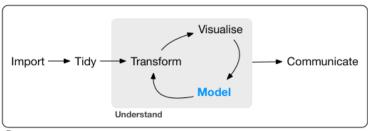


Lecture 7: Modeling I

Data Science for Business Analytics





Program

- This morning:
 - how models work mechanistically (focus on linear models),
 - how to use models to find patterns in real data.
- This afternoon:
 - ▶ how to use **many** simple models,
 - ▶ how to combine modeling and programming tools.

As usual, most of the material is borrowed from R for data science.

Outline



1 Model basics

2 Model building

Hypothesis generation/confirmation



- 1. Each observation can either be used for exploration **OR** confirmation, not both.
- 2. You can use an observation
 - as many times as you like for exploration,
 - only once for confirmation.

When using an observation twice, switch from confirmation to exploration.



Goals:

- Provide a simple low-dimensional summary of a dataset.
- Often partition data into patterns and residuals.
- Help peel back layers of structure (since strong patterns hide subtler trends).

Two parts to a model:

- 1. **Family of models**: a precise, but generic, pattern to capture.
 - A straight line, or a quadatric curve.
 - Equations like y = a_1 * x + a_2 or y = a_1 * x ^ a_2 (with x and y known variables and a_1 and a_2 parameters).
- 2. **Fitted model**: member of the family that is closest to the data.
 - $y = 3 * x + 7 \text{ or } y = 9 * x ^ 2.$

Word of caution



All models are wrong, but some are useful. —George Box

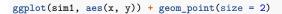
- A fitted model is "just" the closest model to the data from a family of models.
- The "best" model (according to some criteria):
 - isn't necessarily a good model,
 - isn't necessarily "true".

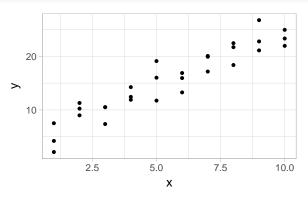
The goal is not to uncover truth, but to discover useful approximations.

```
library(tidyverse)
library(modelr)
```

A simulated dataset

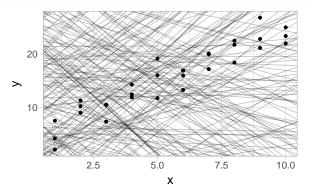






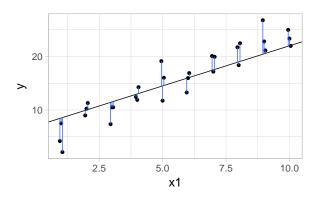
Linear family?





Distance between data and model





This distance is the difference between

- the y value given by the model (the prediction),
- and the actual y value in the data (the response).

Model family and RMSE



The model family:

```
model1 <- function(a, data) a[1] + data$x * a[2]
model1(c(7, 1.5), sim1)
## [1] 8.5 8.5 8.5 10.0 10.0 10.0 11.5 11.5 11.5 13.0 13.0 13.0 14.5
## [14] 14.5 14.5 16.0 16.0 16.0 17.5 17.5 17.5 19.0 19.0 19.0 20.5 20.5
## [27] 20.5 22.0 22.0 22.0</pre>
```

Root-mean-square error (RMSE):

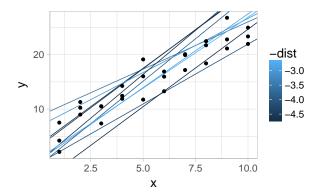
```
measure_distance <- function(mod, data) {
    diff <- data$y - model1(mod, data)
    sqrt(mean(diff ^ 2))}
measure_distance(c(7, 1.5), sim1)</pre>
```

[1] 2.665212



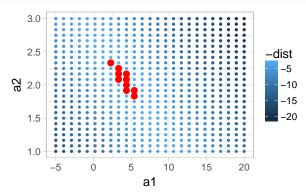
```
sim1_dist <- function(a1, a2) measure_distance(c(a1, a2), sim1)</pre>
(models <- models %>% mutate(dist = map2_dbl(a1, a2, sim1_dist)))
## # A tibble: 250 x 3
##
         а1
                a2 dist
##
      <dbl> <dbl> <dbl>
##
   1 33.8 4.43 43.3
   2 - 4.07 2.62 5.82
##
##
   3 2.33 4.33 12.7
   4 14.4 -0.293 7.58
##
##
   5 34.5 1.04
                   24.9
##
   6 - 7.90 -0.150 25.1
   7 33.9 -3.91 17.5
##
##
   8 36.7 -2.52 15.2
   9 19.6 -0.0149 7.50
##
## 10 17.7 -1.27 10.9
## # ... with 240 more rows
```



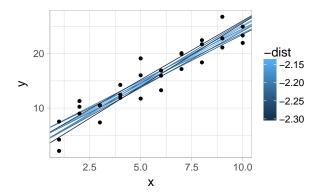


Grid search







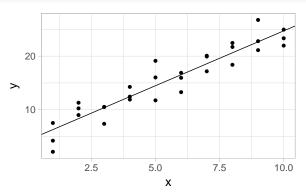


Newton-Raphson search



(best <- optim(c(0, 0), measure_distance, data = sim1)\$par)
[1] 4.222248 2.051204

```
ggplot(sim1, aes(x, y)) + geom_point(size = 2) +
  geom_abline(intercept = best[1], slope = best[2])
```



Linear models



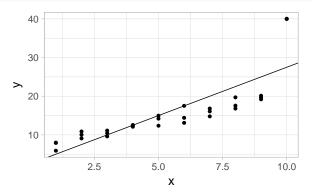
- General form is e.g. $y = a_1 + a_2 * x_1 + a_3 * x_2 + a_3 * x_4 + a_4 * x_4 + a_5 * x_5 * x_6 * x$... + a n * x (n - 1)
- Im() specify the model family using formulas (e.g., y ~ x, which lm() translates to a function like $y = a_1 + a_2 * x$

```
sim1_mod \leftarrow lm(y \sim x, data = sim1)
coef(sim1 mod)
## (Intercept)
```

4.220822 ## 2.051533

What is going on here?





Visualizing models



Two interesting quantities to look at:

- predictions,
- and residuals.

Visualizing predictions: step 1/3



```
(grid <- sim1 %>% modelr::data_grid(x))
## # A tibble: 10 x 1
##
##
      <int>
##
##
##
##
##
          5
          6
##
##
##
##
##
   10
         10
```

Visualizing predictions: step 2/3



```
(grid <- grid %>% add_predictions(sim1_mod))
## # A tibble: 10 x 2
##
          x pred
##
      <int> <dbl>
          1 6.27
##
##
          2 8.32
##
          3 10.4
##
          4 12.4
##
          5 14.5
          6 16.5
##
##
          7 18.6
##
          8 20.6
          9 22.7
##
```

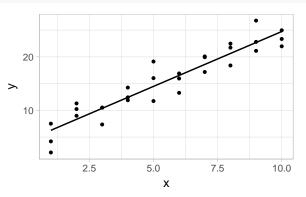
10

10 24.7

Visualizing predictions: step 3/3



```
ggplot(sim1, aes(x, y)) + geom_point(size = 2) +
geom_line(aes(y = pred), data = grid, size = 1)
```





```
(sim1 <- sim1 %>% add_residuals(sim1_mod))
## # A tibble: 30 x 3
##
                     resid
          х
##
      <int> <dbl>
                     <dbl>
##
          1 \quad 4.20 \quad -2.07
##
          1 7.51 1.24
##
          1 2.13 -4.15
##
          2 8.99 0.665
##
          2 10.2 1.92
##
          2 11.3 2.97
          3 7.36 -3.02
##
         3 10.5 0.130
##
##
         3 10.5 0.136
## 10
         4 12.4 0.00763
    ... with 20 more rows
```

Visualizing residuals: step 2/2



```
ggplot(sim1, aes(resid)) + geom_freqpoly(binwidth = 0.5)
ggplot(sim1, aes(x, resid)) + geom_ref_line(h = 0) + geom_point()
                                                5.0
      5
      4
                                                2.5
    count 2
                                             esid
                                                0.0
                                               -2.5
       -5.0
                -2.5
                         0.0
                                 2.5
                                          5.0
                                                         2.5
                                                                  5.0
                                                                           7.5
                                                                                   10.0
                         resid
```

Exercises



- 1. Instead of using lm() to fit a straight line, you can use loess() to fit a smooth curve. Repeat the process of model fitting, grid generation, predictions, and visualisation on sim1 using loess() instead of lm(). How does the result compare to geom_smooth()?
- 2. add_predictions() is paired with gather_predictions() and spread_predictions(). How do these three functions differ?
- 3. What does geom_ref_line() do? What package does it come from? Why is displaying a reference line in plots showing residuals useful and important?
- 4. Why might you want to look at a frequency polygon of absolute residuals? What are the pros and cons compared to looking at the raw residuals?



- A way of getting "special behavior".
- "Capture variables" so they can be interpreted by the function.
- Sometimes called "Wilkinson-Rogers notation" from Symbolic Description of Factorial Models for Analysis of Variance

Behind the scenes:



Without intercept:

Adding a second variable:

Categorical variables



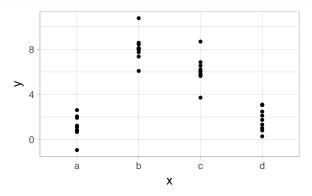
```
df <- tribble(~ sex, ~ response,
            "male". 1.
            "female", 2,
            "male", 1)
model_matrix(df, response ~ sex)
## # A tibble: 3 x 2
##
    `(Intercept)` sexmale
##
           <dbl> <dbl>
## 1
          1.00 1.00
## 2
          1.00 0
## 3
          1.00 1.00
```

Why doesn't R also create a sexfemale column?

Another simulated dataset







Linear model and predictions



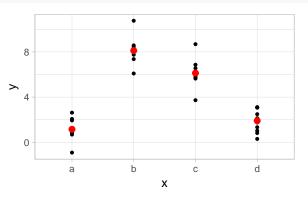
```
mod2 <- lm(y ~ x, data = sim2)
(grid <- sim2 %>% data_grid(x) %>% add_predictions(mod2))

## # A tibble: 4 x 2
## x pred
## <chr> <dbl>
## 1 a    1.15
## 2 b    8.12
## 3 c    6.13
## 4 d    1.91
```

Visualize the results



```
ggplot(sim2, aes(x)) + geom_point(aes(y = y), size = 2) +
geom_point(data = grid, aes(y = pred), color = "red", size = 4)
```



What's happening here?

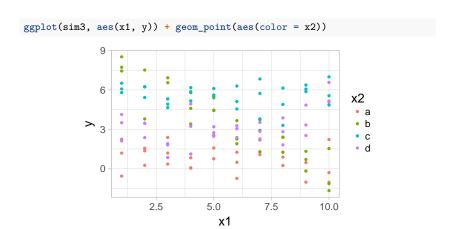


```
tibble(x = "e") %>% add_predictions(mod2)
```

Error in model.frame.default(Terms, newdata, na.action = na.action, xlev = o

Interactions (cont. and cat.)





Two possible models



```
mod1 <- lm(y ~ x1 + x2, data = sim3)
mod2 <- lm(y ~ x1 * x2, data = sim3)
```

Note that:

- $y \sim x1 + x2$ is translated to $y = a_0 + a_1 * x1 + a_2 * x2$.
- $y \sim x1 * x2$ is translated to $y = a_0 + a_1 * x1 + a_2 * x2 + a_12 * x1 * x2.$

Two new tricks to visualize them



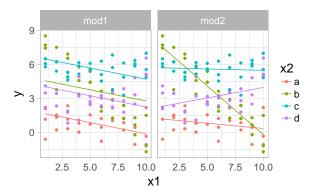
- Give data_grid() both variables.
- 2. To generate predictions from both models simultaneously, use
 - gather_predictions() to add predictions as rows,
 - or spread_predictions() to add predictions as columns.

```
(grid <- sim3 %>% data_grid(x1, x2) %>% gather_predictions(mod1, mod2))
## # A tibble: 80 x 4
     model
              x1 x2
##
                       pred
##
     <chr> <int> <fct> <dbl>
##
   1 mod1
               1 a
                       1.67
   2 mod1
               1 b
                       4.56
##
##
   3 mod1 1 c
                       6.48
   4 mod1 1 d
                       4.03
##
          2 a
   5 mod1
                    1.48
##
          2 b
##
   6 mod1
                    4.37
   7 mod1
              2 c
                    6.28
##
##
   8 mod1
               2 d
                       3.84
##
   9 mod1
               3 a
                      1.28
## 10 mod1
               3 b
                       4.17
## # ... with 70 more rows
```

Using facetting



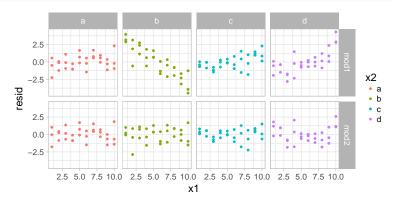
```
ggplot(sim3, aes(x1, y, color = x2)) + geom_point() +
  geom_line(data = grid, aes(y = pred)) + facet_wrap(~ model)
```





```
sim3 <- sim3 %>% gather_residuals(mod1, mod2)

ggplot(sim3, aes(x1, resid, color = x2)) + geom_point() +
  facet_grid(model ~ x2)
```



Interactions (two continuous)



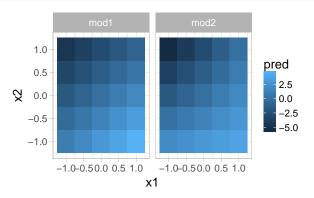
```
mod1 \leftarrow lm(y \sim x1 + x2, data = sim4)
mod2 \leftarrow lm(y \sim x1 * x2, data = sim4)
(grid <- sim4 %>%
       data_grid(x1 = seq_range(x1, 5), x2 = seq_range(x2, 5)) \%
       gather_predictions(mod1, mod2))
## # A tibble: 50 x 4
##
    model x1
                     x2 pred
## <chr> <dbl> <dbl> <dbl> <dbl>
   1 mod1 -1.00 -1.00 0.996
##
   2 mod1 -1.00 -0.500 -0.395
##
   3 mod1 -1.00 0 -1.79
##
   4 mod1 -1.00 0.500 -3.18
##
   5 mod1 -1.00 1.00 -4.57
##
##
   6 mod1 -0.500 -1.00 1.91
## 7 mod1 -0.500 -0.500 0.516
## 8 mod1 -0.500 0 -0.875
##
   9 mod1 -0.500 0.500 -2.27
## 10 mod1 -0.500 1.00 -3.66
## # ... with 40 more rows
```

?seq_range for other arguments (e.g., pretty = TRUE for tables).



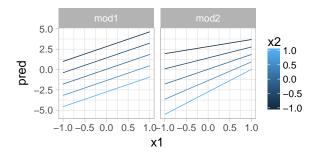


```
ggplot(grid, aes(x1, x2)) + geom_tile(aes(fill = pred)) +
facet_wrap(~ model)
```





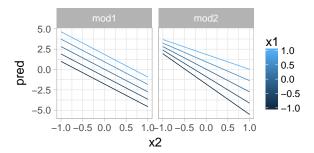
```
ggplot(grid, aes(x1, pred, color = x2, group = x2)) + geom_line() +
facet_wrap(~ model)
```



Slices with respect to x1



ggplot(grid, aes(x2, pred, color = x1, group = x1)) + geom_line() +
 facet_wrap(~ model)



model_matrix(df, y ~ x^2 + x)



- $log(y) \sim sqrt(x1) + x2$ is transformed to $log(y) = a_1 + a_2 * sqrt(x1) + a_3 * x2$.
- If the transformation involves +, *, ^, or -, wrap it in I():

```
y \sim x + I(x ^2) \equiv y = a_1 + a_2 * x + a_3 * x^2.
```

 $y \sim x ^2 + x \equiv y \sim x * x + x \equiv y = a_1 + a_2 * x.$

```
model_matrix(df, y \sim I(x^2) + x)
## # A tibble: 3 x 2
## `(Intercept)` x
##
     <dbl> <dbl>
## 1 1.00 1.00
## 2 1.00 2.00
## 3 1.00 3.00
## # A tibble: 3 x 3
## `(Intercept)` `I(x^2)` x
##
      <dbl> <dbl> <dbl>
## 1 1.00 1.00 1.00
## 2
   1.00 4.00 2.00
## 3
    1.00 9.00 3.00
```

df <- tribble(~y, ~x, 1, 1, 2, 2, 3, 3)

Polynomial approximations with poly Columbia University in the city of New York



```
To get y = a_1 + a_2 * x + a_3 * x^2:
model_matrix(df, y ~ poly(x, 2))
## # A tibble: 3 x 3
   ##
##
        <dbl>
                         <dbl>
                               <dbl>
## 1
        1.00 -0.707
                                  0.408
## 2 1.00 -0.000000000000000785
                              -0.816
## 3
         1.00 0.707
                                  0.408
```

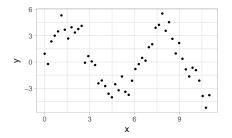
Natural splines



```
library(splines)
model_matrix(df, y ~ ns(x, 2))
## # A tibble: 3 x 3
    `(Intercept)` `ns(x, 2)1` `ns(x, 2)2`
##
##
           <dbl>
                     <dbl>
                               <dbl>
## 1
           1.00
                     0
                                0
## 2
          1.00 0.566 -0.211
## 3
           1.00
                   0.344
                              0.771
```

A non-linear function





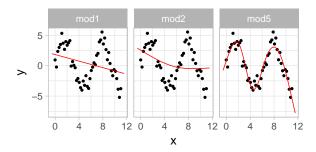
Three models using splines:

```
mod1 <- lm(y ~ ns(x, 1), data = sim5)
mod2 <- lm(y ~ ns(x, 2), data = sim5)
mod5 <- lm(y ~ ns(x, 5), data = sim5)
```



```
grid <- sim5 %>%
  data_grid(x = seq_range(x, n = 50, expand = 0.1)) %>%
  gather_predictions(mod1, mod2, mod5, .pred = "y")

ggplot(sim5, aes(x, y)) + geom_point() +
  geom_line(data = grid, color = "red") +
  facet_wrap(~ model)
```



Missing values



```
options(na.action = na.warn)
df <- tribble(~x, ~y,
               1, 2.2,
               2, NA,
               3, 3.5,
               4, 8.3,
               NA, 10)
mod \leftarrow lm(y \sim x, data = df)
## Warning: Dropping 2 rows with missing values
mod \leftarrow lm(y \sim x, data = df, na.action = na.exclude)
nobs(mod)
## [1] 3
```

Other model families



- Generalised linear models, e.g. stats::glm():
 - ▶ LMs assume continuous responses and Gaussian errors.
 - GLMs extend LMs to other distributions, including non-continuous responses (e.g. binary data or counts).
- Generalised additive models, e.g. mgcv::gam():
 - Extend GLMs to incorporate arbitrary smooth functions.
 - A formula like $y \sim s(x)$ becomes an equation like y = f(x).
- Penalized linear models, e.g. glmnet::glmnet():
 - Add penalties to favor simpler models.
 - "Generalize" better to new datasets.
- Robust linear models, e.g. MASS:rlm():
 - Tweaks distance to downweight outliers.
 - Less sensitive to outliers, but sligthly worse without outliers.
- **Trees**, e.g. rpart::rpart():
 - ▶ A piece-wise constant model splitting the data into small pieces.
 - Powerful when aggregated as random forests (e.g. randomForest::randomForest()) or gradient boosting machines (e.g. xgboost::xgboost()).

Outline



1 Model basics

2 Model building

Model building



To partition data into pattern and residuals:

- 1. Find patterns with visualisation.
- 2. Make them concrete and precise with a model.
- 3. Repeat 1. and 2. after replacing the old response variable with the residuals from the model.

How about large and complex datasets?

- ML approaches "simply" focus on predictive ability.
- Issues:
 - black boxes,
 - (sometimes) hard to use domain knowledge,
 - (often) difficult to assess whether or not the model will continue to work in the long-term
- Usually, combinations of both approaches are preferred.

The diamonds dataset

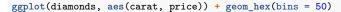


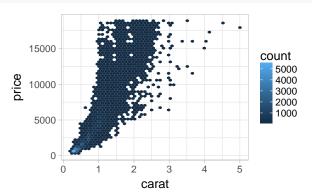
```
ggplot(diamonds, aes(cut, price)) + geom_boxplot()
ggplot(diamonds, aes(color, price)) + geom_boxplot()
ggplot(diamonds, aes(clarity, price)) + geom_boxplot()
                                                               15000
  15000
                                15000
10000
                                                              10000
                                10000
                                                               5000
  5000
                                5000
                                                                      Siz
                                                                            VS2 VS1 VVS2 VVS1
                                               color
                                                                            clarity
                 cut
```

Why are low quality diamonds more expensive?

Price and carat







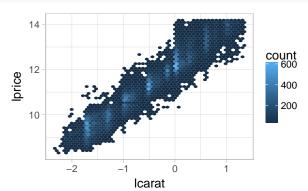
A couple of tweaks



- 1. Focus on diamonds < 2.5 carats (99.7% of the data).
- 2. Log-transform the carat and price.

```
diamonds2 <- diamonds %>% filter(carat <= 2.5) %>%
  mutate(lprice = log2(price), lcarat = log2(carat))

ggplot(diamonds2, aes(lcarat, lprice)) + geom_hex(bins = 50)
mod_diamond <- lm(lprice ~ lcarat, data = diamonds2)</pre>
```

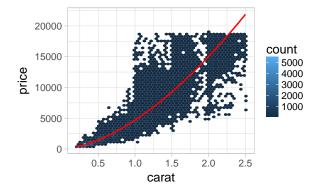


Visualize the predictions



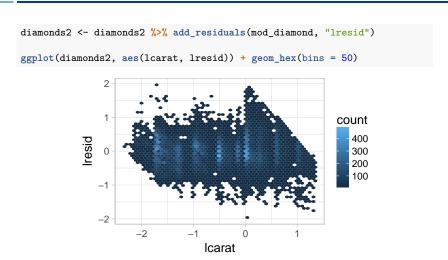
```
grid <- diamonds2 %>% data_grid(carat = seq_range(carat, 20)) %>%
  mutate(lcarat = log2(carat)) %>%
  add_predictions(mod_diamond, "lprice") %>%
  mutate(price = 2 ^ lprice)

ggplot(diamonds2, aes(carat, price)) + geom_hex(bins = 50) +
  geom_line(data = grid, color = "red", size = 1)
```



Visualize the residuals





Replace price by residuals



```
ggplot(diamonds2, aes(cut, lresid)) + geom_boxplot()
ggplot(diamonds2, aes(color, lresid)) + geom_boxplot()
ggplot(diamonds2, aes(clarity, lresid)) + geom_boxplot()
```

A more complicated model



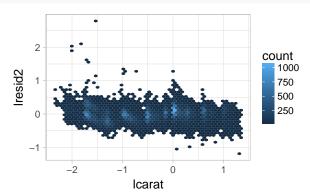
```
mod_diamond2 <- lm(lprice ~ lcarat + color + cut + clarity,</pre>
                data = diamonds2)
(grid <- diamonds2 %>%
       data grid(cut, lcarat = -0.515,
               color = "G", clarity = "SI1") %>%
       add_predictions(mod_diamond2))
## # A tibble: 5 x 5
##
    cut lcarat color clarity
                                pred
##
    <ord>
            <dbl> <chr> <chr>
                               <dbl>
## 1 Fair -0.515 G
                        ST1 11.0
## 2 Good -0.515 G SI1 11.1
## 3 Very Good -0.515 G SI1 11.2
## 4 Premium -0.515 G SI1 11.2
## 5 Ideal -0.515 G
                        SI1
                                11.2
```

Visualize the residuals



```
diamonds2 <- diamonds2 %>%
  add_residuals(mod_diamond2, "lresid2")

ggplot(diamonds2, aes(lcarat, lresid2)) +
  geom_hex(bins = 50)
```



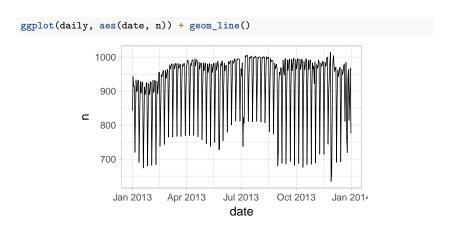
The number of daily flights



```
daily <- flights %>%
    mutate(date = make_date(year, month, day)) %>%
    group_by(date) %>%
    summarise(n = n())
```

What affects this number?

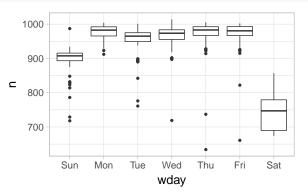




Day of week



```
daily <- daily %>% mutate(wday = wday(date, label = TRUE))
ggplot(daily, aes(wday, n)) + geom_boxplot()
mod <- lm(n ~ wday, data = daily)</pre>
```

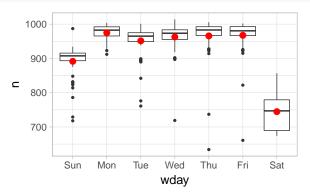


Visualize the predictions



```
grid <- daily %>% data_grid(wday) %>%
  add_predictions(mod, "n")

ggplot(daily, aes(wday, n)) + geom_boxplot() +
  geom_point(data = grid, color = "red", size = 4)
```

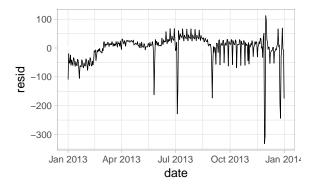


Visualize the residuals



```
daily <- daily %>% add_residuals(mod)

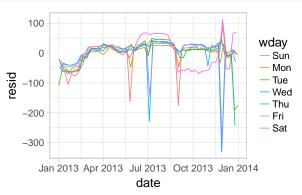
daily %>% ggplot(aes(date, resid)) +
  geom_ref_line(h = 0) + geom_line()
```



What happens here?



```
ggplot(daily, aes(date, resid, colour = wday)) +
  geom_ref_line(h = 0) + geom_line()
```



What happens here?

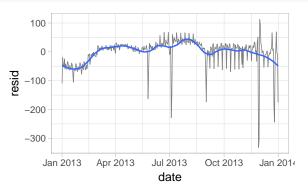


```
daily %>% filter(resid < -100)
## # A tibble: 11 x 4
##
      date
                     n wday
                             resid
##
      <date>
                 <int> <ord> <dbl>
##
    1 2013-01-01
                   842 Tue
                              -109
##
   2 2013-01-20 786 Sun
                              -105
##
   3 2013-05-26
                   729 Sun
                              -162
##
   4 2013-07-04
                  737 Thu
                              -229
##
    5 2013-07-05
                   822 Fri
                              -145
##
   6 2013-09-01
                   718 Sun
                              -173
    7 2013-11-28
                   634 Thu
                              -332
##
##
   8 2013-11-29
                   661 Fri
                              -306
##
   9 2013-12-24
                   761 Tue
                              -190
## 10 2013-12-25
                   719 Wed
                              -244
## 11 2013-12-31
                   776 Tue
                              -175
```

What happens here?



```
daily %>%
    ggplot(aes(date, resid)) +
    geom_ref_line(h = 0) +
    geom_line(colour = "grey50") +
    geom_smooth(se = FALSE, span = 0.20)
```



Seasonal Saturday effect

⊂ 750

700



```
daily %>% filter(wday == "Sat") %>%
  ggplot(aes(date, n)) + geom_point() + geom_line() +
  scale_x_date(NULL, date_breaks = "1 month", date_labels = "%b")
850
800
```

Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec Jan

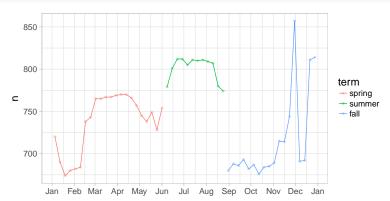
State's school terms: summer break in 2013 was Jun 26-Sep 9.

The three school terms



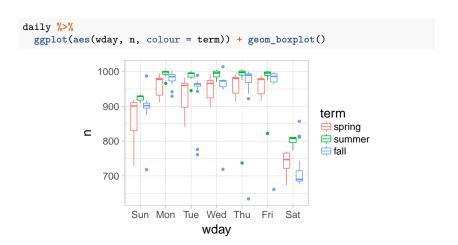
```
term <- function(date) {
  cut(date, breaks = ymd(20130101, 20130605, 20130825, 20140101),
        labels = c("spring", "summer", "fall"))}
daily <- daily %>% mutate(term = term(date))

daily %>% filter(wday == "Sat") %>% ggplot(aes(date, n, colour = term)) +
        geom_point(alpha = 1/3) + geom_line() +
        scale_x_date(NULL, date_breaks = "1 month", date_labels = "%b")
```



School terms and day of week



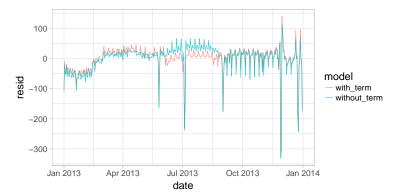


An improved model



```
mod1 <- lm(n ~ wday, data = daily)
mod2 <- lm(n ~ wday * term, data = daily)

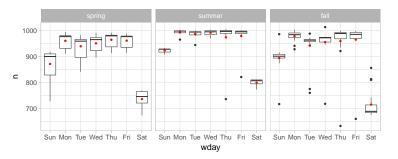
daily %% gather_residuals(without_term = mod1, with_term = mod2) %>%
    ggplot(aes(date, resid, colour = model)) + geom_line(alpha = 0.75)
```





```
grid <- daily %>% data_grid(wday, term) %>%
   add_predictions(mod2, "n")

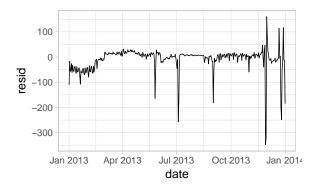
ggplot(daily, aes(wday, n)) + geom_boxplot() +
   geom_point(data = grid, colour = "red") + facet_wrap(~ term)
```



Robust fit



```
mod3 <- MASS::rlm(n ~ wday * term, data = daily)
daily %>% add_residuals(mod3, "resid") %>% ggplot(aes(date, resid)) +
  geom_hline(yintercept = 0, size = 2, colour = "white") + geom_line()
```



Computed variables



Either bundled up into a function:

Or directly in the model formula:

```
wday2 <- function(x) wday(x, label = TRUE)
mod3 <- lm(n ~ wday2(date) * term(date), data = daily)</pre>
```

Time of year: an alternative approach COLUMBIA UNIVERSITY

```
library(splines)
mod <- MASS::rlm(n ~ wday * ns(date, 5), data = daily)</pre>
daily %>% data_grid(wday, date = seq_range(date, n = 13)) %>%
  add_predictions(mod) %>%
  ggplot(aes(date, pred, colour = wday)) + geom_line() + geom_point()
```

