mod_C4 <- ols(cesd ~ rcs(pcs, 4),
              data = day7, x = TRUE, y = TRUE)
mod_C5 <- ols(cesd ~ rcs(pcs, 5),
              data = day7, x = TRUE, y = TRUE)
```

# Model C3 (3-knot spline in pcs)

```
mod_C3
```

```
> mod_C3
Linear Regression Model

 ols(formula = cesd ~ rcs(pcs, 3), data = day7, x = TRUE, y = TRUE)

                  Model Likelihood     Discrimination
                        Ratio Test            Indexes
 Obs       453     LR chi2     40.79    R2       0.086
 sigma11.9901     d.f.             2    R2 adj   0.082
 d.f.      450     Pr(> chi2) 0.0000    g        4.206

 Residuals

      Min       1Q   Median       3Q      Max
 -28.3462  -7.7005   0.5098   8.6376  29.8454


           Coef    S.E.   t     Pr(>|t|)
 Intercept 47.3631 4.7053 10.07 <0.0001
 pcs       -0.2908 0.1187 -2.45 0.0146
 pcs'      -0.0624 0.1363 -0.46 0.6471
```

# Model C4 (4-knot spline in pcs)

```
mod_C4
```

```
> mod_C4
Linear Regression Model

 ols(formula = cesd ~ rcs(pcs, 4), data = day7, x = TRUE, y = TRUE)

                  Model Likelihood    Discrimination
                        Ratio Test           Indexes
 Obs       453    LR chi2     51.31    R2       0.107
 sigma11.8648    d.f.            3    R2 adj   0.101
 d.f.      449    Pr(> chi2) 0.0000    g        4.590

 Residuals

      Min       1Q   Median       3Q      Max
 -28.3147  -8.2830   0.8559   8.8866  26.5458


           Coef    S.E.    t     Pr(>|t|)
 Intercept 33.3298 6.5742  5.07 <0.0001
 pcs        0.1464 0.1856  0.79 0.4308
 pcs'      -1.4383 0.4497 -3.20 0.0015
 pcs''      6.2561 1.9076  3.28 0.0011
```

# Model C5 (5-knot spline in pcs)

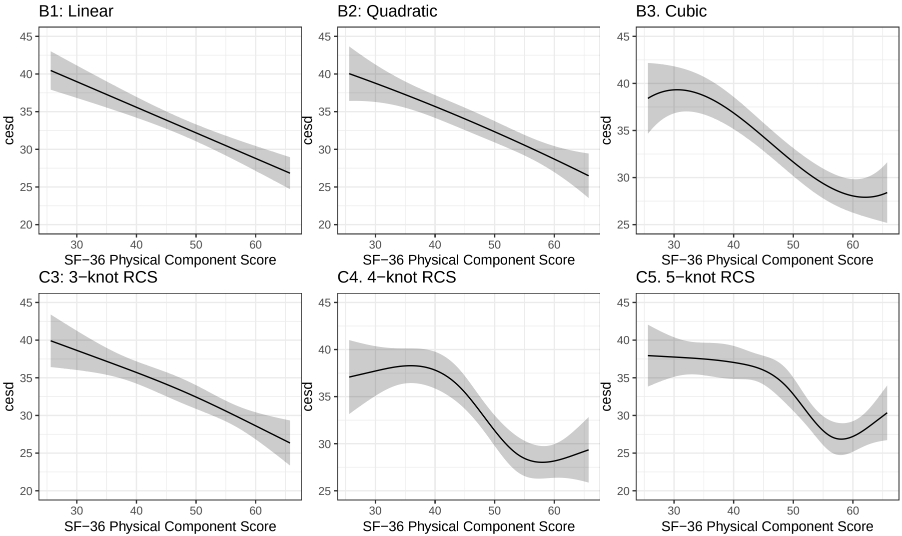
```
mod_C5
```

```
> mod_C5
Linear Regression Model

 ols(formula = cesd ~ rcs(pcs, 5), data = day7, x = TRUE, y = TRUE)

                    Model Likelihood    Discrimination
                          Ratio Test           Indexes
 Obs        453     LR chi2     54.64    R2       0.114
 sigma11.8345     d.f.            4    R2 adj   0.106
 d.f.       448     Pr(> chi2) 0.0000    g        4.744

 Residuals

     Min       1Q  Median       3Q      Max
 -29.396  -7.928   1.016   8.762   26.974


           Coef    S.E.   t     Pr(>|t|)
 Intercept 39.0631 7.8282  4.99 <0.0001
 pcs       -0.0436 0.2332 -0.19 0.8517
 pcs'      -0.2952 1.0079 -0.29 0.7697
 pcs''     -3.1835 4.8079 -0.66 0.5082
 pcs'''    14.4216 8.3721  1.72 0.0857
```

# Code to plot all six fits

```r
p1 <- ggplot(Predict(mod_B1)) + ggtitle("B1: Linear")
p2 <- ggplot(Predict(mod_B2)) + ggtitle("B2: Quadratic")
p3 <- ggplot(Predict(mod_B3)) + ggtitle("B3. Cubic")
p4 <- ggplot(Predict(mod_C3)) + ggtitle("C3: 3-knot RCS")
p5 <- ggplot(Predict(mod_C4)) + ggtitle("C4. 4-knot RCS")
p6 <- ggplot(Predict(mod_C5)) + ggtitle("C5. 5-knot RCS")

(p1 + p2 + p3) / (p4 + p5 + p6)
```

# Visualizing the fits better?



# Which of these models looks better?

- Compare our six models for the `cesd` to `pcs` association
- I used `set.seed(432)` then `validate(mod_B1)` etc.

| Model | Index-Corrected $R^2$ | Corrected MSE |
|---|---|---|
| B1 (linear) | 0.0848 | 143.25 |
| B2 (quadratic) | 0.0752 | 142.49 |
| B3 (cubic) | 0.0909 | 143.73 |
| C3 (3-knot RCS) | 0.0732 | 143.31 |
| C4 (4-knot RCS) | 0.0870 | 144.00 |
| C5 (5-knot RCS) | 0.0984 | 141.44 |

- So which model has the best (validated) summaries?
- We'd need to look at residual plots, too, of course.

# Data Spending: Non-Linearity Prior to Fits

# 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 = 453 observations on 6 candidate 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?

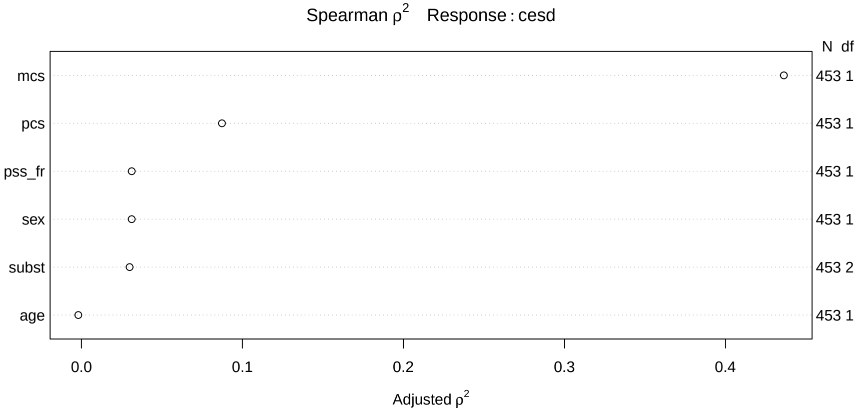
Spearman's $\rho^2$ is an indicator (not a perfect one) of potential predictive punch, but doesn't give away the game.

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

```
spear_cesd <- spearman2(cesd ~ mcs + subst + pcs +
                            age + sex + pss_fr,
                        data = day7)
```

# Spearman's $\rho^2$ Plot

```
plot(spear_cesd)
```



# Conclusions from Spearman $\rho^2$ Plot

- `mcs` 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.
  - This **does not** mean that `mcs` actually needs a non-linear term, or will show meaningfully better results if a non-linear term is included. We'd have to fit a model with and without non-linearity in `mcs` to know that.
  - Non-linearity will often take the form of a product term, a polynomial term, or a restricted cubic spline.
- `pcs`, also quantitative, has the next most potential predictive punch
- these are followed by `pss_fr` and `sex`.

# Grim Reality

With 453 observations (452 df) we should be thinking about models with modest 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 to include non-linear terms in just two or three variables (and that's it) and even that would be tough to justify with this modest sample size.

# Contents of spear_cesd

```
spear_cesd
```

```
Spearman rho^2    Response variable:cesd

        rho2      F df1 df2      P Adjusted rho2   n
mcs    0.438 350.89   1 451 0.0000         0.436 453
subst  0.034   7.97   2 450 0.0004         0.030 453
pcs    0.089  44.22   1 451 0.0000         0.087 453
age    0.000   0.12   1 451 0.7286        -0.002 453
sex    0.033  15.56   1 451 0.0001         0.031 453
pss_fr 0.033  15.57   1 451 0.0001         0.031 453
```

# Proposed New Model

Fit a model to predict `cesd` using:

- a 5-knot spline on `mcs`
- a 3-knot spline on `pcs`
- a linear term on `pss_fr`
- a linear term on `age`
- an interaction of `sex` with the main effect of `mcs` (restricting our model so that terms that are non-linear in both `sex` and `mcs` are excluded), and
- a main effect of `subst`

Perhaps more than we can reasonably do with 453 observations, but let's see how it looks.

# Our new model `mod2`

```r
dd <- datadist(day7)
options(datadist = "dd")

mod2 <- ols(cesd ~ rcs(mcs, 5) + rcs(pcs, 3) + sex +
                mcs %ia% sex + pss_fr + age + subst,
            data = day7, x = TRUE, y = TRUE)
```

- `%ia%` tells R to fit an interaction term with `sex` and the main effect of `mcs`.
- We have to include `sex` as a main effect for the interaction term (%ia%) to work here.

# Our new, more complex model `mod2`

```
mod2
```

```
> mod2
Linear Regression Model

 ols(formula = cesd ~ rcs(mcs, 5) + rcs(pcs, 3) + sex + mcs %ia%
     sex + pss_fr + age + subst, data = day7, x = TRUE, y = TRUE)

                  Model Likelihood    Discrimination
                        Ratio Test           Indexes
 Obs      453     LR chi2     349.44    R2         0.538
 sigma8.6248      d.f.            12    R2 adj     0.525
 d.f.     440     Pr(> chi2) 0.0000     g         10.439

 Residuals

      Min       1Q    Median       3Q      Max
 -26.7893  -5.9000   0.1545   5.5884  26.1304


                Coef    S.E.    t     Pr(>|t|)
 Intercept      76.3346 6.2540 12.21 <0.0001
 mcs            -0.9306 0.2315 -4.02 <0.0001
 mcs'            1.6607 2.5040  0.66 0.5075
 mcs''          -2.8854 8.3945 -0.34 0.7312
 mcs'''          0.2942 7.9390  0.04 0.9705
 pcs            -0.2341 0.0883 -2.65 0.0083
 pcs'           -0.0151 0.1000 -0.15 0.8797
 sex=male       -2.0330 2.5456 -0.80 0.4249
 mcs * sex=male -0.0129 0.0783 -0.17 0.8690
 pss_fr         -0.2569 0.1046 -2.46 0.0144
 age            -0.0466 0.0569 -0.82 0.4139
 subst=cocaine  -2.6999 0.9965 -2.71 0.0070
 subst=heroin   -2.1741 1.0677 -2.04 0.0423
```

# ANOVA for this model

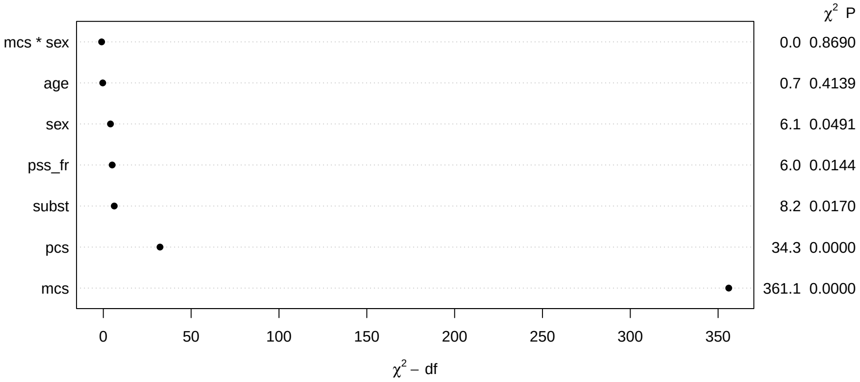
```
anova(mod2)
```

```
> anova(mod2)
                Analysis of Variance          Response: cesd

 Factor                                        d.f. Partial SS    MS          F     P
 mcs   (Factor+Higher Order Factors)             5  26857.364670 5371.472934 72.21 <.0001
  All Interactions                               1      2.026255    2.026255  0.03 0.8690
  Nonlinear                                      3    293.502251   97.834084  1.32 0.2688
 pcs                                             2   2548.388579 1274.194290 17.13 <.0001
  Nonlinear                                      1      1.705031    1.705031  0.02 0.8797
 sex   (Factor+Higher Order Factors)             2    451.578352  225.789176  3.04 0.0491
  All Interactions                               1      2.026255    2.026255  0.03 0.8690
 mcs * sex  (Factor+Higher Order Factors)        1      2.026255    2.026255  0.03 0.8690
 pss_fr                                          1    448.812293  448.812293  6.03 0.0144
 age                                             1     49.758786   49.758786  0.67 0.4139
 subst                                           2    611.625952  305.812976  4.11 0.0170
 TOTAL NONLINEAR                                 4    293.512204   73.378051  0.99 0.4146
 TOTAL NONLINEAR + INTERACTION                   5    294.601803   58.920361  0.79 0.5558
 REGRESSION                                     12  38058.315322 3171.526277 42.64 <.0001
 ERROR                                         440  32730.174744   74.386761
```

- Remember that this ANOVA testing is sequential, other than the TOTALs.
- We can also plot the ANOVA results, for example…

# Plotting ANOVA results for `mod2`

```
plot(anova(mod2))
```



# Validation of Summary Statistics

```r
set.seed(432); validate(mod2)
```

```
> set.seed(432); validate(mod2)
          index.orig training    test optimism index.corrected  n
R-square      0.5376   0.5513  0.5233   0.0280          0.5096 40
MSE          72.2520  69.8358 74.4984  -4.6627         76.9147 40
g            10.4392  10.5053 10.2718   0.2335         10.2056 40
Intercept     0.0000   0.0000  0.7893  -0.7893          0.7893 40
Slope         1.0000   1.0000  0.9751   0.0249          0.9751 40
```

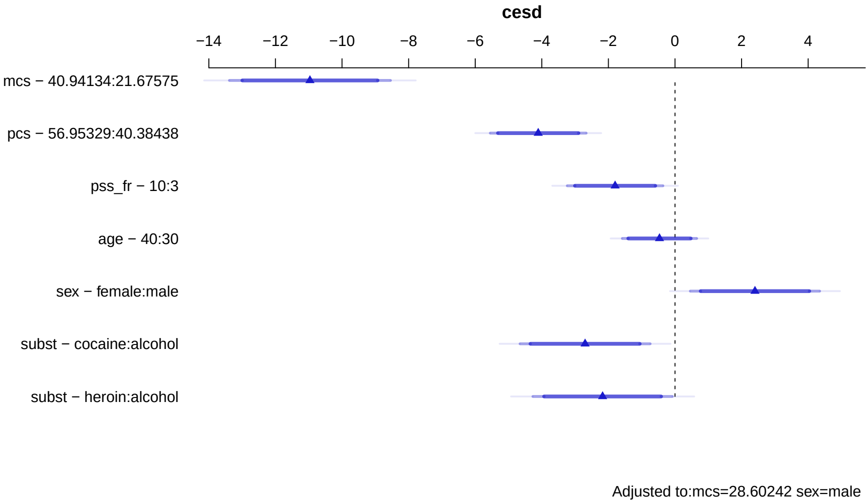
# `summary` results for `mod2`

```
summary(mod2)
```

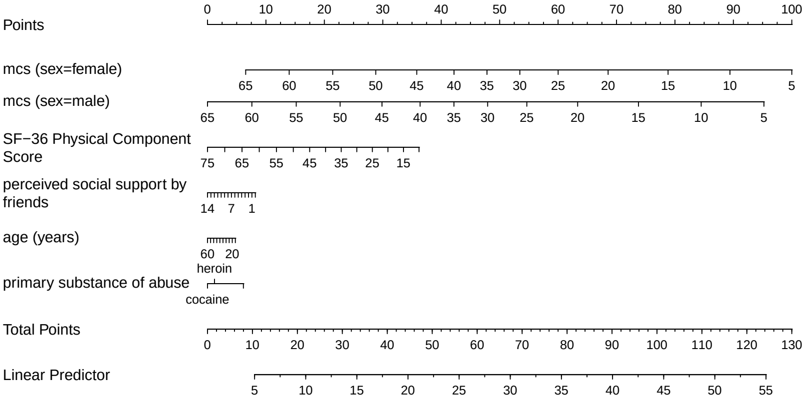
```
> summary(mod2)
             Effects              Response : cesd

 Factor                   Low    High   Diff.  Effect    S.E.    Lower 0.95 Upper 0.95
 mcs                      21.676 40.941 19.266 -10.96400 1.23340 -13.38800  -8.539800
 pcs                      40.384 56.953 16.569  -4.10790 0.73381  -5.55010  -2.665700
 pss_fr                    3.000 10.000  7.000  -1.79860 0.73225  -3.23780  -0.359500
 age                      30.000 40.000 10.000  -0.46552 0.56918  -1.58420   0.653130
 sex - female:male         2.000  1.000     NA   2.40260 0.99054   0.45577   4.349300
 subst - cocaine:alcohol   1.000  2.000     NA  -2.69990 0.99647  -4.65830  -0.741430
 subst - heroin:alcohol    1.000  3.000     NA  -2.17410 1.06770  -4.27250  -0.075632

Adjusted to: mcs=28.60242 sex=male
```

# Plot of summary results for mod2

```
plot(summary(mod2))
```

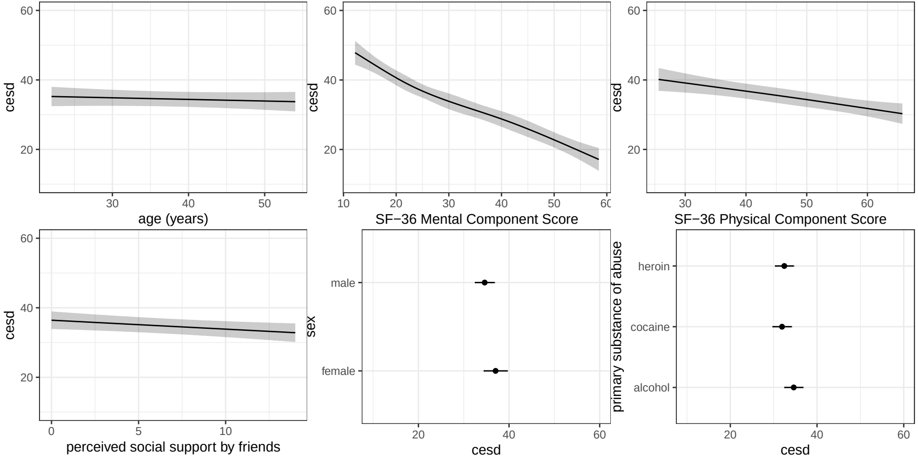


```
plot(nomogram(mod2))
```



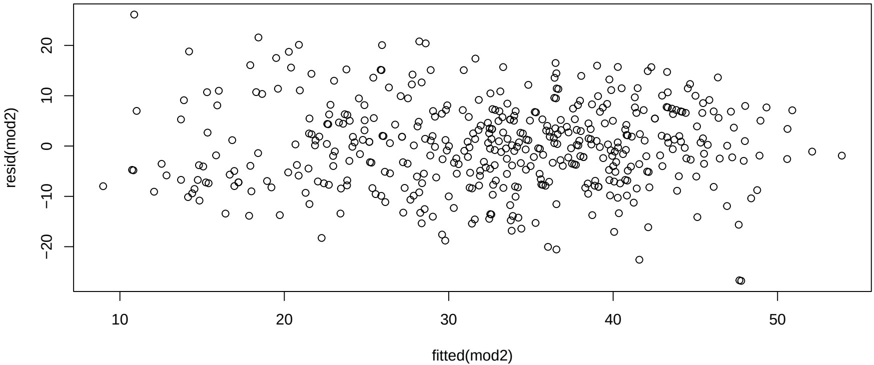
# Seeing the impact of the modeling another way

```
ggplot(Predict(mod2))
```



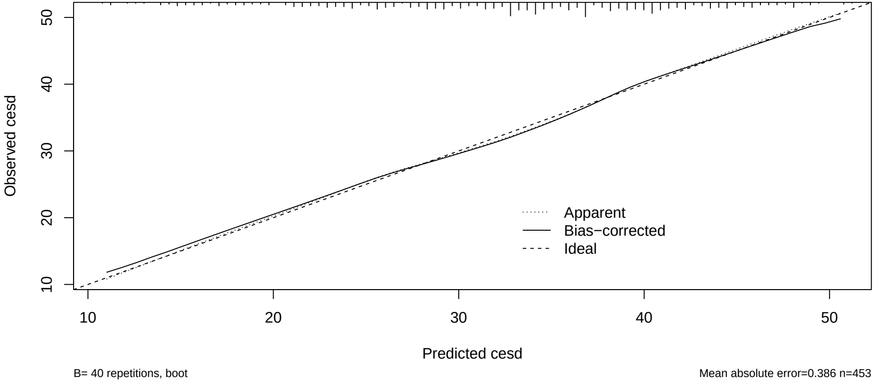
# Residuals vs. Fitted Values to check assumptions

```
plot(resid(mod2) ~ fitted(mod2))
```



# Checking the model's calibration

```
set.seed(432); plot(calibrate(mod2))
```




```
n=453   Mean absolute error=0.386   Mean squared error=0.19775
0.9 Quantile of absolute error=0.704
```

# Limitations of `lm` for fitting complex linear models

We can certainly assess this big, complex model using `lm`, too:

- with in-sample summary statistics like adjusted $R^2$, 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`.

- In Project A, we expect some results that are most easily obtained using `lm` and others that are most easily obtained using `ols`.

# Next Time

- The HERS data
- Fitting a more complex linear regression model
- Adding missing data into all of this, and running multiple imputation

Please remember to participate in the brief poll on Piazza about Chapter 2 of *The Signal and the Noise*.