431 Class 24

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Agenda for Today

- Linear Regression for Prediction in our dm431 data
 - Pre-Modeling Considerations
 - Consideration of Outcome Transformations
 - (Simple) Imputation to deal with Missing Data
 - Partitioning the Data (Development vs. Testing)
 - Building the Model
 - Evaluating Fit in the Development Sample
 - Considering Regression Assumptions
 - Post-Modeling Considerations
 - Evaluating Prediction Quality (Test Sample)
 - Back-Transformation of Outcome Predictions

In today's class, we will start with slide 48.

```
library(simputation) # for simple imputation
library(car) # for Box-Cox plot
library(GGally) # for scatterplot matrix

library(here); library(magrittr)
library(patchwork); library(janitor); library(broom)
library(tidyverse) # always load tidyverse last

theme_set(theme_bw()) # now all applots use theme_bw()
```

Things discussed in Class 22 and 23

A change to the data!

All this time, we've had an error in the dm431 data, which I'll now call dm431_old.Rds. Can you spot it?

```
dm431_old <- readRDS(here("data", "dm431_old.Rds"))
head(dm431_old, 8)</pre>
```

```
# A tibble: 8 \times 21
 subject practice
                    age race eth sex
                                        alc insurance
                  <dbl> <fct> <fct> <dbl> <fct>
 <chr> <fct>
1 S-001
         Arlingt~
                     62 Black o~ F
                                        6.3 Commerci~
         Bristol
                     54 Black o~ F
2 S-002
                                       11
                                            Uninsured
3 S-003
         Chester
                     47 Black o~ F
                                        8.7 Uninsured
4 S-004
         Dover
                    53 Non-His~ M
                                        6.5 Commerci~
5 S-005
         Franklin
                     64 Non-His~ F
                                        6.7 Commerci~
6 S-006
         Bristol
                     48 Black o~ F
                                        5.8 Medicare
7 S-006
         Franklin
                     49 Black o~ M
                                        9.6 Commerci~
8 S-008
                     63 Black o~ F
                                        6.1 Medicaid
         Dover
```

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```
dm431 old %>% nrow()
[1] 431
dm431 old %%% n distinct(subject)
[1] 430
dm431_old %>% slice(6:7) %>% select(subject, age)
# A tibble: 2 \times 2
  subject age
  <chr> <dbl>
1 S-006 48
2 S-006 49
```

```
dm431_fixed <- dm431_old %>%
 mutate(subject = ifelse(subject == "S-006" & age == 49,
                         "S-007", subject))
dm431_fixed %>% slice(6:7) %>% select(subject, age)
# A tibble: 2 x 2
 subject age
 <chr> <dbl>
1 S-006 48
2 S-007 49
saveRDS(dm431 fixed, file = here("data", "dm431 fixed.Rds"))
```

Focus on Four Variables (+ Subject)

```
dm431 <- readRDS(here("data", "dm431_fixed.Rds"))

dm_1 <- dm431 %>%
    select(a1c, a1c_old, age, income, subject)
```

Summarizing the dm_1 data set

summary(dm_1)

```
a1c
             a1c_old
                                age
Min. : 4.300 Min. : 4.200
                            Min. :31.00
1st Qu.: 6.500 1st Qu.: 6.500
                            1st Qu.:51.00
Median: 7.300 Median: 7.300
                            Median :57.00
Mean : 7.884 Mean : 7.712 Mean : 56.14
3rd Qu.: 8.600 3rd Qu.: 8.400
                            3rd Qu.:62.00
Max. :16.700 Max. :16.300 Max. :70.00
NA's :3 NA's :14
          income subject
Below 30K :146 Length:431
Between 30-50K:171 Class:character
Higher_than_50K:110 Mode :character
NA's
```

```
dm_1 %>% skimr::skim()
Skim summary statistics
n obs: 431
n variables: 5
-- Variable type:character -----
variable missing complete n min max empty n_unique subject 0 431 431 5 5 0 431
variable missing complete n n_unique
                                               top_counts ordered
  income 4 427 431 3 Bet: 171, Bel: 146, Hig: 110, NA: 4 FALSE
-- Variable type:numeric ----
variable missing complete n mean sd p0 p25 p50 p75 p100 hist
    alc 3 428 431 7.88 2.03 4.3 6.5 7.3 8.6 16.7
 alc old 14
                 417 431 7.71 1.77 4.2 6.5 7.3 8.4 16.3
                  431 431 56.14 8.41 31
    age
                                     51
                                             62
                                                 70
```

What roles will these variables play?

a1c is our outcome, which we'll predict with ...

- Model 1: Use a1c old alone to predict a1c
- Model 2: Use a1c old and age together to predict a1c
- Model 3: Use alc old, age, and income together to predict alc

What will we do about missing data?

```
dm_1 %>% summarise_all(~ sum(is.na(.)))
# A tibble: 1 x 5
   a1c a1c_old age income subject
 <int> <int> <int> <int> <int>
   3 14 0 4
```

- We're missing 3 values of a1c, our outcome
- and 14 values of a1c_old, a predictor (Models 1-3)
- and 4 values of income, another predictor (Model 3)

Dealing with outcome missingness

I don't want to impute the outcome. We'll drop the 3 observations missing a1c from our data set.

```
dm_2 <- dm_1 %>% filter(complete.cases(a1c))
dm_2 %>% summarise_all(~ sum(is.na(.)))
```

How should we deal with the remaining missing values?

Simple Imputation of Missing a1c_old Values

We could use a robust linear model method to impute our quantitative a1c_old values on the basis of age, which is missing no observations in common with a1c_old (in fact, age is missing no observations.)

```
dm_3a <- impute_rlm(dm_2, a1c_old ~ age)

dm_3a %>% select(a1c_old, income) %>% summary()

a1c_old income
Min. : 4.200 Below_30K :146
```

Min. : 4.200 Below_30K :146

1st Qu.: 6.500 Between_30-50K :169

Median : 7.300 Higher_than_50K:109

Mean : 7.711 NA's : 4

3rd Qu.: 8.400 Max. :16.300

Simple Imputation of Missing income Values

We could use a decision tree (CART) method to impute our missing categorical income values, on the basis of age.

```
dm_3b <- impute_cart(dm_2, income ~ age)
dm_3b %>% select(a1c_old, income) %>% summary()
```

```
a1c_old income
Min. : 4.200 Below_30K :148
1st Qu.: 6.500 Between_30-50K:171
Median : 7.300 Higher_than_50K:109
Mean : 7.716
3rd Qu.: 8.400
Max. :16.300
NA's :12
```

Chaining our Simple Imputations

Or we could put all of our imputations together in a chain. I encourage you to try rlm for quantitative variables, and cart for categorical variables, for now.

```
dm_4 <- dm_2 %>%
  impute_rlm(a1c_old ~ age) %>%
  impute_cart(income ~ age + a1c_old)

dm_4 %>% select(a1c, a1c_old, income) %>%
  summarise_all(~(sum(is.na(.))))
```

What did we do? What is the result?

dm_4 %>% skimr::skim() results

```
dm_4 %>% skimr::skim()
Skim summary statistics
n obs: 428
n variables: 5
-- Variable type:character ------
variable missing complete n min max empty n_unique
 subject
             0 428 428
-- Variable type:factor ------
variable missing complete n n_unique
                                                         top_counts ordered
             0 428 428 3 Bet: 171. Bel: 148. Hig: 109. NA: 0
  income
-- Variable type:numeric ------
variable missing complete n mean
                                     p0
                                                               hist
                                  sd
                                         p25 p50 p75 p100
               428 428 7.88 2.03 4.3
                                          6.5 7.3 8.6 16.7
     a1c
 a1c old
                                          6.5 7.3 8.4 16.3
                   428 428 7.71 1.75 4.2
                    428 428 56.09 8.42 31
                                         50.75 57
                                                   62
                                                       70
     age
```

OK. Ready to proceed?

How will we decide which of the models is "best"?

Our goal is accurate prediction of a1c values.

Which of these models gives us the "best" result?

- Model 1: Use alc old alone to predict alc
- Model 2: Use alc old and age together to predict alc
- Model 3: Use a1c_old, age, and income together to predict a1c

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How shall we be guided by our data?

It can scarcely be denied that the supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience. (A. Einstein)

- often this is reduced to "make everything as simple as possible but no simpler"
 - Entities should not be multiplied without necessity. (Occam's razor)
- often this is reduced to "the simplest solution is most likely the right one"

George Box's aphorisms

On Parsimony: Since all models are wrong the scientist cannot obtain a "correct" one by excessive elaboration. On the contrary following William of Occam he should seek an economical description of natural phenomena. Just as the ability to devise simple but evocative models is the signature of the great scientist so overelaboration and overparameterization is often the mark of mediocrity.

On Worrying Selectively: Since all models are wrong the scientist must be alert to what is importantly wrong. It is inappropriate to be concerned about mice when there are tigers abroad.

- and, the most familiar version...
 - ... all models are approximations. Essentially, all models are wrong, but some are useful. However, the approximate nature of the model must always be borne in mind.

431 approach: Which model is "most useful"?

- Split the data into a model development (training) sample of about 70-80% of the observations, and a model test (holdout) sample, containing the remaining observations.
- Oevelop candidate models using the development sample.
- Assess the quality of fit for candidate models within the development sample.
- Oheck adherence to regression assumptions in the development sample.
- When you have candidates, assess them based on the accuracy of the predictions they make for the data held out (and thus not used in building the models.)
- Select a "final" model for use based on the evidence in steps 3, 4 and especially 5.

Split the data into a model development (training) sample of about 70-80% of the observations, and a model test (holdout) sample, containing the remaining observations.

Partition the imputed data into development/test samples

```
set.seed(20191114)
dm4 dev <- sample frac(dm 4, 0.75, replace = FALSE)
dm4 test <- anti join(dm 4, dm4 dev, by = "subject")
nrow(dm 4); nrow(dm4 dev); nrow(dm4 test)
[1] 428
[1] 321
Γ1 107
```

Develop candidate models using the development sample.

A look at the outcome (a1c) distribution

We'll study the outcome variable (a1c) in the development sample, to consider whether a transformation might be in order.

I did a little fancy work with the code (continues next slide)...

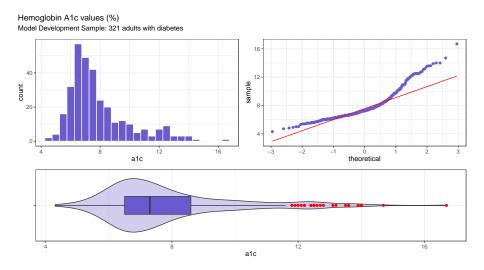
```
p1 \leftarrow ggplot(dm4_dev, aes(x = a1c)) +
  geom_histogram(binwidth = 0.5,
                  fill = "slateblue", col = "white")
p2 <- ggplot(dm4_dev, aes(sample = a1c)) +
  geom_qq(col = "slateblue") + geom_qq_line(col = "red")
p3 \leftarrow ggplot(dm4_dev, aes(x = "", y = a1c)) +
  geom_violin(fill = "slateblue", alpha = 0.3) +
  geom_boxplot(fill = "slateblue", width = 0.3.
                outlier.color = "red") +
  labs(x = "") + coord_flip()
```

A look at the outcome (a1c) distribution

Putting the plots together, and titling them meaningfully...

Result on the next slide...

Outcome (a1c): Model Development Sample



Why Transform the Outcome?

We want to try to identify a good transformation for the conditional distribution of the outcome, given the predictors, in an attempt to make the linear regression assumptions of linearity, Normality and constant variance more appropriate.

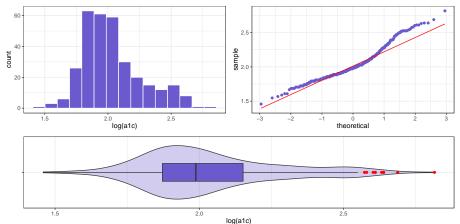
Ladder of Especially Useful (and often interpretable) transformations

Transformation	y ²	у	\sqrt{y}	log(y)	1/ <i>y</i>	$1/y^2$
λ	2	1	0.5	0	-1	-2

 We see some sign of right skew in the a1c data. Let's try a log transformation.

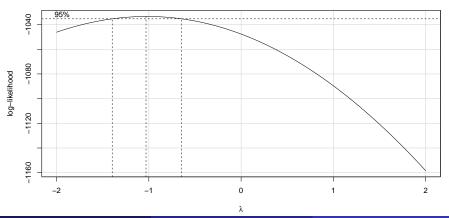
Consider a log transformation?

Natural Logarithm of Hemoglobin A1c Model Development Sample: 321 adults with diabetes



Using Box-Cox to help select a transformation?

```
mod_0 <- lm(a1c ~ a1c_old + age + income, data = dm4_dev)
boxCox(mod_0)</pre>
```



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Using Box-Cox to help select a transformation?

```
summary(powerTransform(mod_0))
```

bcPower Transformation to Normality

```
Est Power Rounded Pwr Wald Lwr Bnd Wald Upr Bnd
Y1 -1.019 -1 -1.3953 -0.6427
```

Likelihood ratio test that transformation parameter is equal (log transformation)

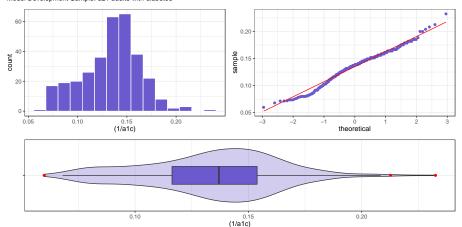
```
LRT df pval LR test, lambda = (0) 28.53961 1 9.1801e-08
```

Likelihood ratio test that no transformation is needed LRT df pval LR test, lambda = (1) 112.3945 1 < 2.22e-16

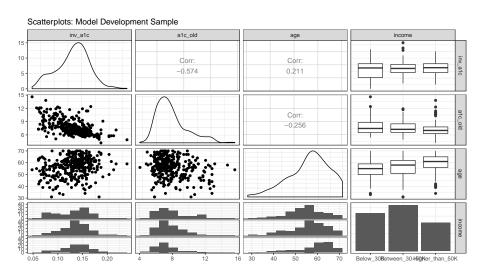
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Consider the inverse?

Inverse of Hemoglobin A1c Model Development Sample: 321 adults with diabetes



Scatterplot Matrix



Scatterplot Matrix (Code)

Note that ggpairs comes from the GGally package.

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Three Regression Models We'll Fit

Remember we're using the model development sample here.

Assess the quality of fit for candidate models within the development sample.

```
Call:
lm(formula = (1/alc) \sim alc_old, data = dm4_dev)
Residuals:
     Min
          10 Median 30 Max
-0.068553 -0.014349 0.000183 0.013117 0.078923
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 0.2099494 0.0061836 33.95 <2e-16 ***
alc old -0.0098553 0.0007868 -12.53 <2e-16 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
Residual standard error: 0.02409 on 319 degrees of freedom
Multiple R-squared: 0.3297, Adjusted R-squared: 0.3276
F-statistic: 156.9 on 1 and 319 DF, p-value: < 2.2e-16
```

Summary of Fit Quality (mod_1)

name	r.squared	adj.r.squared	sigma	AIC	BIC
mod_1	0.33	0.328	0.024	-1477	-1466

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Tidied coefficients (mod_1)

term	estimate	std.error	p.value	conf.low	conf.high
(Intercept)	0.2099	0.0062	0	0.1978	0.2221
a1c_old	-0.0099	0.0008	0	-0.0114	-0.0083

```
Call:
lm(formula = (1/a1c) \sim a1c_old + age, data = dm4_dev)
Residuals:
     Min
           10 Median 30
                                          Max
-0.068387 -0.013588 0.000058 0.013243 0.076861
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 0.1939204 0.0126114 15.377 <2e-16 ***
a1c_old -0.0095521 0.0008125 -11.756 <2e-16 ***
age 0.0002429 0.0001667 1.458 0.146
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 0.02405 on 318 degrees of freedom
Multiple R-squared: 0.3341, Adjusted R-squared: 0.3299
F-statistic: 79.78 on 2 and 318 DF, p-value: < 2.2e-16
```

Summary of Fit Quality (mod_2)

name	r.squared	adj.r.squared	sigma	AIC	BIC
mod_2	0.334	0.33	0.024	-1477	-1462

Tidied coefficients (mod_2)

term	estimate	std.error	p.value	conf.low	conf.high
(Intercept)	0.1939	0.0126	0.000	0.1691	0.2187
a1c_old	-0.0096	0.0008	0.000	-0.0112	-0.0080
age	0.0002	0.0002	0.146	-0.0001	0.0006

```
Call:
lm(formula = (1/alc) \sim alc_old + age + income, data = dm4_dev)
Residuals:
    Min
          10 Median 30
                                       Max
-0.067448 -0.013845 0.000413 0.012895 0.077722
Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)
                 0.1924566 0.0127526 15.092 <2e-16 ***
alc old
               0.0002489 0.0001692 1.471 0.142
age
incomeBetween_30-50K  0.0024669  0.0031434  0.785  0.433
incomeHigher_than_50K -0.0001717 0.0036244 -0.047 0.962
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
Residual standard error: 0.02409 on 316 degrees of freedom
Multiple R-squared: 0.3359, Adjusted R-squared: 0.3275
F-statistic: 39.96 on 4 and 316 DF, p-value: < 2.2e-16
```

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Summary of Fit Quality (mod_3)

name	r.squared	adj.r.squared	sigma	AIC	BIC
mod_3	0.336	0.328	0.024	-1474	-1451

Tidied coefficients (mod_3)

term	est	se	p	low95	high95
(Intercept)	0.1925	0.0128	0.000	0.1674	0.2175
a1c_old	-0.0095	0.0008	0.000	-0.0111	-0.0079
age	0.0002	0.0002	0.142	-0.0001	0.0006
incomeBetween_30-50K	0.0025	0.0031	0.433	-0.0037	0.0087
incomeHigher_than_50K	-0.0002	0.0036	0.962	-0.0073	0.0070

Could we have fit other predictor sets?

Perhaps an automated procedure like stepwise regression would suggest a better alternative?

- Three predictor candidates, so we could have used any of these predictor sets:
- a1c_old alone (our mod_1)
- age alone
- income alone
- a1c_old and age (our mod_2)
- a1c_old and income
- age and income
- a1c_old, age and income (our mod_3)

```
step(mod_3)
```

```
Start: AIC=-2387.04
(1/a1c) \sim a1c \text{ old} + age + income
         Df Sum of Sa RSS
                                 AIC
- income 2 0.000502 0.18392 -2390.2
<none>
                      0.18342 -2387.0
- age 1 0.001256 0.18468 -2386.8
- alc old 1 0.078742 0.26216 -2274.4
Step: AIC=-2390.16
(1/a1c) \sim a1c_old + age
         Df Sum of Sq
                          RSS
                                 AIC
                      0.18392 - 2390.2
<none>
      1 0.001229 0.18515 -2390.0
– age
- a1c_old 1 0.079935 0.26386 -2276.3
Call:
lm(formula = (1/alc) \sim alc_old + age, data = dm4_dev)
Coefficients:
(Intercept) alc_old
                                 age
 0.1939204 -0.0095521 0.0002429
```

Comparing Summary Measures of Fit

in the development sample...

name	r2	adj_r2	sigma	AIC	BIC	df	df_resid
mod_1	0.3297	0.3276	0.0241	-1477.1	-1466	2	319
mod_2	0.3341	0.3299	0.0240	-1477.2	-1462	3	318
mod_3	0.3359	0.3275	0.0241	-1474.1	-1451	5	316

OK. What do we think?

Check adherence to regression assumptions in the development sample.

Checking Regression Assumptions

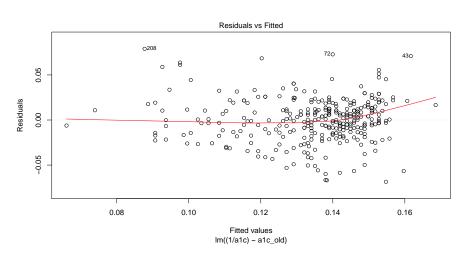
Four key assumptions we need to think about:

- Linearity
- Constant Variance (Homoscedasticity)
- Normality
- Independence

How do we assess 1, 2, and 3? Residual plots.

Residuals vs. Fitted Values Plot (Model mod_1)

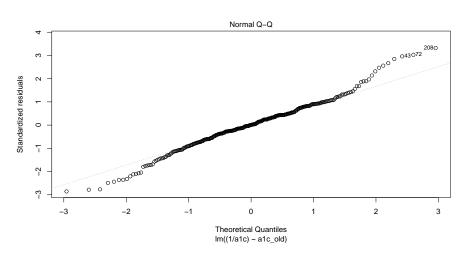
plot(mod_1, which = 1)



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Normal Q-Q of Standardized Residuals (mod_1)

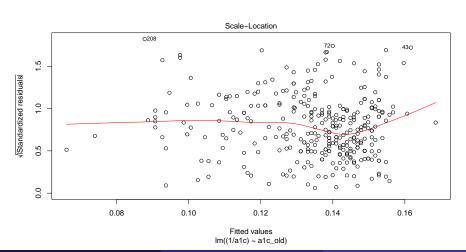
plot(mod_1, which = 2)



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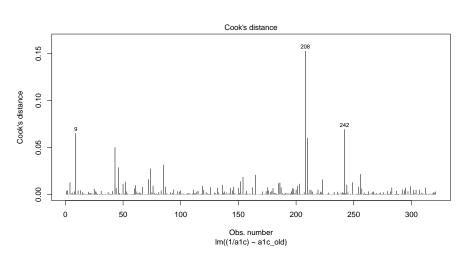
Scale-Location: Non-constant variance check (mod_1)

plot(mod_1, which = 3)



Index plot of Cook's distance for influence (mod_1)

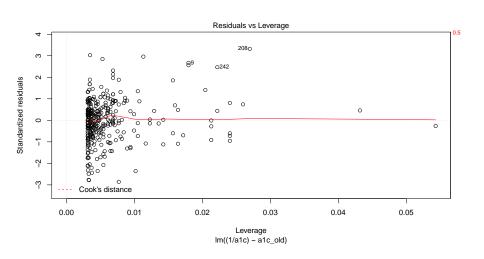
plot(mod_1, which = 4)



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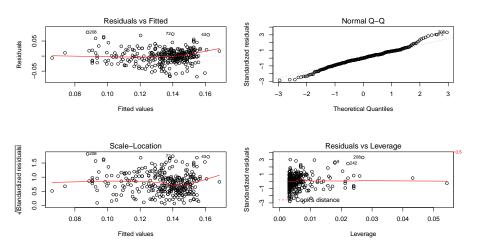
Residuals, Leverage and Influence plot (mod_1)

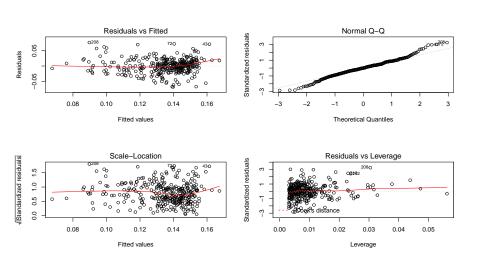
plot(mod_1, which = 5)

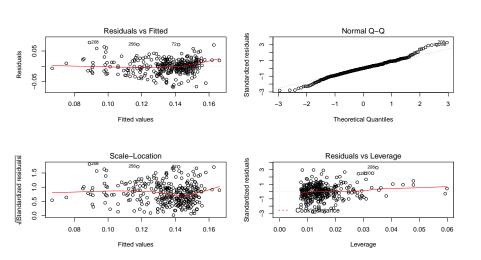


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$$par(mfrow = c(2,2)); plot(mod_1); par(mfrow = c(1,1))$$







Conclusions so far?

- In-sample model predictions are about equally accurate for each of the three models. It's not clear yet that we need anything more than the simple regression on a1c_old.
- Residual plots look similarly reasonable for linearity, Normality and constant variance in all three models.
- Probably worth considering all three models further, but it would depend on the context.

When you have candidates, assess them based on the accuracy of the predictions they make for the data held out (and thus not used in building the models.)

Calculate prediction errors for mod_1 in test sample

The augment function in the broom package will create predictions within our new sample, but we want to back-transform these predictions so that they are on the original scale (a1c, rather than our transformed regression outcome 1/a1c). Since the way to back out of the inverse transformation is to take the inverse again, we will take the inverse of the fitted values provided by augment and then calculate residuals on the original scale, as follows...

What does test_m1 now include?

subject	a1c	fit_a1c	res_a1c	a1c_old	age	income
S-002	11.0	20.28	-9.28	16.3	54	Between_30-50K
S-005	6.7	6.76	-0.06	6.3	64	Between_30-50K
S-006	5.8	6.85	-1.05	6.5	48	Below_30K
S-009	12.9	7.46	5.44	7.7	55	Below_30K
S-013	8.1	6.95	1.15	6.7	55	Higher_than_50K
S-016	8.4	7.46	0.94	7.7	44	Between_30-50K

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Combine test sample results from the three models

name	subject	a1c	fit_a1c	res_a1c	a1c_old	age	income
mod_1	S-002	11.0	20.28	-9.28	16.3	54	Between_30-5
mod_2	S-002	11.0	19.48	-8.48	16.3	54	Between_30-5
mod_3	S-002	11.0	18.87	-7.87	16.3	54	Between_30-5
mod_1	S-006	5.8	6.85	-1.05	6.5	48	Below_30K
mod_2	S-006	5.8	6.97	-1.17	6.5	48	Below_30K
mod_3	S-006	5.8	7.02	-1.22	6.5	48	Below_30K

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What do we do to compare the test-sample errors?

Given this tibble, including predictions and residuals from the three models on our test data, we can now:

- Visualize the prediction errors from each model.
- Summarize those errors across each model.
- Identify the "worst fitting" subject for each model in the test sample.

```
ggplot(test_comp, aes(x = res_a1c, fill = name)) +
  geom_histogram(bins = 20, col = "white") +
  facet_grid (name ~ .) + guides(fill = FALSE)
or maybe
ggplot(test_comp, aes(x = name, y = res_a1c, fill = name)) +
  geom violin(alpha = 0.3) +
  geom_boxplot(width = 0.3, outlier.shape = NA) +
  geom_jitter(height = 0, width = 0.1) +
  guides(fill = FALSE)
```

Test-Sample Prediction Errors

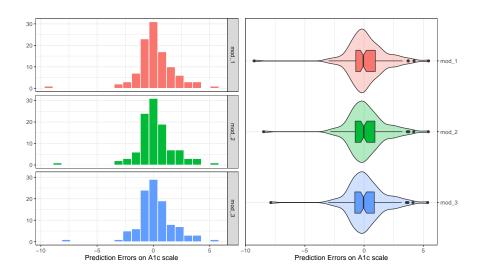


Table Comparing Model Prediction Errors

Calculate the mean absolute prediction error (MAPE), the mean squared prediction error (MSPE) and the maximum absolute error across the predictions made by each model.

Identify the largest errors

Identify the subject(s) where that maximum prediction error was made by each model, and the observed and model-fitted values of a1c in each case.

```
temp1 <- test_m1 %>%
  filter(abs(res_a1c) == max(abs(res_a1c)))

temp2 <- test_m2 %>%
  filter(abs(res_a1c) == max(abs(res_a1c)))

temp3 <- test_m3 %>%
  filter(abs(res_a1c) == max(abs(res_a1c)))
```

Identify the largest errors (Results)

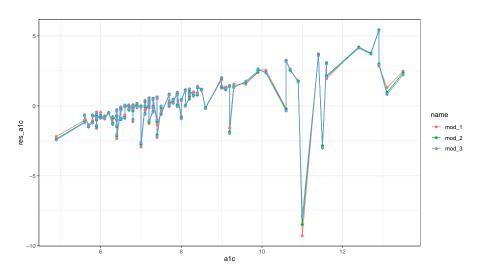
Identify the subject(s) where that maximum prediction error was made by each model, and the observed and model-fitted values of a1c in each case.

```
bind_rows(temp1, temp2, temp3) %>%
select(subject, a1c, fit_a1c, res_a1c)
```

Line Plot of the Errors?

Compare the errors that are made at each level of observed A1c?

Line Plot of the Errors?



What if we ignored S-002 for a moment?

All three miss this subject substantially, but without S-002, we have:

With the exception of subject S-002, the three models seem to make very similar errors in the test sample.

Conclusions now?

- In-sample model predictions are about equally accurate for each of the three models. It's not clear yet that we need anything more than the simple regression on a1c_old. The addition of the other two predictors doesn't add predictive value that is statistically detectable.
- Residual plots look similarly reasonable for linearity, Normality and constant variance in all three models.
- Excluding a bad miss on one subject in the test sample, all three models do about equally well, with perhaps mod_3 very slightly better according to all three metrics (MAPE, MSPE and max_error) in the test sample.

So, what should our "most useful" model be?

Repeating our 431 Strategy

Which model is "most useful" in a prediction context?

- Split the data into a model development (training) sample of about 70-80% of the observations, and a model test (holdout) sample, containing the remaining observations.
- Oevelop candidate models using the development sample.
- Assess the quality of fit for candidate models within the development sample.
- Check adherence to regression assumptions in the development sample.
- When you have candidates, assess them based on the accuracy of the predictions they make for the data held out (and thus not used in building the models.)
- Select a "final" model for use based on the evidence in steps 3, 4 and especially 5.