Using splines in regression

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Today's Lecture

- Assessing model accuracy
- Overfitting
- Fitting smooth curves to data

More info:

- For more gory details: *Intro to Statistical Learning* Chapter 7

Assessing model accuracy: Regression setting

- The mean squared error (MSE) is the most commonly used measure of the performance of a statistical learning method in the regression setting:

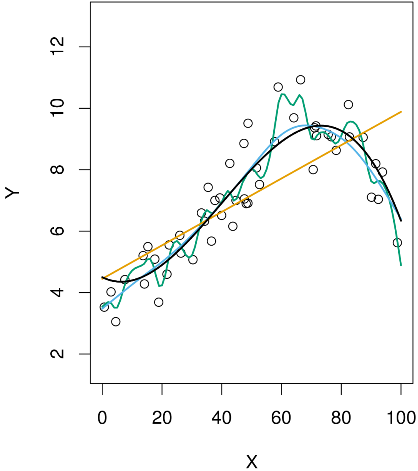
$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

- The MSE will be small if the observed and predicted responses are close to one another, and it will be large if these differ substantially, in at least some instances.

Low MSE is not always a good thing!

Each of the lines represented a model fit to the data to make good predictions of the mean of y, given some x values.

- Which color line/model do you think has the lowest MSE?
- Which color line/model would you trust the most to predict a new observation?



How to find the "sweet spot"?

- Ideally, your model should predict observations well in your dataset ("in-sample") and in a new dataset ("out-of-sample").
- While this is not often possible in practice, ideally the new dataset should be completely separately collected from the initial dataset.
- Example 1: a study done by investigators at Institution A shows that in a sample of 100 cancer patients, a specific set of commonly collected biomarkers accurately classified cancer patients based on severity of outcome at 1 year follow-up. What would be a good replication study?

Often, an ‘internal‘ test sample is used

- In general, we are interested in the accuracy of the predictions that we obtain when we apply our method to previously unseen data $\rightarrow$ called the test sample.
- Often, obtaining an external validation or testing dataset is infeasible or expensive.
- In these cases, investigators may set aside a portion of the observations from the original dataset as a test sample.
- Test samples can be particularly useful in diagnosing whether your model was “overfit“ to the particular features of the training dataset.

Hands-on example: FEV dataset

The FEV dataset describes a sample of 654 youths, aged 3 to 19, in the area of East Boston during middle to late 1970's. Data includes the following variables (among others)

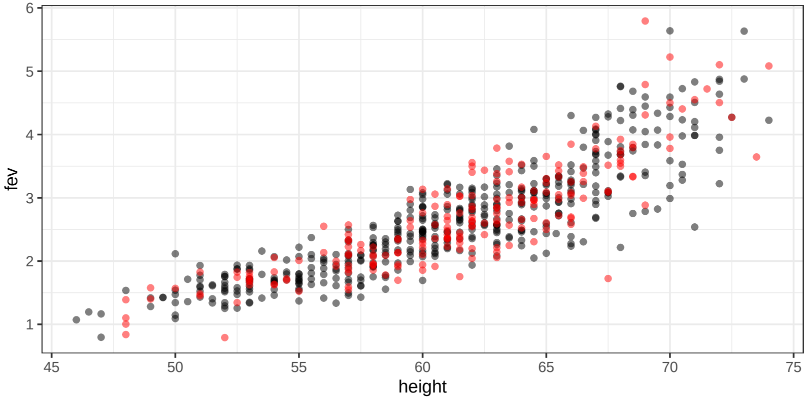
- fev - forced expiratory volume, a measure of lung capacity and strength (in liters)
- height (in inches)

```
library("Hmisc")
getHdata(FEV)
head(FEV)

##     id age   fev height    sex               smoke
## 1  301   9 1.708   57.0 female non-current smoker
## 2  451   8 1.724   67.5 female non-current smoker
## 3  501   7 1.720   54.5 female non-current smoker
## 4  642   9 1.558   53.0   male non-current smoker
## 5  901   9 1.895   57.0   male non-current smoker
## 6 1701   8 2.336   61.0 female non-current smoker
```

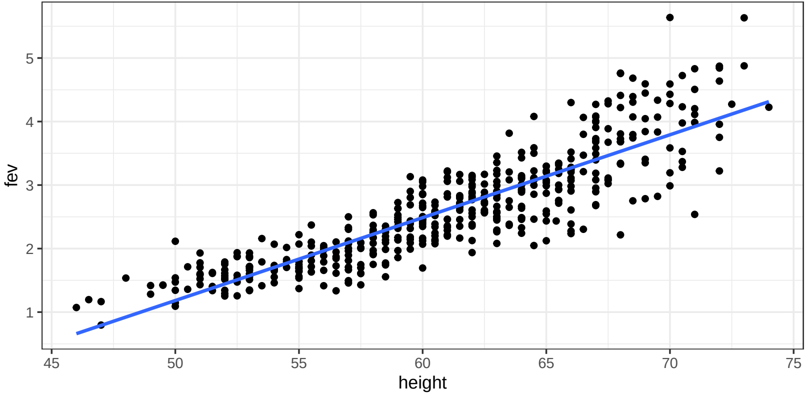
Creating an FEV training/testing split

```
set.seed(756)  ## so we all get the same result
idx_test <- sample(1:nrow(FEV), size=200) ## 200 test observations
fev_train <- FEV[-idx_test,]     ## removing all test observations
fev_test <- FEV[idx_test,]       ## leaving all test observations
ggplot(mapping = aes(x=height, y=fev)) +
  geom_point(data=fev_train, alpha=0.5) +
  geom_point(data=fev_test, color="red", alpha=0.5)
```



Plotting the FEV training sample

```
ggplot(fev_train, aes(height, fev)) + geom_point() +
  geom_smooth(method="lm", se=FALSE)
```



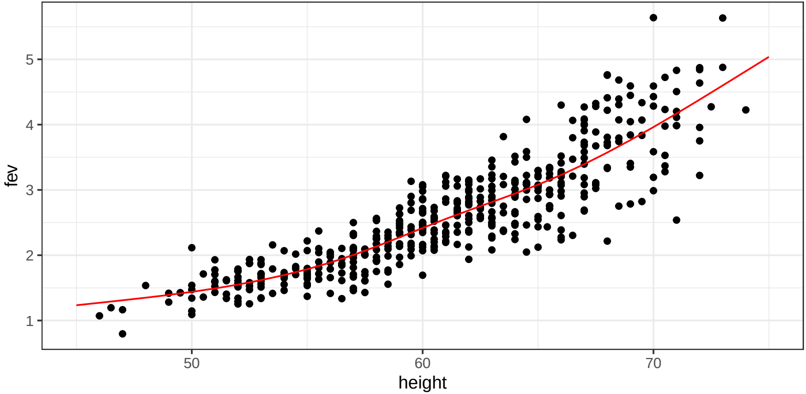
Using a smooth model for *fev* $\sim$ *height*

Let's fit a model to the data that can capture some of what appears to be a non-linear relationship between height and fev. The `ns()` function in the splines package uses a "natural spline" to model a flexible, non-linear relationship bewteen a covariate and an outcome by splicing together polynomial functions. The larger the "degrees of freedom" (`df`) parameter is, the more functions it pieces together and therefore the more wiggly the fitted model becomes.

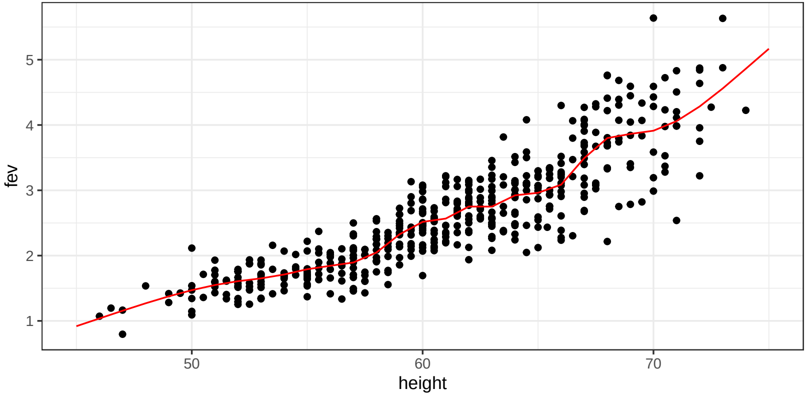
```
library(splines)
spline_mdl <- lm(fev ~ ns(height, df = 4), data=fev_train)
```

Visualizing the smooth model

```
spline_x_vals <- seq(45, 75, by=1)
spline_y_vals <- predict(spline_mdl,
  newdata = data.frame(height=spline_x_vals))
ggplot() +
  geom_point(aes(x=height, y=fev), data=fev_train) +
  geom_line(aes(x = spline_x_vals, y=spline_y_vals), color="red")
```



What is the right level of smoothness?



Find the Goldilocks zone!

That model looks good, but how to we know what degree of smoothness is just the right amount? We can compare MSE between our training and our test set for different levels of smoothness.

```
fev_train$spline_preds <- predict(spline_mdl)
fev_test$spline_preds <- predict(spline_mdl, newdata = fev_test)
( mse_train <- mean((fev_train$fev - fev_train$spline_preds)^2) )

## [1] 0.1549225

( mse_test <- mean((fev_test$fev - fev_test$spline_preds)^2) )

## [1] 0.1905708
```

With your group

- In your breakout rooms, pick a set of `df` to test as a group. Work together to make sure that at least one `df` is run on everyone's computer.
- Compile a dataset on the note-catcher with the `df` value and the associated MSEs for both the training and testing samples.
- Discuss your results as a table and decide on an optimal `df` to choose.

Using a test sample avoids "overfitting"

- A good rule of thumb of a good model is that it will generalize to another setting.
- Therefore, a good model is one that **minimizes the test sample MSE.**
- The mean squared error will always get lower with the training sample as we add more features to our model.
- Overfitting refers to the situation in which a less complex or "wiggly" model would result in a smaller test sample MSE.

MSE: learning versus test sample

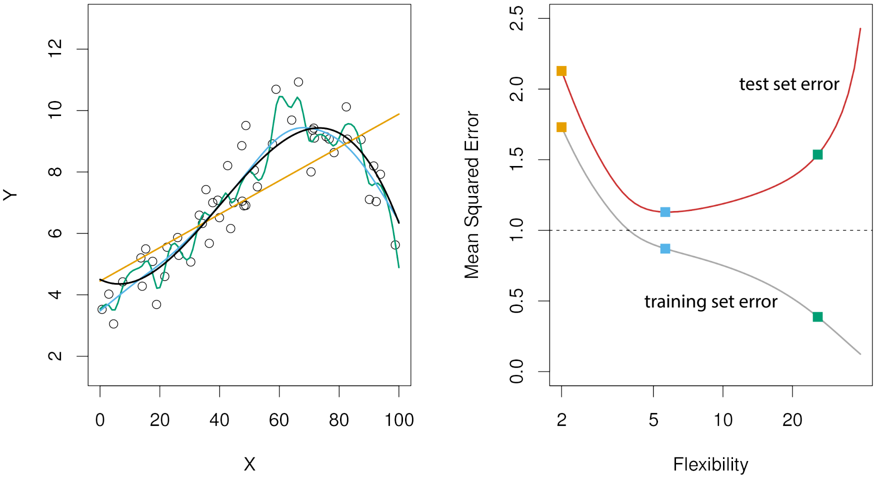


Figure 2.9 from ISL. Black line is the true relationship from which data are simulated

MSE: learning versus test sample

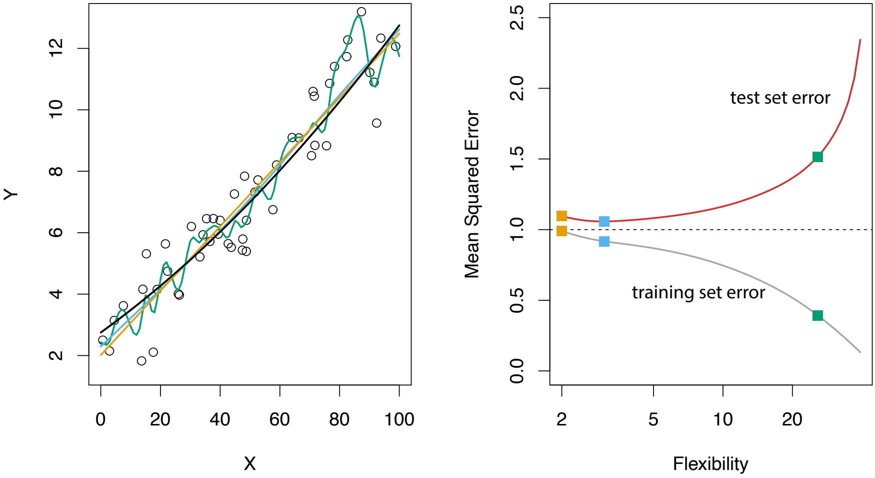


Figure 2.10 from ISL.

Summary

Validating potential models on external data is critical to understanding how well your model will generalize to another dataset.