Lecture 6: Data modeling and linear regression

CME/STATS 195

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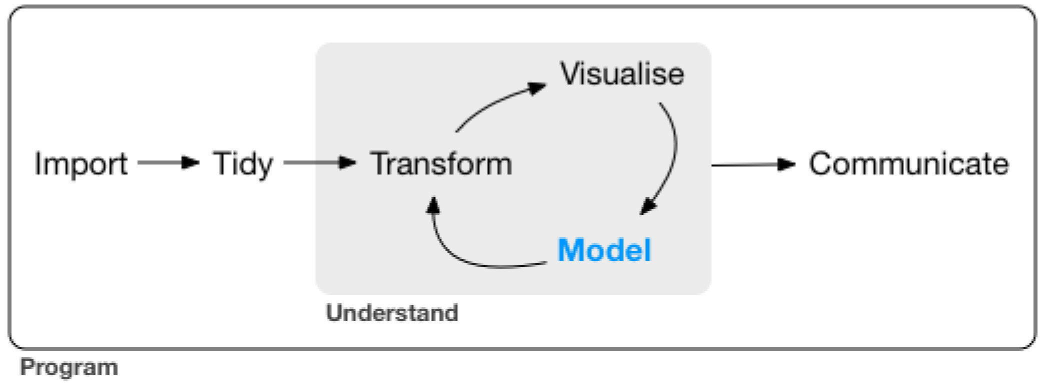


Data Modeling

Introduction to models

> *“**All models are wrong, but some are useful**. Now it would be very remarkable if any system existing in the real world could be exactly represented by any simple model. However, **cunningly chosen parsimonious models often do provide remarkably useful approximations** (…). For such a model there is no need to ask the question”Is the model true?“. If”truth" is to be the “whole truth” the answer must be “No”. The only question of interest is “Is the model illuminating and useful?” – George E.P. Box, 1976*

- The goal of a model is to **provide a simple low-dimensional summary of a dataset**.
- Models can be used to **partition data into patterns of interest and residuals** (other sources of variation and random noise).

Hypothesis generation vs. hypothesis confirmation

- Usually models are used for inference or confirmation of a pre-specified hypothesis.
- Doing inference correctly is hard. The key idea you must understand is that: **Each observation can either be used for exploration or confirmation, NOT both.**
- Observation can be used many times for exploration, but only once for confirmation.
- There is nothing wrong with exploration, but you should **never sell an exploratory analysis as a confirmatory analysis** because it is fundamentally misleading.

Confirmatory analysis

If you plan to do confirmatory analysis at some point after EDA, one approach is to split your data into three pieces before you begin the analysis:

- **Training set** – the bulk (e.g. 60%) of the dataset which can be used to do anything: visualizing, fitting multiple models.
- **Validation set** – a smaller set (e.g. 20%) used for manually comparing models and visualizations.
- **Test set** – a set (e.g. 20%) held back used only ONCE to test and asses your final model.

Confirmatory analysis

- Partitioning the dataset allows you to explore the training data, generate a number of candidate hypotheses and models.
- You can select a final model based on its performance on the validation set.
- Finally, when you are confident with the chosen model you can check how good it is using the test data.
- *Note that even when doing confirmatory modeling, you will still need to do EDA. If you don't do any EDA you might remain blind to some quality problems with your data.*

Model Basics

There are two parts to data modeling:

- **defining a family of models**: deciding on a set of models that can express a type of pattern you want to capture, e.g. a straight line, or a quadratic curve.
- **fitting a model**: finding a model within the family that the closest to your data.

A fitted model is just the best model from a chosen family of models, i.e. the "best" according to some set criteria.

This does not necessarily imply that the model is a good and certainly does NOT imply that the model is true.

The `modelr` package

- The `modelr` package, provides a few useful functions that are wrappers around base R's modeling functions.
- These functions facilitate the data analysis process as they are nicely integrated with the `tidyverse` pipeline.
- `modelr` is not automatically loaded when you load in `tidyverse` package, you need to do it separately:

```r
library(modelr)
```

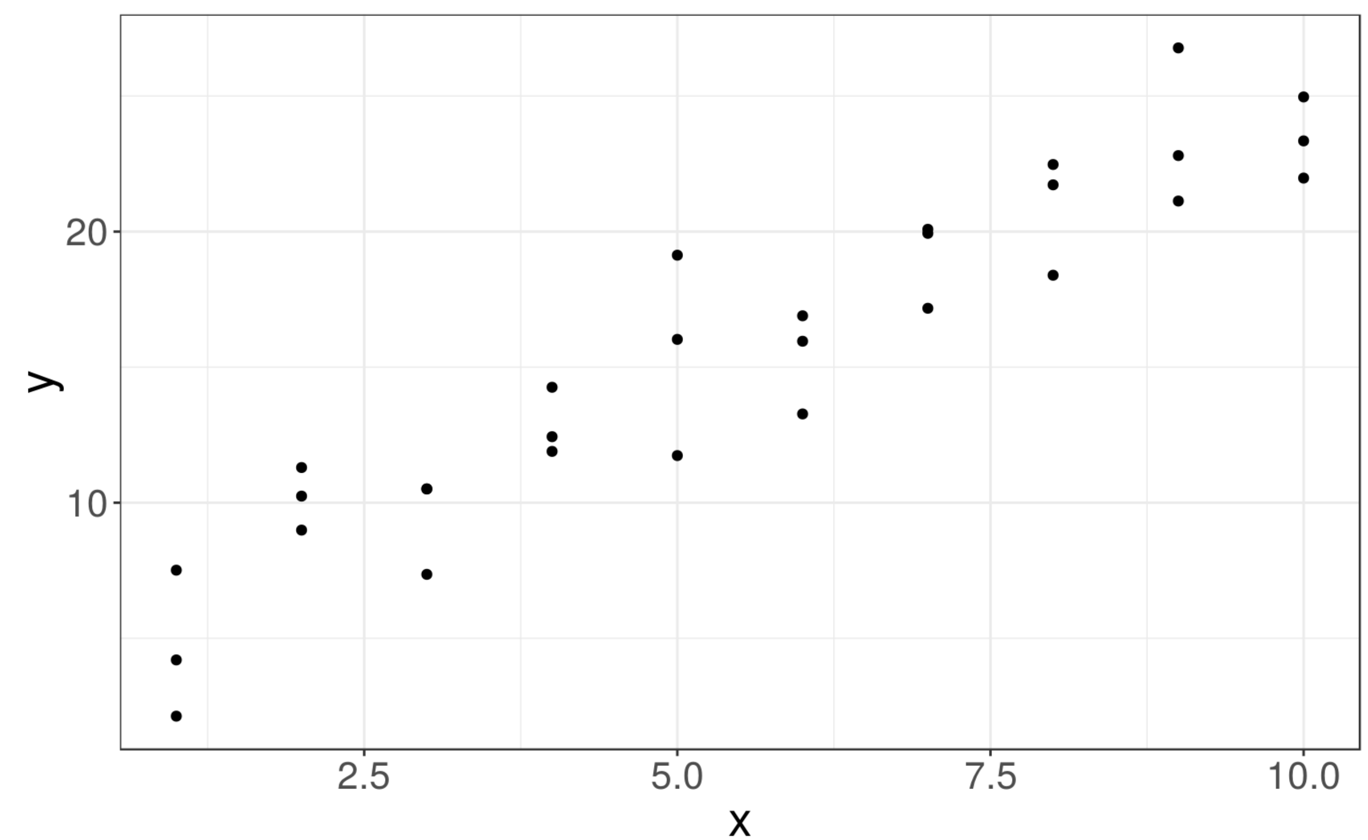
A toy dataset

We will work with a simulated dataset `sim1` from `modelr`:

```
sim1
```

```
## # A tibble: 30 x 2
##        x     y
##    <int> <dbl>
##  1     1  4.20
##  2     1  7.51
##  3     1  2.13
##  4     2  8.99
##  5     2 10.2
##  6     2 11.3
##  7     3  7.36
##  8     3 10.5
##  9     3 10.5
## 10     4 12.4
## # ... with 20 more rows
```

```
ggplot(sim1, aes(x, y)) + geom_point()
```



Defining a family of models

The relationship between x and y for the points in `sim1` look linear. So, will look for models which belong to **a family of models** of the following form:

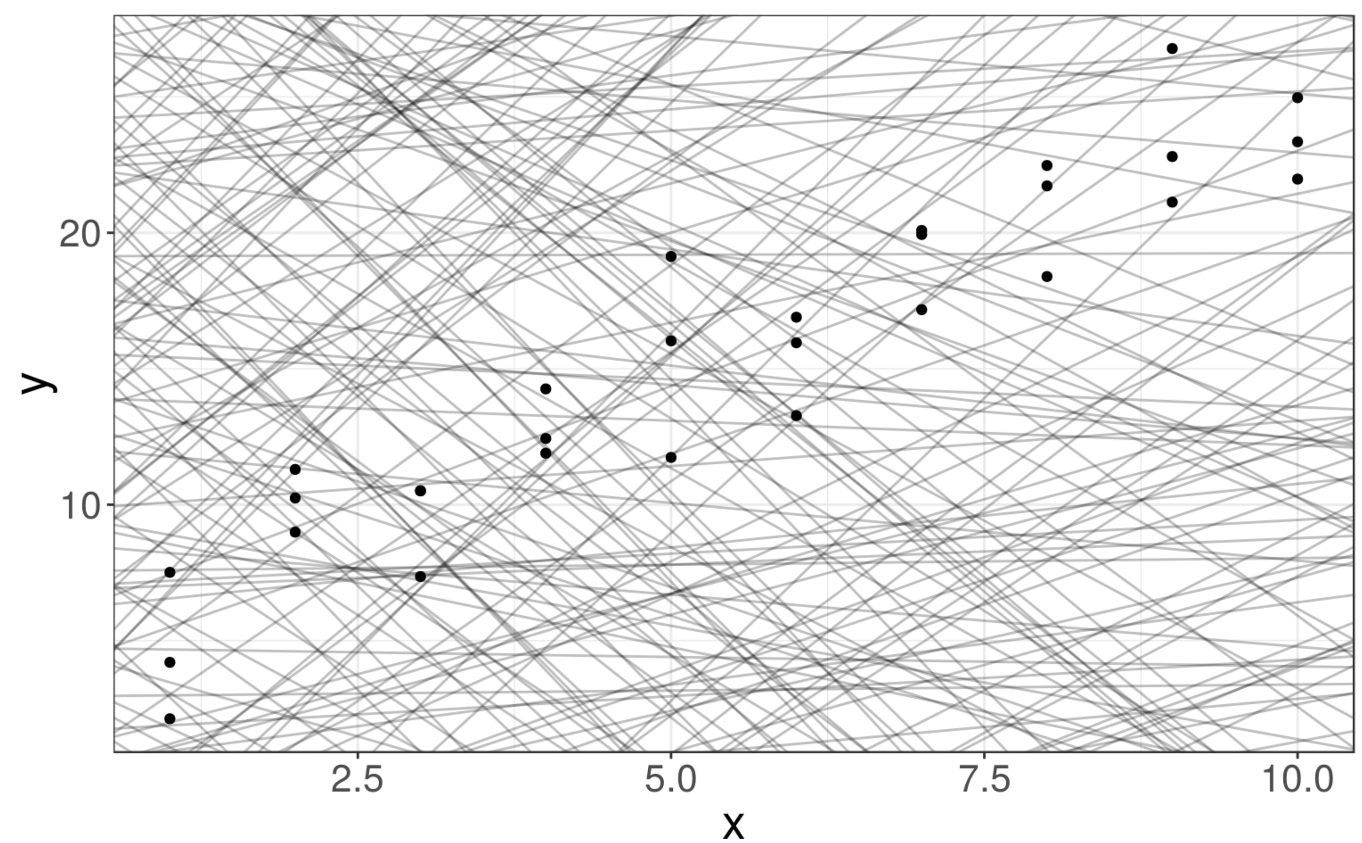
$$y = \beta_0 + \beta_1 \cdot x$$

The models that can be expressed by the above formula, can adequately capture a linear trend.

We generate a few examples of the models from this family on the right.

```
models <- tibble(
    b0 = runif(250, -20, 40),
    b1 = runif(250, -5, 5))

ggplot(sim1, aes(x, y)) +
  geom_abline(
      data = models,
      aes(intercept = b0, slope = b1),
      alpha = 1/4) +
  geom_point()
```



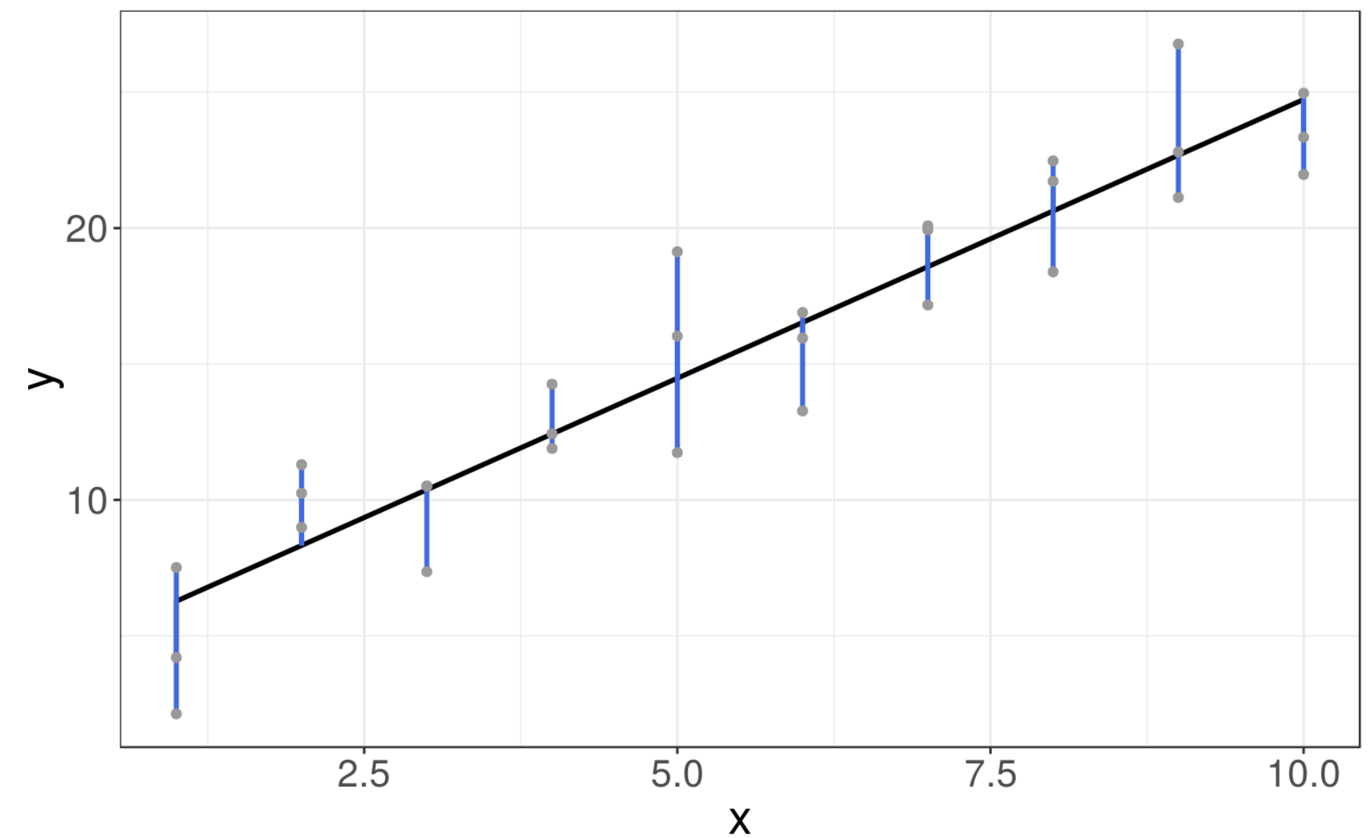
Fitting a model

From all the lines in the linear family of models, we need to find the best one, i.e. the one that is **the closest to the data**.

This means that we need to find parameters $\hat{a}_0$ and $\hat{a}_1$ that identify such a fitted line.

The closest to the data can be defined as the one with the minimum distance to the data points in the y direction (the minimum residuals):

$$
\begin{aligned}
\|\hat{e}\|_2^2 &= \|\vec{y} - \hat{y}\|_2^2 \\
&= \|\vec{y} - (\hat{\beta}_0 + \hat{\beta}_1 x)\|_2^2 \\
&= \sum_{i=1}^{n} (y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2
\end{aligned}
$$



Linear Regression

Linear Regression

- Regression is a supervised learning method, whose goal is inferring the relationship between input data, x, and a **continuous** response variable, y.
- Linear regression is a type of regression where **y is modeled as a linear function of x**.
- **Simple linear regression** predicts the output y from a single predictor x.

$$y = \beta_0 + \beta_1 x + \epsilon$$

- **Multiple linear regression** assumes y relies on many covariates:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p + \epsilon$$

$$= \beta^T x + \epsilon$$

- here ϵ denotes a random noise term with zero mean.

Objective function

Linear regression seeks a solution $\hat{y} = \hat{\beta} \cdot \vec{x}$ that **minimizes the difference between the true outcome y and the prediction $\hat{y}$**, in terms of the residual sum of squares (RSS).

$$\arg\min_{\hat{\beta}} \sum_i \left(y_i - \hat{\beta}^T x_i\right)^2$$

Simple Linear Regression

- Predict the mileage per gallon using the weight of the car.
- In R the linear models can be fit with a `lm()` function.

```r
# convert 'data.frame' to 'tibble':
mtcars <- tbl_df(mtcars)

# Separate the data into train and test:
set.seed(123)
n <- nrow(mtcars)
idx <- sample(1:n, size = floor(n/2))
mtcars_train <- mtcars[idx, ]
mtcars_test <- mtcars[-idx, ]

# Fit a simple linear model:
mtcars_fit <- lm(mpg ~ wt, mtcars_train)
# Extract the fitted model coefficients:
coef(mtcars_fit)
```

```
## (Intercept)          wt
##   36.469815   -5.406813
```

```r
# check the details on the fitted model:
summary(mtcars_fit)
```

```
##
## Call:
## lm(formula = mpg ~ wt, data = mtcars_train)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -3.5302 -1.9952  0.0179  1.3017  3.5194
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|
## (Intercept)   36.470      2.108  17.299 7.61e
## wt            -5.407      0.621  -8.707 5.04e
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0
##
## Residual standard error: 2.2 on 14 degrees of
## Multiple R-squared:  0.8441, Adjusted R-squar
## F-statistic: 75.81 on 1 and 14 DF,  p-value:
```

Fitted values

We can compute the fitted values $\hat{y}$, a.k.a. the predicted `mpg` values for existing observations using `modelr::add_predictions()` function.

```
mtcars_train <- mtcars_train %>% add_predictions(mtcars_fit)
mtcars_train
```

```
## # A tibble: 16 x 12
##      mpg   cyl  disp    hp  drat    wt  qsec    vs    am  gear  carb  pred
##    <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
##  1  19.2     6 168.    123  3.92  3.44  18.3     1     0     4     4 17.9
##  2  19.2     8 400     175  3.08  3.84  17.0     0     0     3     2 15.7
##  3  17.3     8 276.    180  3.07  3.73  17.6     0     0     3     3 16.3
##  4  27.3     4  79      66  4.08  1.94  18.9     1     1     4     1 26.0
##  5  26       4 120.     91  4.43  2.14  16.7     0     1     5     2 24.9
##  6  21       6 160     110  3.9   2.88  17.0     0     1     4     4 20.9
##  7  15.2     8 276.    180  3.07  3.78  18       0     0     3     3 16.0
##  8  15.2     8 304     150  3.15  3.44  17.3     0     0     3     2 17.9
##  9  15.8     8 351     264  4.22  3.17  14.5     0     1     5     4 19.3
## 10  17.8     6 168.    123  3.92  3.44  18.9     1     0     4     4 17.9
## 11  15.5     8 318     150  2.76  3.52  16.9     0     0     3     2 17.4
## 12  21.4     4 121     109  4.11  2.78  18.6     1     1     4     2 21.4
## 13  13.3     8 350     245  3.73  3.84  15.4     0     0     3     4 15.7
## 14  15       8 301     335  3.54  3.57  14.6     0     1     5     8 17.2
## 15  30.4     4  95.1   113  3.77  1.51  16.9     1     1     5     2 28.3
## 16  10.4     8 460     215  3     5.42  17.8     0     0     3     4  7.14
```

Predictions for new observations

To predict the `mpg` for **new observations**, e.g. cars not in the dataset, we first need to generate a data table with predictors `x`, in this case the car weights:

```
newcars <- tibble(wt = c(2, 2.1, 3.14, 4.1, 4.3))
newcars <- newcars %>% add_predictions(mtcars_fit)
newcars
```

```
## # A tibble: 5 x 2
##      wt  pred
##   <dbl> <dbl>
## 1  2     25.7
## 2  2.1   25.1
## 3  3.14  19.5
## 4  4.1   14.3
## 5  4.3   13.2
```

Predictions for the test set

Remember that we already set aside a test set check our model:

```
mtcars_test <- mtcars_test %>% add_predictions(mtcars_fit)
head(mtcars_test, 3)
```

```
## # A tibble: 3 x 12
##     mpg   cyl  disp    hp  drat    wt  qsec    vs    am  gear  carb  pred
##   <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1  21       6   160   110  3.9   2.62  16.5     0     1     4     4  22.3
## 2  22.8     4   108    93  3.85  2.32  18.6     1     1     4     1  23.9
## 3  21.4     6   258   110  3.08  3.22  19.4     1     0     3     1  19.1
```

Compute the root mean square error:

$$\mathrm{RMSE} = \frac{1}{\sqrt{n}}\|\vec{y} - \hat{\vec{y}}\| = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

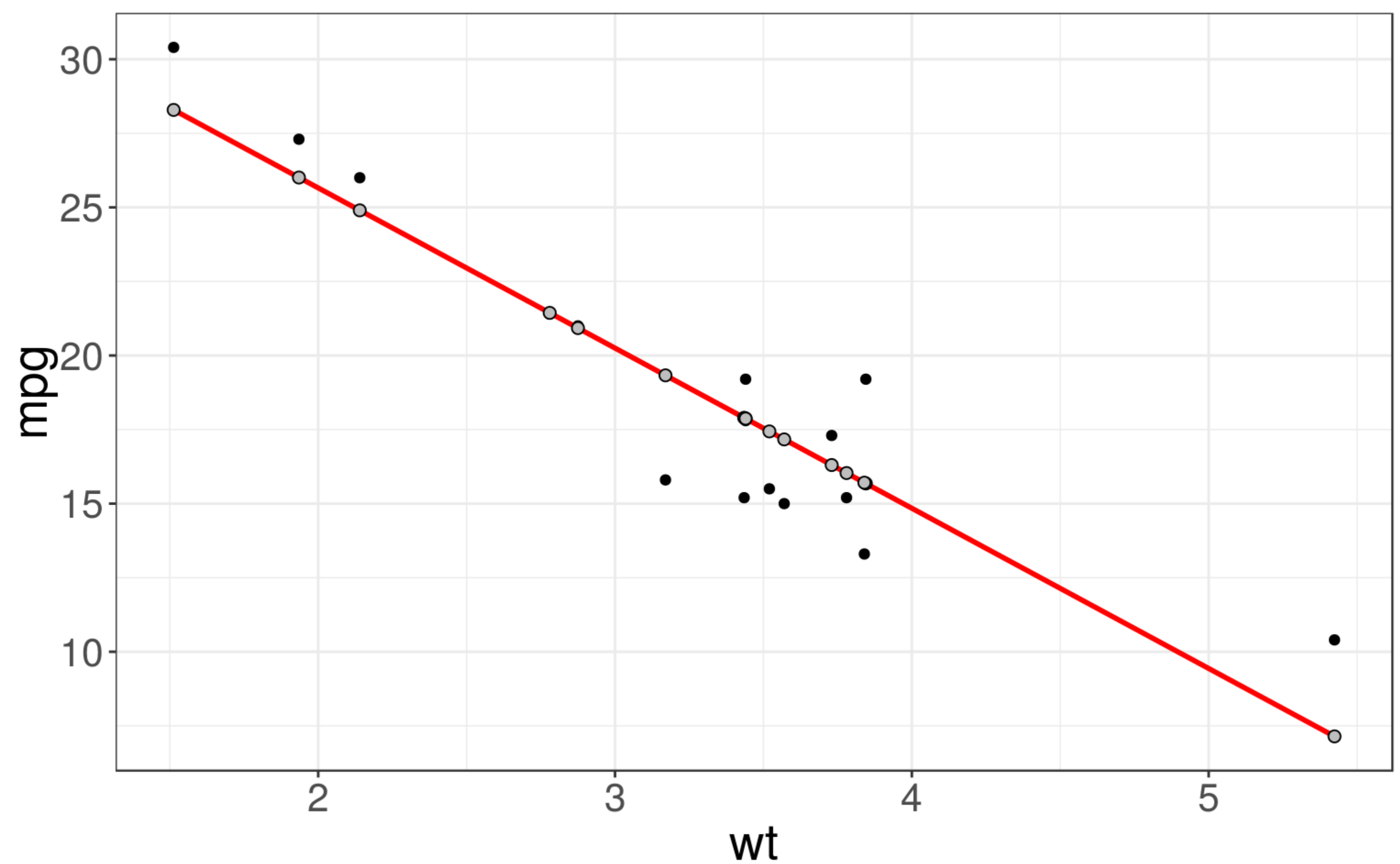
```
sqrt(mean(mtcars_test$mpg - mtcars_test$pred))
```

```
## [1] 1.425397
```

Visualizing the model

Now we can compare our predictions (grey) to the observed (black) values.

```
ggplot(mtcars_train, aes(wt)) + geom_point(aes(y = mpg)) +
    geom_line(aes(y = pred), color = "red", size = 1) +
    geom_point(aes(y = pred), fill = "grey", color = "black", shape = 21, size = 2)
```



Visualizing the residuals

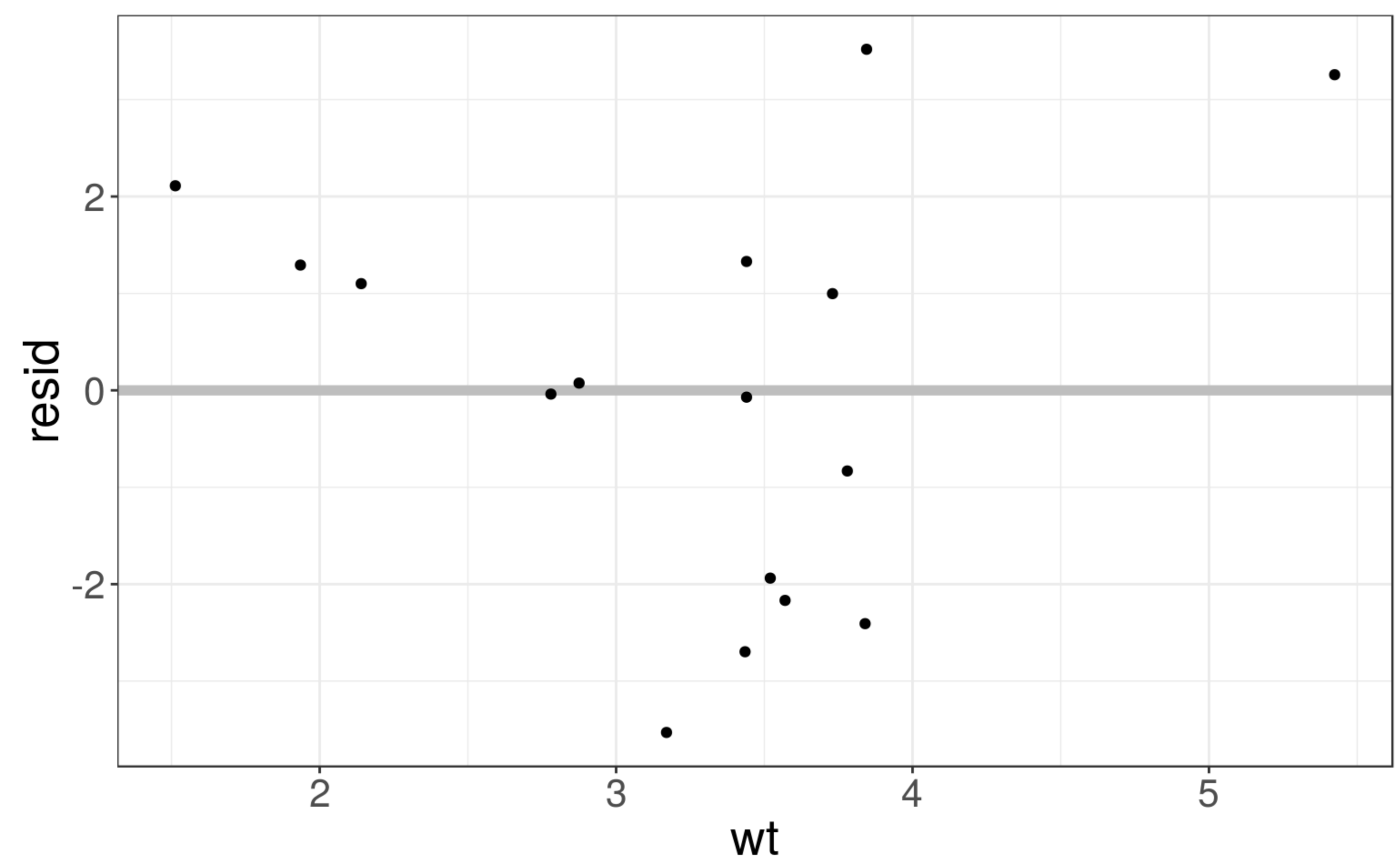
The residuals tell you what the model has missed. We can compute and add residuals to data with `add_residuals()` from `modelr` package:

Plotting residuals is a good practice – you want the residuals to look like random noise.

```
mtcars_train <- mtcars_train %>%
    add_residuals(mtcars_fit)
mtcars_train %>%
    select(mpg, mpg, resid, pred)
```

```
## # A tibble: 16 x 3
##      mpg   resid  pred
##    <dbl>   <dbl> <dbl>
##  1  19.2  1.33   17.9
##  2  19.2  3.52   15.7
##  3  17.3  0.998  16.3
##  4  27.3  1.29   26.0
##  5  26    1.10   24.9
##  6  21    0.0748 20.9
##  7  15.2 -0.832  16.0
##  8  15.2 -2.70   17.9
##  9  15.8 -3.53   19.3
## 10  17.8 -0.0704 17.9
## 11  15.5 -1.94   17.4
## 12  21.4 -0.0389 21.4
## 13  13.3 -2.41   15.7
## 14  15   -2.17   17.2
## 15  30.4  2.11   28.3
## 16  10.4  3.26    7.14
```

```
ggplot(mtcars_train, aes(wt, resid)) +
    geom_ref_line(h = 0, colour = "grey") +
    geom_point()
```



Formulae in R

You have seen that `lm()` takes in a formula relation `y ~ x` as an argument.

You can take a look at what R actually does, you can use the `model_matrix()`.

```
sim1
```

```
## # A tibble: 30 x 3
##        x     y  pred
##    <int> <dbl> <dbl>
##  1     1  4.20  6.27
##  2     1  7.51  6.27
##  3     1  2.13  6.27
##  4     2  8.99  8.32
##  5     2 10.2   8.32
##  6     2 11.3   8.32
##  7     3  7.36 10.4
##  8     3 10.5  10.4
##  9     3 10.5  10.4
## 10     4 12.4  12.4
## # ... with 20 more rows
```

```
model_matrix(sim1, y ~ x)
```

```
## # A tibble: 30 x 2
##    `(Intercept)`     x
##            <dbl> <dbl>
##  1             1     1
##  2             1     1
##  3             1     1
##  4             1     2
##  5             1     2
##  6             1     2
##  7             1     3
##  8             1     3
##  9             1     3
## 10             1     4
## # ... with 20 more rows
```

Formulae with categorical variables

- It doesn't make sense to parametrize the model with categorical variables, as we did before.
- `trans` variable is not a number, so R creates **an indicator column** that is 1 if "male", and 0 if "female".

```
(df <- tibble(
    sex = c("male", "female", "female",
            "female", "male", "male"),
     response = c(2, 5, 1, 3, 6, 8)
))
```

```
## # A tibble: 6 x 2
##   sex    response
##   <chr>     <dbl>
## 1 male          2
## 2 female        5
## 3 female        1
## 4 female        3
## 5 male          6
## 6 male          8
```

```
model_matrix(df, response ~ sex)
```

```
## # A tibble: 6 x 2
##   `(Intercept)` sexmale
##           <dbl>   <dbl>
## 1             1       1
## 2             1       0
## 3             1       0
## 4             1       0
## 5             1       1
## 6             1       1
```

- In general, it creates k−1 columns, where k is the number of categories.

```
(df <- tibble(
    rating = c("good", "bad", "average", "bad",
               "average", "good", "bad", "good"),
    score = c(2, 5, 1, 3, 6, 8, 10, 6)
))
```

```
## # A tibble: 8 x 2
##   rating  score
##   <chr>   <dbl>
## 1 good        2
## 2 bad         5
## 3 average     1
## 4 bad         3
## 5 average     6
## 6 good        8
## 7 bad        10
## 8 good        6
```

```
model_matrix(df, score ~ rating)
```

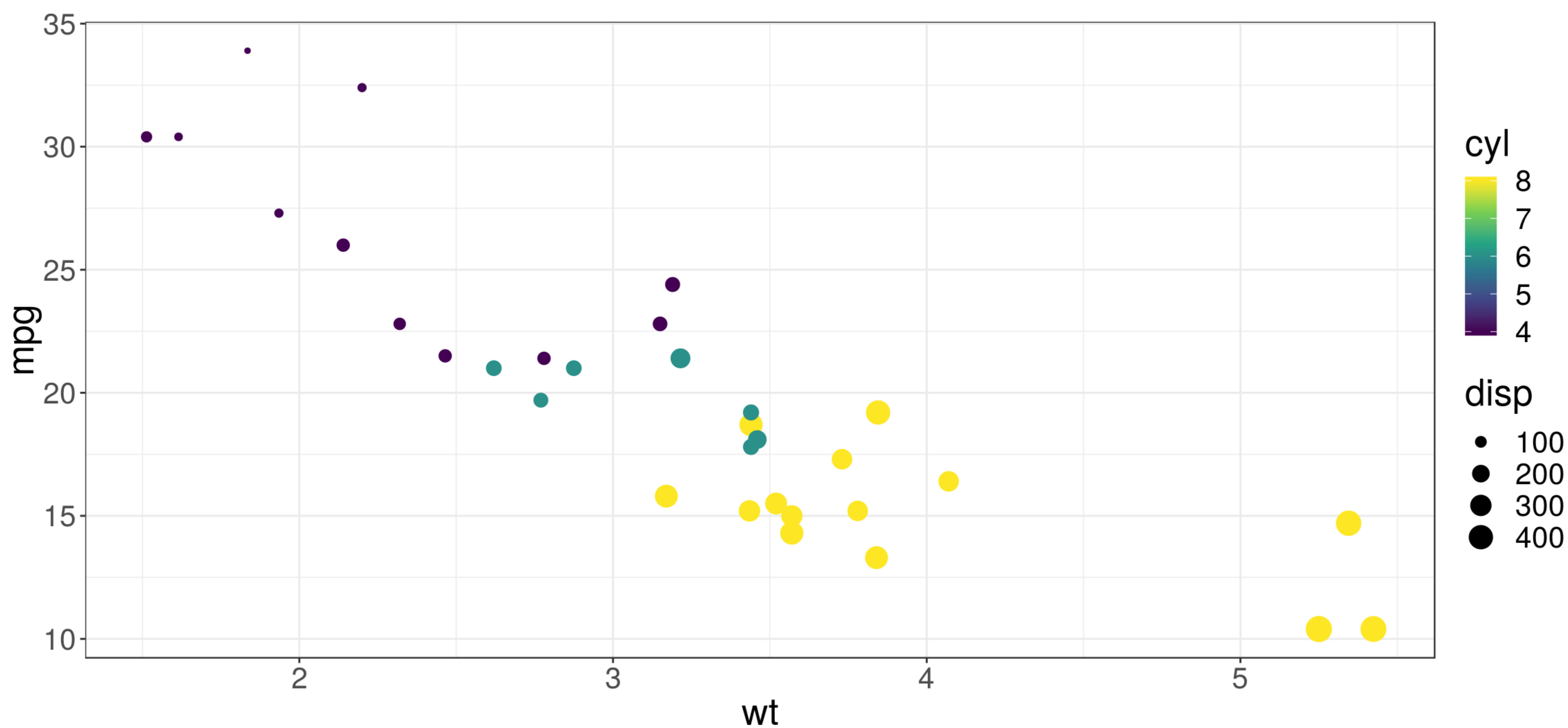
```
## # A tibble: 8 x 3
##   `(Intercept)` ratingbad ratinggood
##           <dbl>     <dbl>      <dbl>
## 1             1         0          1
## 2             1         1          0
## 3             1         0          0
## 4             1         1          0
## 5             1         0          0
## 6             1         0          1
## 7             1         1          0
## 8             1         0          1
```

But you don't need to worry about the parametrization to make predictions.

Multiple Linear Regression

Models often include **multiple predictors**, e.g. we might like to predict `mpg` using three variables: `wt`, `disp` and `cyl`.

```
ggplot(mtcars, aes(x=wt, y=mpg, col=cyl, size=disp)) +
    geom_point() +
    scale_color_viridis_c()
```



```r
mtcars_mult_fit <- lm(mpg ~ wt + disp + cyl, data = mtcars_train)

# Summarize the results
summary(mtcars_mult_fit)
```

```
##
## Call:
## lm(formula = mpg ~ wt + disp + cyl, data = mtcars_train)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.4016 -0.9539  0.0017  0.6243  3.4510
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 40.259994   2.692593  14.952 4.03e-09 ***
## wt          -3.986230   0.984659  -4.048  0.00162 **
## disp         0.009933   0.010756   0.924  0.37394
## cyl         -1.644638   0.629635  -2.612  0.02272 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.818 on 12 degrees of freedom
## Multiple R-squared:  0.9088, Adjusted R-squared:  0.886
## F-statistic: 39.88 on 3 and 12 DF,  p-value: 1.616e-06
```

To **predict `mpg` for new cars**, you must first create a data frame describing the attributes of the new cars, before computing predicted `mpg` values.

```
newcars <- expand.grid(
    wt = c(2.1, 3.6, 5.1),
    disp = c(150, 250),
    cyl = c(4, 6)
)
newcars
```

```
##      wt disp cyl
## 1   2.1  150   4
## 2   3.6  150   4
## 3   5.1  150   4
## 4   2.1  250   4
## 5   3.6  250   4
## 6   5.1  250   4
## 7   2.1  150   6
## 8   3.6  150   6
## 9   5.1  150   6
## 10  2.1  250   6
## 11  3.6  250   6
## 12  5.1  250   6
```

```
newcars <- newcars %>%
    add_predictions(mtcars_mult_fit)
newcars
```

```
##      wt disp cyl     pred
## 1   2.1  150   4 26.80031
## 2   3.6  150   4 20.82097
## 3   5.1  150   4 14.84162
## 4   2.1  250   4 27.79361
## 5   3.6  250   4 21.81427
## 6   5.1  250   4 15.83492
## 7   2.1  150   6 23.51104
## 8   3.6  150   6 17.53169
## 9   5.1  150   6 11.55235
## 10  2.1  250   6 24.50434
## 11  3.6  250   6 18.52499
## 12  5.1  250   6 12.54565
```

Predictions for the test set

```
mtcars_test_mult <- mtcars_test %>% add_predictions(mtcars_mult_fit)
head(mtcars_test_mult, 3)
```

```
## # A tibble: 3 x 12
##     mpg   cyl  disp    hp  drat    wt  qsec    vs    am  gear  carb  pred
##   <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1  21       6   160   110  3.9   2.62  16.5     0     1     4     4  21.5
## 2  22.8     4   108    93  3.85  2.32  18.6     1     1     4     1  25.5
## 3  21.4     6   258   110  3.08  3.22  19.4     1     0     3     1  20.1
```

Compute the root mean square error:

$$\text{RMSE} = \frac{1}{\sqrt{n}}\|\vec{y} - \hat{\vec{y}}\| = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

```
sqrt(mean(mtcars_test_mult$mpg - mtcars_test_mult$pred))
```

```
## [1] 1.039002
```

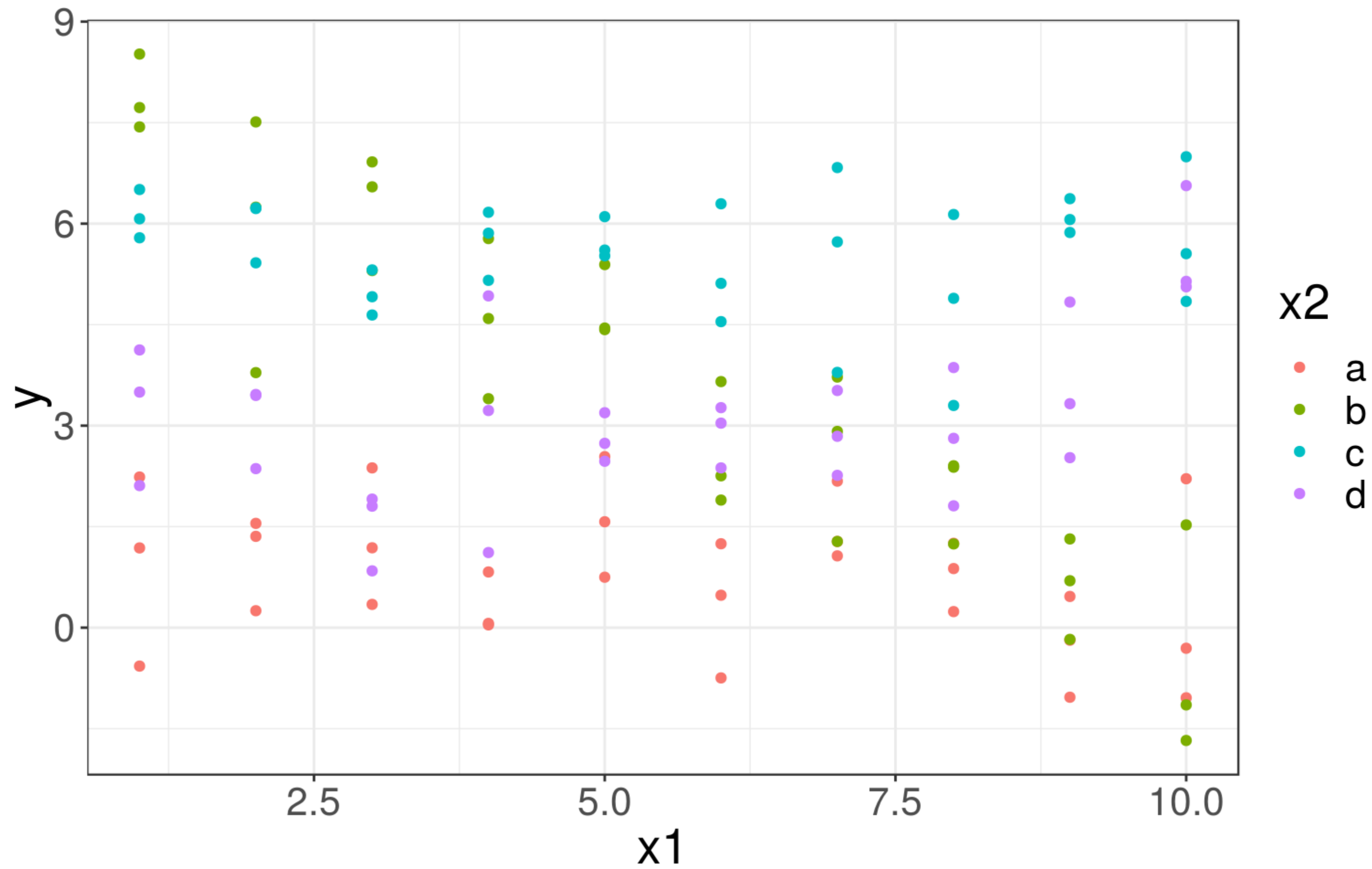
Interaction terms

- An interaction occurs when **an independent variable has a different effect on the outcome depending on the values of another independent**. variable.
- For example, one variable, x_1 might have a different effect on y within different categories or groups, given by variable x_2.
- If you are not familiar with the concept of the interaction terms, read this.

Formulas with interactions

In the `sim3` dataset, there is a categorical, `x2`, and a continuous, `x1`, predictor.

```
ggplot(sim3, aes(x=x1, y=y)) + geom_point(aes(color = x2))
```



Models with interactions

We could fit two different models, one without and one with (`mod2`) different slopes and intercepts for each line (for each `x2` category).

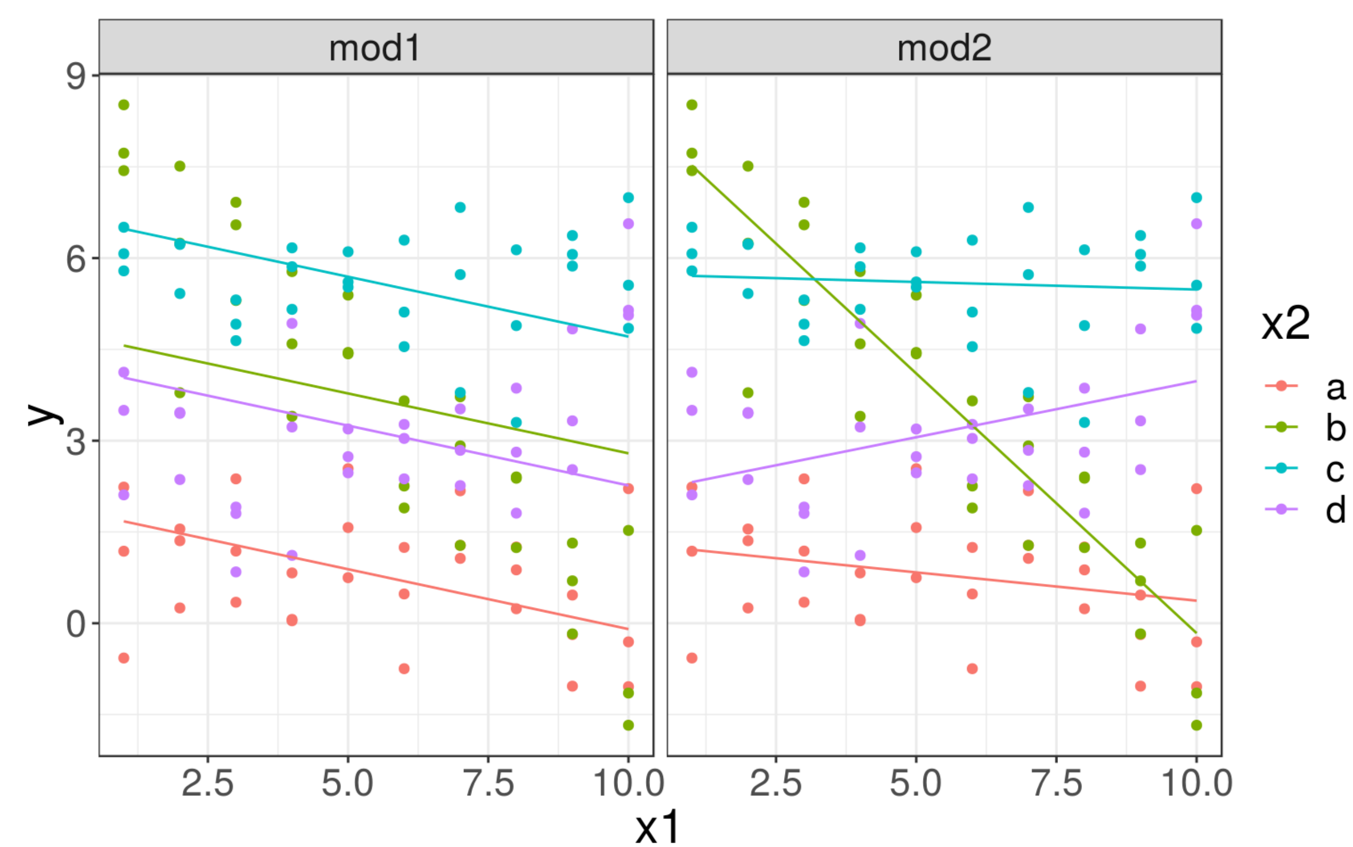
```
# Model without interactions:
mod1 <- lm(y ~ x1 + x2, data = sim3)
# Model with interactions:
mod2 <- lm(y ~ x1 * x2, data = sim3)
# Generate a data grid for two variables
# and compute predictions from both models
grid <- sim3 %>% data_grid(x1, x2) %>%
    gather_predictions(mod1, mod2)
head(grid, 3)
```

```
## # A tibble: 3 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
```

```
tail(grid, 3)
```

```
## # A tibble: 3 x 4
##   model    x1 x2      pred
##   <chr> <int> <fct>  <dbl>
## 1 mod2     10 b     -0.162
## 2 mod2     10 c      5.48
## 3 mod2     10 d      3.98
```

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



Now, we fit **interaction effects** for the `mtcars` dataset. Note the ‘`:`’-notation for the interaction term.

```
mfit_inter <- lm(mpg ~ am * wt, mtcars_train)
names(coefficients(mfit_inter))
```

```
## [1] "(Intercept)" "am"          "wt"          "am:wt"
```

```
summary(mfit_inter)
```

```
##
## Call:
## lm(formula = mpg ~ am * wt, data = mtcars_train)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.5603 -1.0064  0.0679  0.7265  3.3565
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  28.7955     3.7796   7.619 6.18e-06 ***
## am           13.7636     4.5621   3.017  0.01072 *
## wt           -3.3685     0.9759  -3.452  0.00479 **
## am:wt        -4.4730     1.3701  -3.265  0.00677 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.721 on 12 degrees of freedom
## Multiple R-squared:  0.9183, Adjusted R-squared:  0.8978
## F-statistic: 44.94 on 3 and 12 DF,  p-value: 8.43e-07
```

Exercise 1

- Go to the “Lec6_Exercises.Rmd” file, which can be downloaded from the class website under the Lecture tab.
- Complete Exercise 1.

Lasso Regression

Choosing a model

- Modern datasets often have “too” many variables, e.g. predict the risk of a disease from the single nucleotide polymorphisms (SNPs) data.
- **Issue:** $n \ll p$ i.e. no. of predictors is much larger than than the no. of observations.
- **Lasso regression** is especially useful for problems, where

> *the number of available covariates is extremely large, but only a handful of them are relevant for the prediction of the outcome.*

Lasso Regression

- Lasso regression is simply regression with L_1 penalty.
- That is, it solves the problem:

$$\hat{\beta} = \arg\min_{\beta} \sum_{i} \left(y^{(i)} - \beta^T x^{(i)}\right)^2 + \lambda \|\beta\|_1$$

- It turns out that the L_1 norm $\|\vec{\beta}\|_1 = \sum_i |\, beta_i \,|$ **promotes sparsity**, i.e. only a handful of $\hat{\beta}_i$ will actually be non-zero.
- The number of non-zero coefficients depends on the choice of the tuning parameter, λ. The higher the λ the fewer non-zero coefficients.

`glmnet`

- Lasso regression is implemented in an R package `glmnet`.
- An introductory tutorial to the package can be found here.

```
# install.packages("glmnet")
library(glmnet)
```

- We go back to `mtcars` datasets and use Lasso regression to predict the `mpg` using all variables.
- Lasso will pick a subset of predictors that best predict the `mpg`.
- This means that we technically allow for all variables to be included, but due to penalization, most of the fitted coefficients will be zero.

```
mtcars <- as.data.frame(mtcars)
class(mtcars)
```

```
## [1] "data.frame"
```

```
head(mtcars)
```

```
##                    mpg cyl disp  hp drat    wt  qsec vs am gear carb
## Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
## Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
## Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
## Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
## Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
## Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

Fitting a sparse model

```r
# Convert to 'glmnet' required input format:
y <- mtcars[, 1]  # response vector, 'mpg'
X <- mtcars[, -1] # all other variables treated as predictors
X <- data.matrix(X, "matrix") # converts to NUMERIC matrix

# Choose a training set
set.seed(123)
idx <- sample(1:nrow(mtcars), floor(0.7 * nrow(mtcars)))
X_train <- X[idx, ]; y_train <- y[idx]
X_test <- X[-idx, ]; y_test <- y[-idx]

# Fit a sparse model
fit <- glmnet(X_train, y_train)
names(fit)
```

```
##  [1] "a0"        "beta"      "df"        "dim"       "lambda"
##  [6] "dev.ratio" "nulldev"   "npasses"   "jerr"      "offset"
## [11] "call"      "nobs"
```

- `glmnet()` compute the Lasso regression for a sequence of different tuning parameters, λ.
- Each row of `print(fit)` corresponds to a particular λ in the sequence.
- column `Df` denotes the number of non-zero coefficients (degrees of freedom),
- `%Dev` is the percentage variance explained,
- `Lambda` is the value of the currently chosen tuning parameter.

```
print(fit)
```

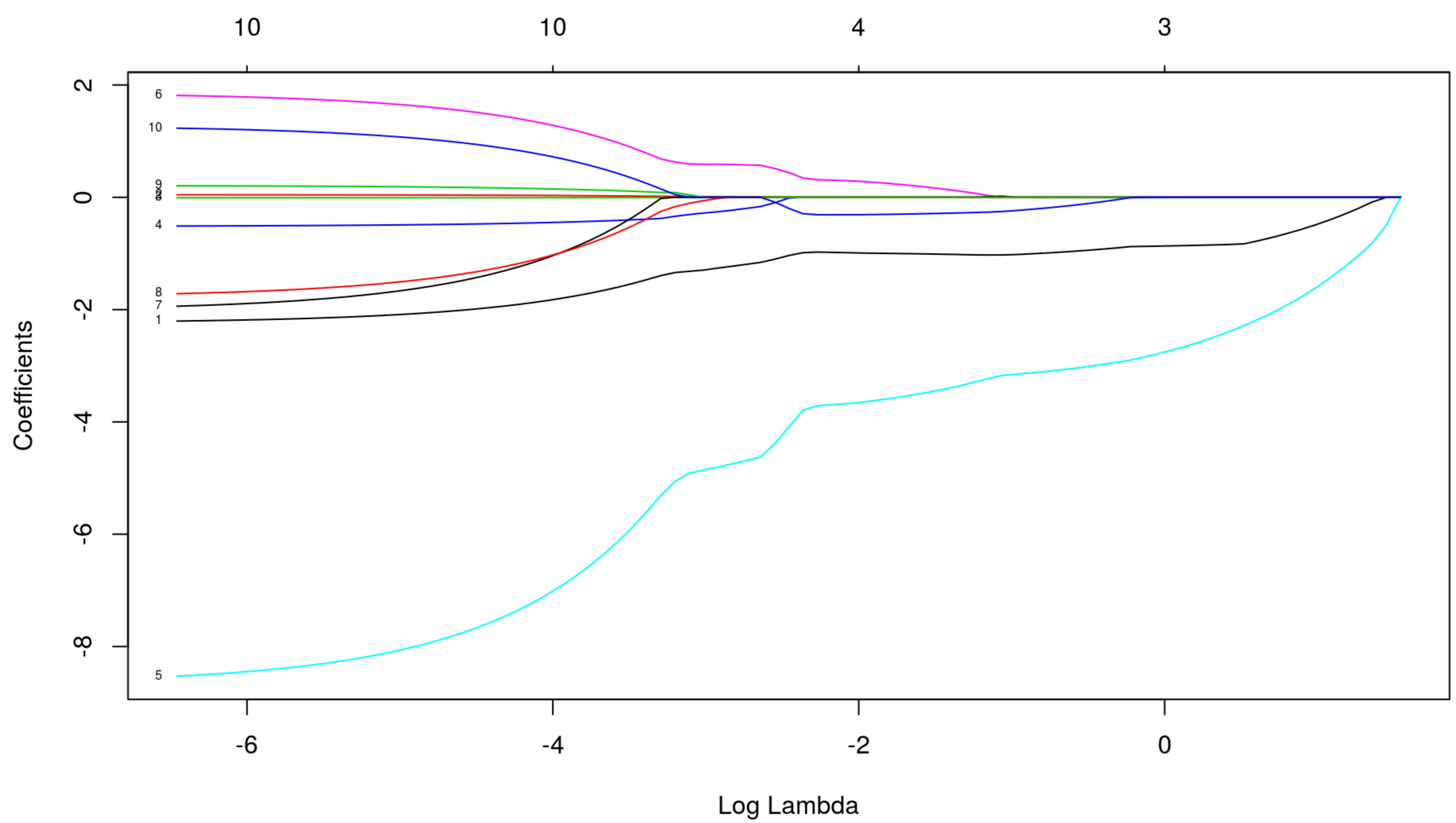
```
##
## Call:  glmnet(x = X_train, y = y_train)
##
##       Df   %Dev   Lambda
##   [1,]  0 0.0000 4.679000
##   [2,]  1 0.1383 4.264000
##   [3,]  2 0.2626 3.885000
##   [4,]  2 0.3700 3.540000
##   [5,]  2 0.4593 3.225000
##   [6,]  2 0.5333 2.939000
##   [7,]  2 0.5948 2.678000
##   [8,]  2 0.6459 2.440000
##   [9,]  2 0.6883 2.223000
##  [10,]  2 0.7235 2.026000
##  [11,]  2 0.7527 1.846000
##  [12,]  2 0.7770 1.682000
##  [13,]  3 0.7993 1.532000
##  [14,]  3 0.8179 1.396000
##  [15,]  3 0.8335 1.272000
##  [16,]  3 0.8463 1.159000
```

```
## [17,]  3 0.8570 1.056000

## [18,]  3 0.8659 0.962300
## [19,]  3 0.8733 0.876800
## [20,]  4 0.8797 0.798900
## [21,]  4 0.8862 0.727900
## [22,]  4 0.8915 0.663300
## [23,]  4 0.8960 0.604300
## [24,]  4 0.8997 0.550700
## [25,]  4 0.9028 0.501700
## [26,]  4 0.9054 0.457200
## [27,]  4 0.9075 0.416600
## [28,]  4 0.9093 0.379500
## [29,]  5 0.9108 0.345800
## [30,]  6 0.9124 0.315100
## [31,]  5 0.9139 0.287100
## [32,]  5 0.9152 0.261600
## [33,]  5 0.9162 0.238400
## [34,]  5 0.9171 0.217200
## [35,]  5 0.9178 0.197900
## [36,]  5 0.9184 0.180300
## [37,]  5 0.9189 0.164300
## [38,]  5 0.9193 0.149700
## [39,]  4 0.9197 0.136400
## [40,]  4 0.9199 0.124300
## [41,]  4 0.9201 0.113200
## [42,]  4 0.9203 0.103200
## [43,]  5 0.9215 0.094020
## [44,]  7 0.9263 0.085660
## [45,]  7 0.9313 0.078050
## [46,]  6 0.9350 0.071120
## [47,]  6 0.9361 0.064800
## [48,]  6 0.9371 0.059050
## [49,]  7 0.9379 0.053800
## [50,]  7 0.9387 0.049020
## [51,]  8 0.9396 0.044670
## [52,]  9 0.9414 0.040700
## [53,] 10 0.9443 0.037080
## [54,] 10 0.9473 0.033790
## [55,] 10 0.9499 0.030790
## [56,] 10 0.9520 0.028050
## [57,] 10 0.9538 0.025560
```

```
## [57,] 10 0.9538 0.025560
## [58,] 10 0.9553 0.023290
## [59,] 10 0.9565 0.021220
## [60,] 10 0.9575 0.019330
## [61,] 10 0.9584 0.017620
## [62,] 10 0.9591 0.016050
## [63,] 10 0.9597 0.014630
## [64,] 10 0.9602 0.013330
## [65,] 10 0.9606 0.012140
## [66,] 10 0.9609 0.011060
## [67,] 10 0.9612 0.010080
## [68,] 10 0.9614 0.009186
## [69,] 10 0.9616 0.008369
## [70,] 10 0.9618 0.007626
## [71,] 10 0.9619 0.006949
## [72,] 10 0.9620 0.006331
## [73,] 10 0.9621 0.005769
## [74,] 10 0.9622 0.005256
## [75,] 10 0.9623 0.004789
## [76,] 10 0.9623 0.004364
## [77,] 10 0.9624 0.003976
## [78,] 10 0.9624 0.003623
## [79,] 10 0.9625 0.003301
## [80,] 10 0.9625 0.003008
## [81,] 10 0.9625 0.002741
## [82,] 10 0.9625 0.002497
## [83,] 10 0.9626 0.002275
## [84,] 10 0.9626 0.002073
## [85,] 10 0.9626 0.001889
## [86,] 10 0.9626 0.001721
## [87,] 10 0.9626 0.001568
```

```r
# label = TRUE makes the plot annotate the curves with the corresponding coeffients labels.
plot(fit, label = TRUE, xvar = "lambda")
```



- the y-axis corresponds the value of the coefficients.
- the x-axis is denoted "Log Lambda" corresponds to the value of λ parameter penalizing the L1 norm of $\hat{\beta}$

- Each curve corresponds to a single variable, and shows the value of the coefficient as the tuning parameter varies.
- $\|\hat{\beta}\|_{L_1}$ increases and λ decreases from left to right.
- When λ is small (right) there are more non-zero coefficients.

The computed Lasso coefficient for a particular choice of λ can be printed using:

```r
# Lambda = 1
coef(fit, s = 1)
```

```
## 11 x 1 sparse Matrix of class "dgCMatrix"
##                        1
## (Intercept) 34.877093111
## cyl         -0.867649618
## disp         .
## hp          -0.005778702
## drat         .
## wt          -2.757808266
## qsec         .
## vs           .
## am           .
## gear         .
## carb         .
```

- Like for `lm()`, we can use a function `predict()` to predict the `mpg` for the training or the test data.
- However, we need specify the value of λ using the argument `s`.

```r
# Predict for the test set:
predict(fit, newx = X_test, s = c(0.5, 1.5, 2))
```

```
##                            1        2        3
## Datsun 710          25.36098 23.87240 23.22262
## Valiant             19.82245 19.42427 19.41920
## Duster 360          16.19324 17.27111 17.74858
## Merc 230            22.62471 21.86937 21.50396
## Merc 450SE          15.20595 16.16123 16.71324
## Cadillac Fleetwood 11.25687 13.28117 14.26985
## Chrysler Imperial  10.81730 13.01570 14.07314
## Fiat 128            25.88928 24.20103 23.47110
## Toyota Corolla      27.01880 25.08206 24.22690
## Toyota Corona       24.89106 23.51713 22.92237
```

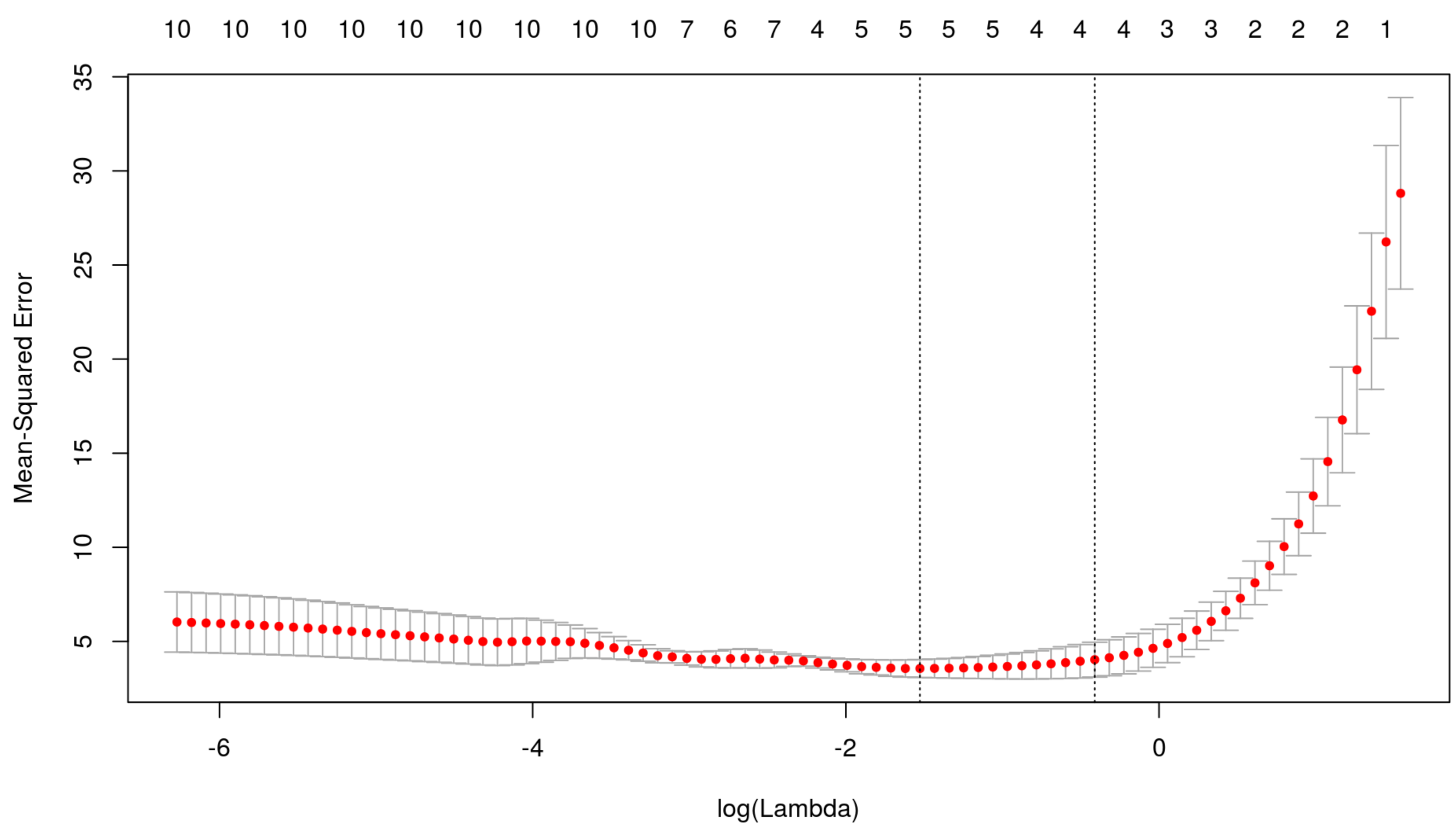
Each of the columns corresponds to a choice of λ.

Choosing λ

- To choose λ can use cross-validation.
- Use `cv.glmnet()` function to perform a k-fold cross validation.

> *In k-fold cross-validation, the original sample is randomly partitioned into k equal sized subsamples. Of the k subsamples, a single subsample is retained as the validation data for testing the model, and the remaining $k - 1$ subsamples are used as training data.* [1]

```r
set.seed(1)
# `nfolds` argument sets the number of folds (k).
cvfit <- cv.glmnet(X_train, y_train, nfolds = 5)
plot(cvfit)
```



- The red dots are the average MSE over the k-folds.
- The two chosen λ values are the one with MSE_{min} and one with $MSE_{min} + sd_{min}$

λ with minimum mean squared error, MSE:

```
cvfit$lambda.min
```

```
## [1] 0.2171905
```

The "best" λ in a practical sense is usually chosen to be the biggest λ whose MSE is within one standard error of the minimum MSE.

```
cvfit$lambda.1se
```

```
## [1] 0.6632685
```

Predictions using the "best" λ:

```
final_pred <- predict(cvfit, newx=X_test, s="lambda.1se")
final_pred
```

```
##                            1
## Datsun 710          25.01062
## Valiant             19.68422
## Duster 360          16.32664
## Merc 230            22.44375
## Merc 450SE          15.35370
## Cadillac Fleetwood 11.58909
## Chrysler Imperial  11.13782
## Fiat 128            25.54984
## Toyota Corolla      26.64431
## Toyota Corona       24.55160
```

More on models

Building Models

Building models is an important part of EDA.

It takes practice to gain an intuition for which patterns to look for and what predictors to select that are likely to have an important effect.

You should go over examples in http://r4ds.had.co.nz/model-building.html to see concrete examples of how a model is built for `diamonds` and `nycflights2013` datasets we have seen before.

Other model families

This chapter has focused exclusively on the class of linear models

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p + \epsilon = \vec{\beta}\vec{x} + \epsilon$$

and penalized linear models.

There are a large set of other model classes.

Extensions of linear models:

- Generalized linear models, `stats::glm()`, binary or count data.
- Generalized additive models, `mgcv::gam()`, extend generalized linear models to incorporate arbitrary smooth functions.
- Robust linear models, `MASS:rlm()`, less sensitive to outliers.

Completely different models:

- Trees, `rpart::rpart()`, fit a piece-wise constant model splitting the data into progressively smaller and smaller pieces.
- Random forests, `randomForest::randomForest()`, aggregate many different trees.
- Gradient boosting machines, `xgboost::xgboost()`, aggregate trees.

Useful Books

- “An introduction to Statistical Learning” [ISL] by James, Witten, Hastie and Tibshirani
- “Elements of statistical learning” [ESL] by Hastie, Tibshirani and Friedman
- “Introduction to Linear Regression Analysis” by Montgomery, Peck, Vinning

1. https://en.wikipedia.org/wiki/Cross-validation_(statistics)#k-fold_cross-validation↩