Model fitting

Katie Schuler

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> ⚠ Under Construction

0.1 You are here

0.2 Model building

0.3 Linear model review

- how would we specify this model
- how would we write it in R
- estimate the free paramters

0.4 Estimate free parameters

```r
# with base R
lm(y ~ 1 + x, data = data)
```

```

Call:
lm(formula = y ~ 1 + x, data = data)

Coefficients:
(Intercept)            x
        0.6          0.7
```

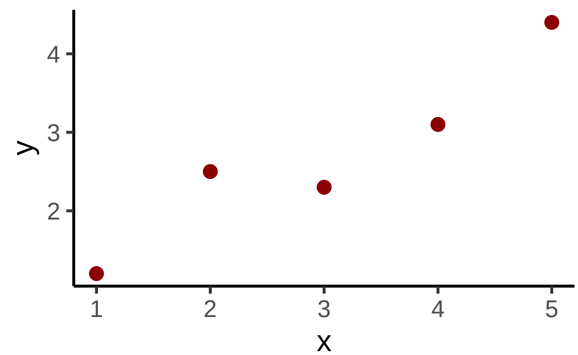
```
# with infer workflow
data %>%
    specify(y ~ 1 + x) %>%
    fit()
```

```
# A tibble: 2 x 2
  term      estimate
  <chr>        <dbl>
1 intercept    0.600
2 x            0.7
```

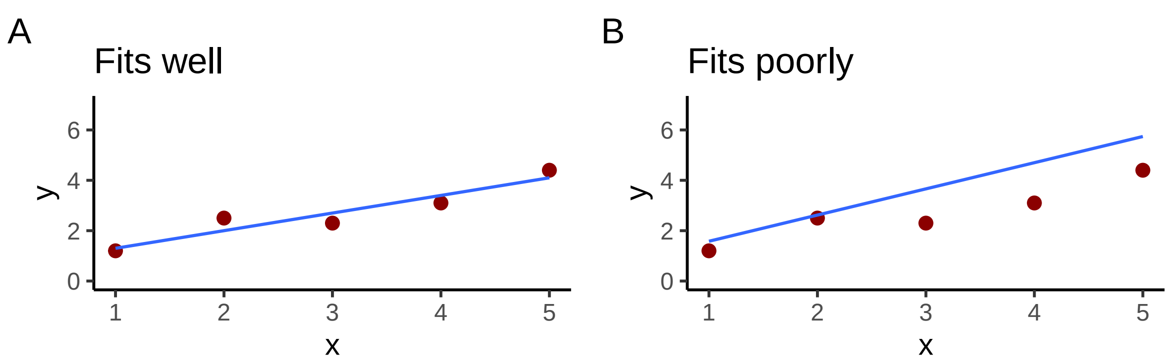
0.5 Model fitting basics

Linear model

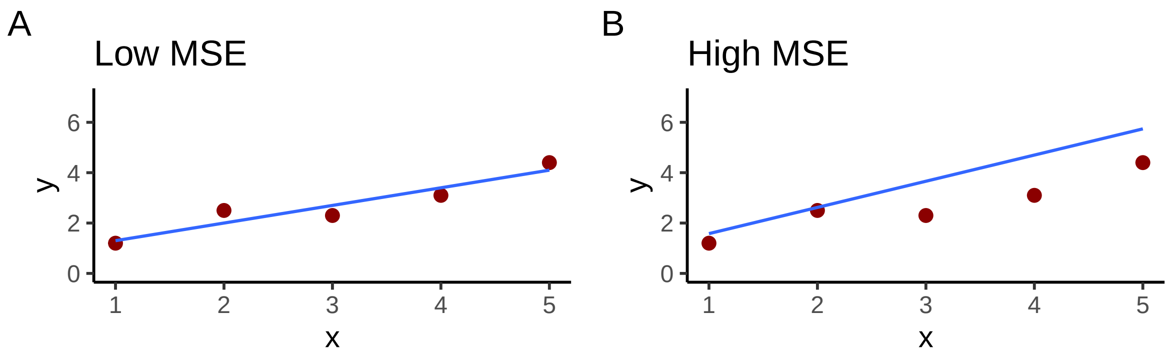
```
# A tibble: 5 x 2
      x     y
  <dbl> <dbl>
1     1   1.2
2     2   2.5
3     3   2.3
4     4   3.1
5     5   4.4
```



We can see which fits better with our eyes.




```
mean(mseA$sq_err)
```



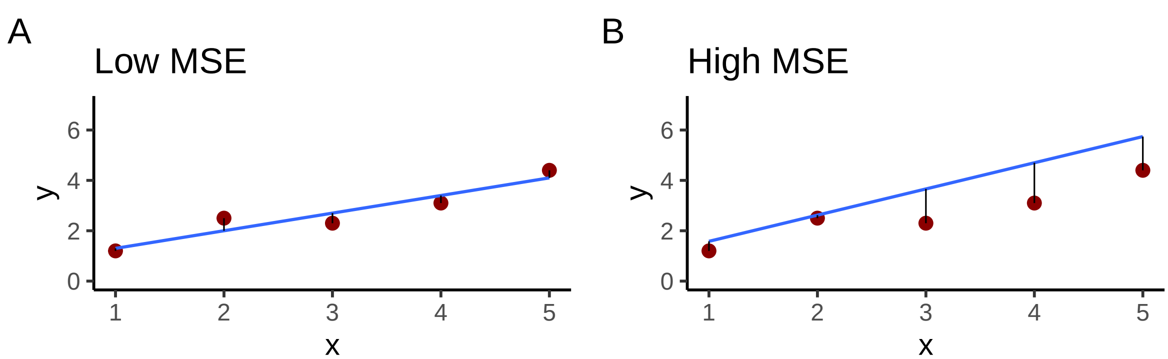
x	y	pred	err	sq_err
1	1.2	1.3	-0.1	0.01
2	2.5	2.0	0.5	0.25
3	2.3	2.7	-0.4	0.16
4	3.1	3.4	-0.3	0.09
5	4.4	4.1	0.3	0.09

x	y	pred	err	sq_err
1	1.2	1.58	-0.38	0.1444
2	2.5	2.62	-0.12	0.0144
3	2.3	3.66	-1.36	1.8496
4	3.1	4.70	-1.60	2.5600
5	4.4	5.74	-1.34	1.7956

```
[1] 0.12
```

```
mean(mseB$sq_err)
```

```
[1] 1.2728
```




```
lm(y ~ 1 + x, data = data)
```

```
Call:
```

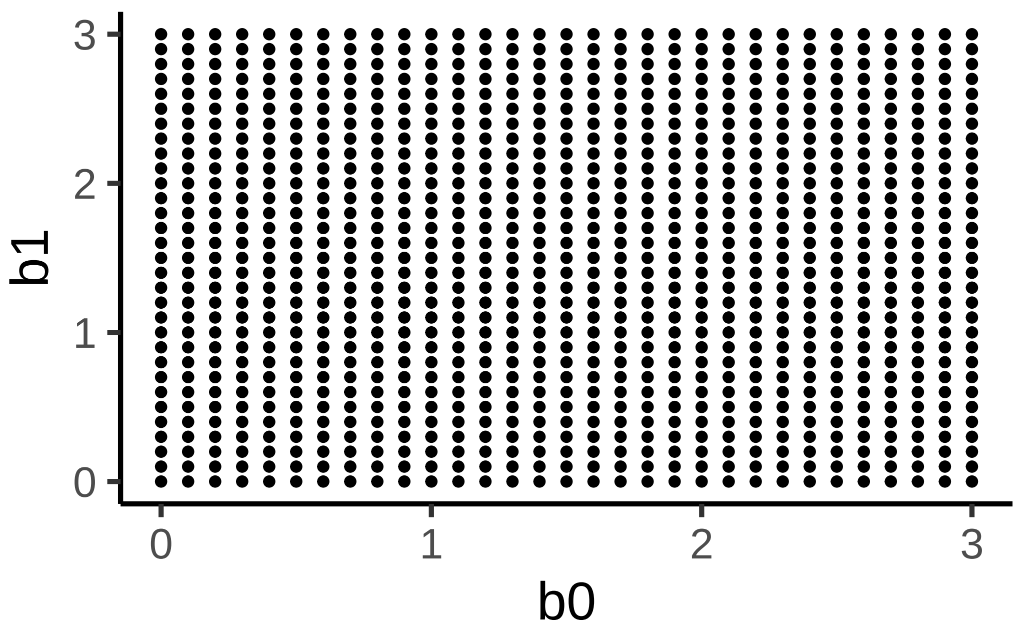
```
lm(formula = y ~ 1 + x, data = data)

Coefficients:
(Intercept)            x
        0.6          0.7
```

```
data %>%
    specify(y ~ 1 + x) %>%
    fit()
```

```
# A tibble: 2 x 2
  term      estimate
  <chr>        <dbl>
1 intercept    0.600
2 x            0.7
```

```
b0 <- seq(from = 0, to = 3, by = 0.1)
b1 <- seq(from = 0, to = 3, by = 0.1)
possible_weights <- expand.grid(b0 = b0, b1 = b1)
```

```
ggplot(data = possible_weights,
    mapping = aes(x = b0, y = b1)) +
    geom_point()
```



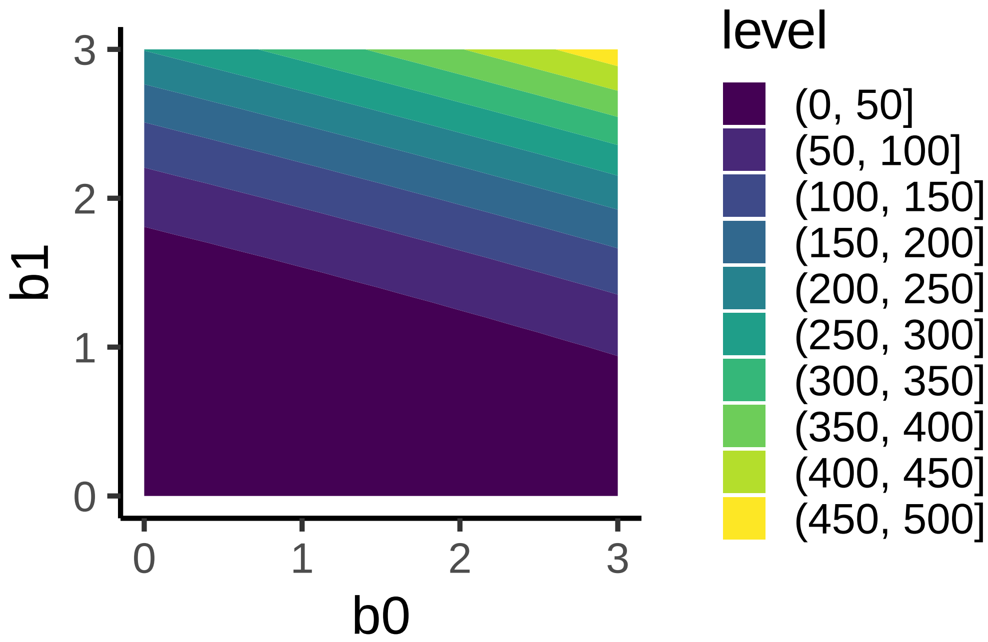
```
# compute the sum of squares for those weights on a dataframe
sum_squares <- function(b0, b1) {

    data %>%
        mutate(pred = b0 + b1*x) %>%
        mutate(err = pred-y) %>%
        mutate(sq_err = err^2) %>%
        select(sq_err) %>%
        sum()

}
error_surf <- possible_weights %>%
    rowwise() %>%
    mutate(sum_sq =  sum_squares(b0, b1)) %>%
    ungroup

error_surf
```

```
# A tibble: 961 x 3
      b0    b1 sum_sq
   <dbl> <dbl>  <dbl>
 1   0       0   42.0
 2   0.1     0   39.3
 3   0.2     0   36.8
 4   0.3     0   34.3
 5   0.4     0   32.0
 6   0.5     0   29.7
 7   0.6     0   27.6
 8   0.7     0   25.5
 9   0.8     0   23.6
10   0.9     0   21.7
# i 951 more rows
```

```
error_surf  %>% filter(sum_sq < 0.608)
```

```
# A tibble: 1 x 3
     b0    b1 sum_sq
  <dbl> <dbl>  <dbl>
1   0.6   0.7  0.600
```

```
ggplot(error_surf, aes(b0, b1, z = sum_sq)) +
    geom_contour_filled()
```




```
        # %>%
        # sum(.$sq_err)
      # summarise(sum_sq = sum(sq_err)) %>%


# return sum of squares as a column next to

# mse <- function(data, b0, b1) {
#   model_value <- b0 + b1*data[1]
#   resid <- data[2] - model_value
#   sq_err <- resid^2
#   sum(sq_err)
# }

# possible_weights %>% mutate(
#     mse = mse(1, 1, b0, b1)
# )
```

- in context of model building more broadly
- a genear overview of the concept

0.6 Mean squared error

Cost function.

0.7 Error surface

- We can visualize the error surface for simple example: 2 parameters, β_0 and β_1, and the cost function (mean square error).
- Show nonlinear model v linear model figs
- goal is to find the minimum point
- notice the nonlinear model can have local minimums but lm has only 1. Because lm is a **convex** function.

0.8 Gradient descent

IF we want to estimate the free parameters in a way that would work broadly, for linear or nonlinear models, we can use **gradient descent**.

- machine learning / optimization.
- If we have a lot of data, we could use **stochastic gradient descent** which is the same except we…

0.9 Ordinary least squares

As we saw above, linear models have the special property that they have a solution, the OLS. Rather than searching the error surface iteratively via gradient descent (optimization), we can solve for this point directly with **linear algebra**.

- matrix approach: we write the 3-step function.
- use lm() in R.
- infer approach:
  - specify(), fit()

0.9.1 Further reading

- Ch. 8 Fitting models to data in Statistical Modeling