# Linear Regression

Max Turgeon

DATA 2010—Tools and Techniques in Data Science

# Lecture Objectives

- Build a model using linear regression
- Explain how parameters can be estimated
- Explore the flexibility of linear regression

# Motivation

- Over the last few lectures we discussed:
    - What are scores and how they can be used for ranking.
    - How to build models and validate them.
- For the rest of the semester, we will look at different methodologies for building models.
    - And we start with **linear regression**.

# Disclaimer

- You’ve probably seen linear regression in other courses.
    - E.g. STAT 1150 and 2150
- In statistics, linear regression is typically presented as a way to study correlation and/or differences in means.
    - I.e. it is used for inference
- In this course, we will focus on linear regression as a *prediction model*.
    - Therefore, we won’t focus on statistical assumptions or model fit.

# General notation

- Linear regression estimates the relationship between a single variable $Y$, called the *outcome variable*, and a series of variables $X_1, \ldots, X_p$, called *covariates*.
    - Machine learning uses the terms “target” and “features”, respectively.
- The outcome $Y$ is typically a continuous variable.
    - Eg. Height, income, blood pressure, etc.
- The covariates $X_1, \ldots, X_p$ can be anything.
- We want to collect all variables $Y, X_1, \ldots, X_p$ on the same unit of observation (e.g. person, school, animal, olive oil).

# Multiple Linear Regression i

- The linear regression equation is

$$E(Y \mid X_1, \ldots, X_p) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p.$$

- Some authors also write the following equation:

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \epsilon.$$

- Here, $\epsilon$ is a random variable with mean 0 and variance $\sigma^2$.
    - You can use either equation; I prefer the first one.

# Multiple Linear Regression ii

- In matrix notation, we have

$$E(Y \mid \mathbf{X}) = \beta^T \mathbf{X},$$

where

$$\beta = (\beta_0, \beta_1, \dots, \beta_p),$$
$$\mathbf{X} = (1, X_1, \dots, X_p).$$

# Least-Squares Estimation

- Let $Y_1, \ldots, Y_n$ be a random sample of size $n$, and let $\mathbf{X}_1, \ldots, \mathbf{X}_n$ be the corresponding sample of covariates.
- We will write $\mathbb{Y}$ for the vector whose $i$-th element is $Y_i$, and $\mathbb{X}$ for the matrix whose $i$-th row is $\mathbf{X}_i$.
- The Least-Squares estimate $\hat{\beta}$ is given by

$$\hat{\beta} = (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T \mathbb{Y}.$$

# Fitted values and residuals i

- After we have estimated the regression coefficients $\beta_0, \beta_1, \ldots, \beta_p$, we can compute **fitted values** and **residuals**.
- We will use the hat notation to indicate that a parameter has been estimated:
  - $\beta_0$ is the (population) parameter.
  - $\hat{\beta}_0$ is the estimate from linear regression.
- Now assume we have our estimates $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$. For a given observation in our dataset, we also have a set of covariate values $X_{i1}, \ldots, X_{ip}$.

# Fitted values and residuals ii

- We get the $i$-th **fitted value** by plugging all these values in the regression equation:

$$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_{i1} + \cdots + \hat{\beta}_p X_{ip}.$$

  - In matrix notation:

$$\widehat{\mathbb{Y}} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}\mathbb{X}.$$

- We get the $i$-th **residual** by taking the difference between the observed value $Y_i$ and the fitted value $\hat{Y}_i$:

$$\hat{e}_i = Y_i - \hat{Y}_i.$$

# Simplest linear regression

- The simplest linear regression only has an outcome variable $Y$, no covariates.
    - It’s equivalent to a one-sample t-test.
    - It’s often a good “baseline model” against which you can compare a more sophisticated model.
- The linear regression equation can be written as

$$E(Y) = \beta_0.$$

- In other words, we are saying the population mean of $Y$ (i.e. $E(Y)$) is equal to a parameter $\beta_0$.

# Example i

```
library(tidyverse)
url <- paste0(”https://web.stanford.edu/~hastie/”,
              ”ElemStatLearn/datasets/prostate.data”)
dataset <- read.table(url)
```

```
# Separate train and test
data_train <- filter(dataset, train)
data_test <- filter(dataset, train)
```

# Example ii

```
# Use function lm
fit1 <- lm(lpsa ~ 1, data = data_train)
fit1
```

```
##
## Call:
## lm(formula = lpsa ~ 1, data = data_train)
##
## Coefficients:
## (Intercept)
##       2.452
```

# Example iii

```r
# Getting predicted values
pred_vals1 <- predict(fit1, newdata = data_test)
head(pred_vals1)
```

```
## 1 2 3 4 5 6
## 2.452345 2.452345 2.452345 2.452345 2.452345
2.452345
```

# One continuous covariate i

- Next we look at the case of a single *continuous* covariate $X$
- The linear regression equation for this situation can also be written as

$$E(Y|X) = \beta_0 + \beta_1 X.$$

- Let's unpack this:
    - When $X = 0$, the RHS still simplifies to $\beta_0$, and we get

$$E(Y|X = 0) = \beta_0.$$

# One continuous covariate ii

- Let's compare two values of $X$ that differ by 1 unit, e.g. $x$ and $x + 1$. We have

$$\begin{aligned} E(Y|X = x) &= \beta_0 + \beta_1 x \\ E(Y|X = x + 1) &= \beta_0 + \beta_1(x + 1) \\ &= (\beta_0 + \beta_1 x) + \beta_1 \\ &= E(Y|X = x) + \beta_1. \end{aligned}$$

# One continuous covariate iii

- Rearranging, we get

$$\beta_1 = E(Y|X = x + 1) - E(Y|X = x).$$

- In other words, $\beta_1$ represents the **difference** in population means between two subgroups that differ by 1 unit in their value of the covariate $X$.
- $\beta_0$ still represents the population mean of $Y$ when $X = 0$.
    - But depending on what $X$ represent (e.g. age, cholesterol), $X = 0$ may not be possible!

# Example

```r
# Use function lm
fit2 <- lm(lpsa ~ age, data = data_train)
fit2
```

```
##
## Call:
## lm(formula = lpsa ~ age, data = data_train)
##
## Coefficients:
## (Intercept)          age
##     0.07945      0.03665
```

# Exercise

Compute the RMSE for this model (i.e. `lpsa ~ age`), and compare to the RMSE we get from only using the intercept. Which model performs better?

# Solution i

```
# Recall from previous lecture
target <- data_test$lpsa
rmse1 <- sqrt(mean((target - pred_vals1)^2))
rmse1
```

```
## [1] 1.198765
```

```
pred_vals2 <- predict(fit2, newdata = data_test)
rmse2 <- sqrt(mean((target - pred_vals2)^2))
c(rmse1, rmse2)
```

# Solution ii

```
## [1] 1.198765 1.167291
```

The second model (with age as a feature) performs slightly better.

# Improving the model

- There are various ways of trying to improve the model:
    - Add more features that can explain the remaining variation.
    - Model the effect of age non-linearly.
    - Regularization (next lecture).
- We will look at these approaches one at a time.

# Multiple features i

- The dataset contains 8 covariates that we can use in our model.
    - Some are continuous (`lcavol`, `lweight`, `age`, `lbph`, `lcp`, `pgg45`).
    - Some are categorical (`svi`, `gleason`).
- We will add all of them in the model.

```r
# Remove column train
data_train <- select(data_train, -train)
# The dot is a short-hand for all variables
fit3 <- lm(lpsa ~ ., data = data_train)
fit3
```

# Multiple features ii

```
##
## Call:
## lm(formula = lpsa ~ ., data = data_train)
##
## Coefficients:
## (Intercept) lcavol lweight age lbph svi
## 0.429170 0.576543 0.614020 -0.019001 0.144848
0.737209
## lcp gleason pgg45
## -0.206324 -0.029503 0.009465
```

# Multiple features iii

```r
pred_vals3 <- predict(fit3, newdata = data_test)
rmse3 <- sqrt(mean((target - pred_vals3)^2))
c(rmse1, rmse2, rmse3)
```

```
## [1] 1.1987646 1.1672908 0.6627215
```

- This was a huge improvement: we reduced the RMSE by almost 50%.
- Note: `gleason` has four levels, but it only has 1 regression coefficient...
    - We would expect 3 coefficients.

# Multiple features iv

- We can fix that by transforming `gleason` from integer to factor.
    - Let's see if that leads to any improvement.

```
# Turn gleason into factor
data_train <- mutate(data_train,
                     gleason = factor(gleason))

fit4 <- lm(lpsa ~ ., data = data_train)
fit4
```

# Multiple features v

```
##
## Call:
## lm(formula = lpsa ~ ., data = data_train)
##
## Coefficients:
## (Intercept) lcavol lweight age lbph svi
## 0.19622 0.56811 0.64616 -0.02218 0.13193
0.70716
## lcp gleason7 gleason8 gleason9 pgg45
## -0.24550 0.18307 0.72688 -0.49720 0.01105
```

# Multiple features vi

```r
# gleason needs to be a factor in the test data too!
data_test <- mutate(data_test,
                    gleason = factor(gleason))
pred_vals4 <- predict(fit4, newdata = data_test)
rmse4 <- sqrt(mean((target - pred_vals4)^2))
c(rmse1, rmse2, rmse3, rmse4)
```

```
## [1] 1.1987646 1.1672908 0.6627215 0.6428274
```

- The effect was marginal.

# Exercise

Consider a model with all covariates except `gleason`. Compute its RMSE. Does it perform better or worse than the model with all 8 covariates?

# Solution i

```r
fit5 <- lm(lpsa ~ lcavol + lweight + age + lbph +
              svi + lcp + pgg45, data = data_train)

pred_vals5 <- predict(fit5, newdata = data_test)
rmse5 <- sqrt(mean((target - pred_vals5)^2))

c(rmse1, rmse2, rmse3, rmse4, rmse5)
```

```
## [1] 1.1987646 1.1672908 0.6627215 0.6428274
0.6628444
```

- It performs slightly worse, but the difference is minimal.

# Splines

# Motivation

- Recall the linear regression equation:

$$E(Y \mid X_1, \ldots, X_p) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p.$$

- We implicitly assume that the $X_i$ are different measurements/features.
  - They more or less match the columns of the dataset.
- However, we can also include transformations of the same covariate (e.g. age and its square).
- For example, we can perform *cubic regression* within the framework of linear regression as follows:

$$E(Y \mid X) = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3.$$

# Example i

```r
# poly gives us the polynomial expansion
head(poly(data_train$age, 3))
```

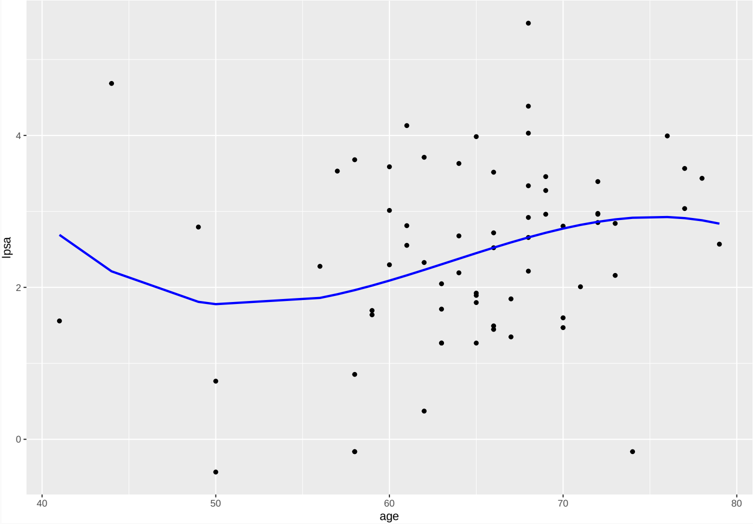
```
##                1           2            3
## [1,] -0.24194745  0.10877056  0.189860637
## [2,] -0.11068851 -0.06639027  0.138164924
## [3,]  0.15182937  0.11396035 -0.009135548
## [4,] -0.11068851 -0.06639027  0.138164924
## [5,] -0.04505904 -0.08763665  0.027096941
## [6,] -0.24194745  0.10877056  0.189860637
```

# Example ii

```
fit_cube <- lm(lpsa ~ poly(age, 3), data = data_train)

data_train |>
  bind_cols(.fitted = fitted(fit_cube)) |>
  ggplot(aes(x = age)) +
  geom_point(aes(y = lpsa)) +
  geom_line(aes(y = .fitted),
            colour = ”blue”, size = 1)
```

# Example iii



# Splines i

- Polynomial regression is simple, but its main drawback is that it requires a global fit.
  - The resulting cubic polynomial is the same over the whole range of values.
- **Splines** increase the flexibility by fitting polynomial over subsets of the range.
  - E.g. a certain cubic polynomial on the range $[0, 10]$, and a different cubic polynomial on the range $[10, 20]$.
- They also have to satisfy extra constraints.
  - They have to be continuous (i.e. the polynomials have to match on the boundary points).

# Splines ii

    - They have to be differentiable everywhere (so no sharp corners on the boundary points).
- However, they require many degrees of freedom.
    - Assume we have $k$ knots (i.e. the boundary points).
    - On each piece, we fit polynomials of degree $d$.
    - Continuity/Differentiability gives use $dk$ constraints.
    - Therefore, we need $(d+1)(k+1) - dk = d + k + 1$ degrees of freedom.

# Example i

- You can manually specify the knots.

```r
library(splines)
head(bs(data_train$age,
        knots = c(62, 65, 69),
        degree = 3))
```

# Example ii

```
## 1 2 3 4 5 6
## [1,] 0.4604136 0.3013393 0.05165816 0.0000000
0.0000000 0.000
## [2,] 0.1432098 0.5017361 0.34814342 0.0000000
0.0000000 0.000
## [3,] 0.0000000 0.0000000 0.05252101 0.3301321
0.4923469 0.125
## [4,] 0.1432098 0.5017361 0.34814342 0.0000000
0.0000000 0.000
## [5,] 0.0156250 0.3281250 0.65625000 0.0000000
0.0000000 0.000
## [6,] 0.4604136 0.3013393 0.05165816 0.0000000
```

# Example iii

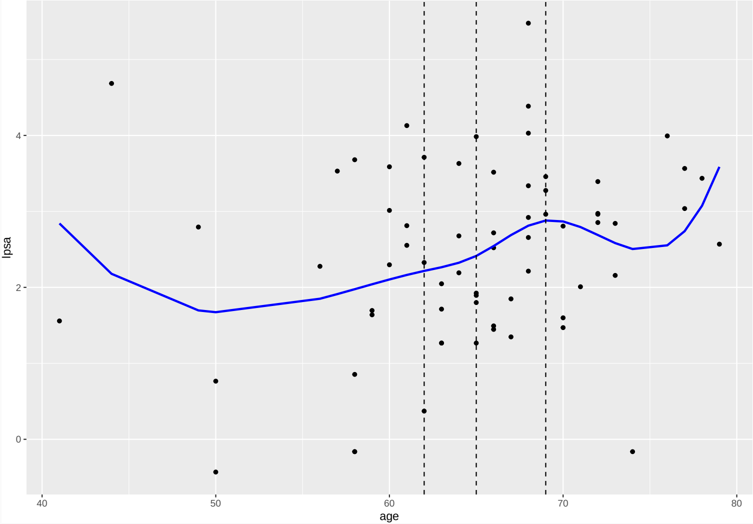
```
0.0000000 0.000
```

```r
fit_spl <- lm(lpsa ~ bs(age, degree = 3,
                        knots = c(62, 65, 69)),
              data = data_train)
```

# Example iv

```r
data_train |>
  bind_cols(.fitted = fitted(fit_spl)) |>
  ggplot(aes(x = age)) +
  geom_point(aes(y = lpsa)) +
  geom_line(aes(y = .fitted),
            colour = ”blue”, size = 1) +
  geom_vline(xintercept = c(62, 65, 69),
             linetype = ”dashed”)
```

# Example v



# Example vi

- Or you can specify the degrees of freedom.

```
# The intercept is the 7th df
spl_mat <- bs(data_train$age, df = 6)
head(spl_mat)
```

```
## 1 2 3 4 5 6
## [1,] 0.46659375 0.3127902 0.05424107
0.000000000 0.0000000 0.000
## [2,] 0.12862153 0.5024529 0.36555060
0.000000000 0.0000000 0.000
## [3,] 0.00000000 0.0000000 0.04960317
```

# Example vii

```
0.333049887 0.4923469 0.125
## [4,] 0.12862153 0.5024529 0.36555060
0.000000000 0.0000000 0.000
## [5,] 0.01171875 0.3007812 0.68576389
0.001736111 0.0000000 0.000
## [6,] 0.46659375 0.3127902 0.05424107
0.000000000 0.0000000 0.000
```

```
attr(spl_mat, ”knots”)
```

```
## 25% 50% 75%
##  61  65  69
```

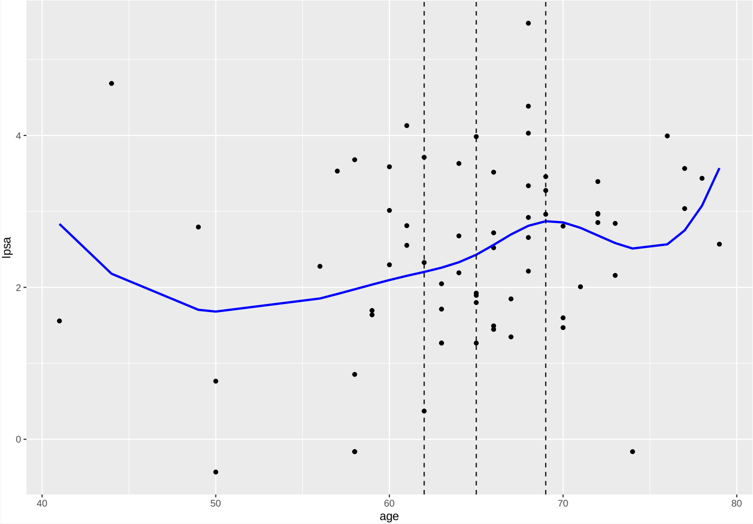
# Example viii

```r
# Same result
fit_spl <- lm(lpsa ~ bs(age, df = 6),
              data = data_train)
```

# Example ix

```
data_train |>
  bind_cols(.fitted = fitted(fit_spl)) |>
  ggplot(aes(x = age)) +
  geom_point(aes(y = lpsa)) +
  geom_line(aes(y = .fitted),
            colour = ”blue”, size = 1) +
  geom_vline(xintercept = c(62, 65, 69),
             linetype = ”dashed”)
```

# Example x



# Exercise

Compute the RMSE for this model, and compare with the model with only age as a covariate (i.e. `fit2`).

# Solution i

```r
pred_vals_spl <- predict(fit_spl, newdata = data_test)
rmse_spl <- sqrt(mean((target - pred_vals_spl)^2))

c(rmse2, rmse_spl)
```

```
## [1] 1.167291 1.140155
```

# Final remarks

- Linear regression is a general framework for building models.
- Its main asset is its high interpretability:
    - The coefficients represent differences in expected outcome.
- It is also quite flexible, especially when combined with splines.
- However, it can be quite sensitive to outliers in the training data, and the number of degrees of freedom we can use is bounded above by the number of observations.
- Next lecture, we will discuss regularization, which tries to address both points.