Linear Regression Basics

Utrecht University Winter School: Regression in R

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Outline

Regression Problem

Simple Linear Regression

- Model Estimation
- Model Fit

Multiple Linear Regression

- Model Comparison

Regression Problem

Some of the most ubiquitous and useful statistical models are *regression models*.

- *Regression* problems (as opposed to *classification* problems) involve modeling a quantitative response.
- The regression problem begins with a random outcome variable, Y.
- We hypothesize that the mean of Y is dependent on some set of fixed covariates, $\mathbf{X}$.

Flavors of Probability Distribution

The distributions we consider in regression problems have *conditional means*.

- The value of Y that we expect for each observation is defined by the observations' individual characteristics.
- This type of distribution is called "conditional."

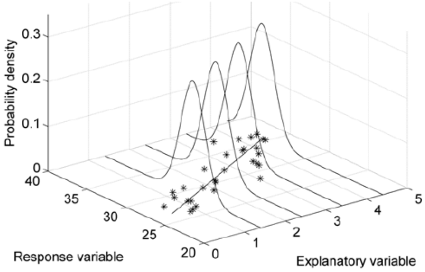
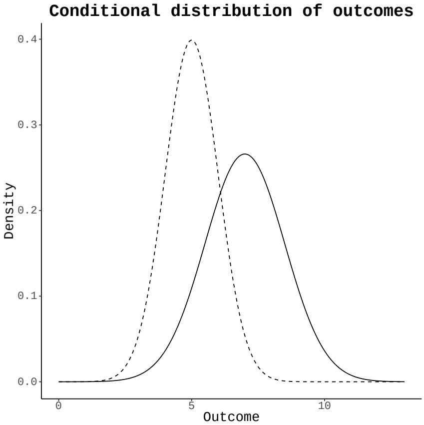


Image retrieved from:
`http://www.seaturtle.org/mtn/archives/mtn122/mtn122p1.shtml`

Flavors of Probability Distribution

Even a simple comparison of means implies a conditional distribution.

- The solid curve corresponds to outcome values for one group.
- The dashed curve represents outcomes from the other group.

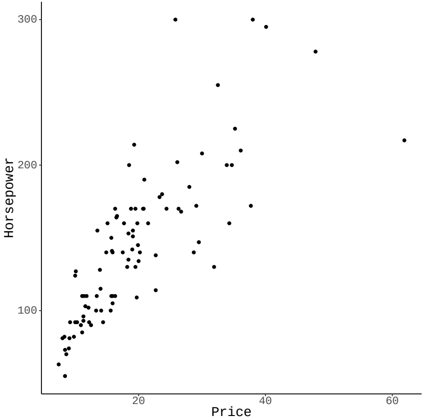


Simple Linear Regression

Projecting a Distribution onto the Plane

In practice, we only interact with the X-Y plane of the previous 3D figure.

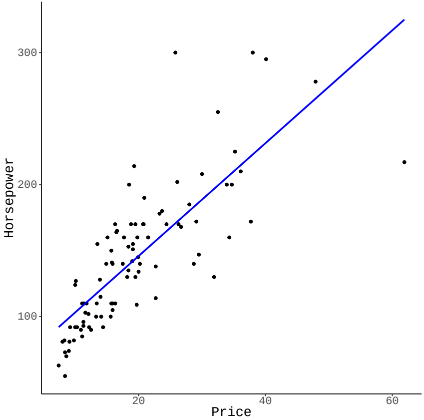
- On the Y-axis, we plot our outcome variable
- The X-axis represents the predictor variable upon which we condition the mean of Y.



Modeling the X–Y Relationship in the Plane

We want to explain the relationship between Y and X by finding the line that traverses the scatterplot as "closely" as possible to each point.

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$$



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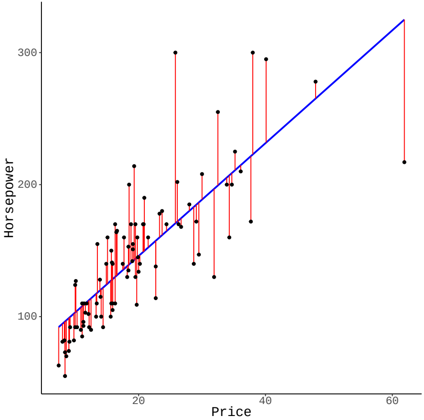
To fully model the relation between Y and X, we still need to account for the estimation error.

$$Y = \hat{\beta}_0 + \hat{\beta}_1 X + \hat{\varepsilon}$$



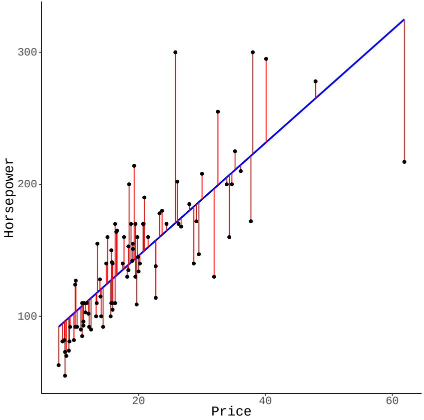
Residuals as the Basis of Estimation

The $\hat{\varepsilon}_n$ are defined in terms of deviations between each observed Y_n value and the corresponding $\hat{Y}_n$.

$$\hat{\varepsilon}_n = Y_n - \hat{Y}_n = Y_n - \left(\hat{\beta}_0 + \hat{\beta}_1 X_n\right)$$

Each $\hat{\varepsilon}_n$ is squared before summing to produce a quadratic objective function.

$$RSS = \sum_{n=1}^{N} \hat{\varepsilon}_n^2 = \sum_{n=1}^{N} \left(Y_n - \hat{Y}_n\right)^2$$
$$= \sum_{n=1}^{N} \left(Y_n - \hat{\beta}_0 - \hat{\beta}_1 X_n\right)^2$$



Least Squares Example

Estimate the least squares coefficients for our example data:

```
#data(Cars93)
out1 <- lm(Horsepower ~ Price, data = Cars93)
coef(out1)

(Intercept)       Price
  60.447578    4.273796
```

The estimated intercept is $\hat{\beta}_0 = 60.45$.

- A free car is expected to have 60.45 horsepower.

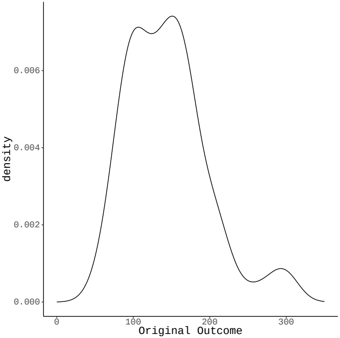
The estimated slope is: $\hat{\beta}_1 = 4.27$.

- For every additional $1000 in price, a car is expected to gain 4.27 horsepower.

Model Fit

We may also want to know how well our model explains the outcome.

- Our model explains some proportion of the outcome's variability.
- The residual variance $\hat{\sigma}^2 = \mathrm{Var}(\hat{\varepsilon})$ will be less than $\mathrm{Var}(Y)$.



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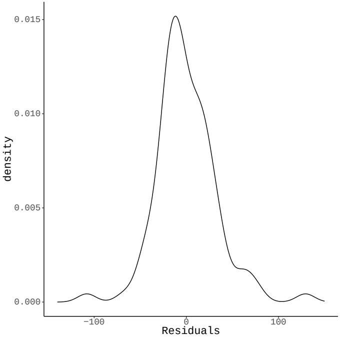

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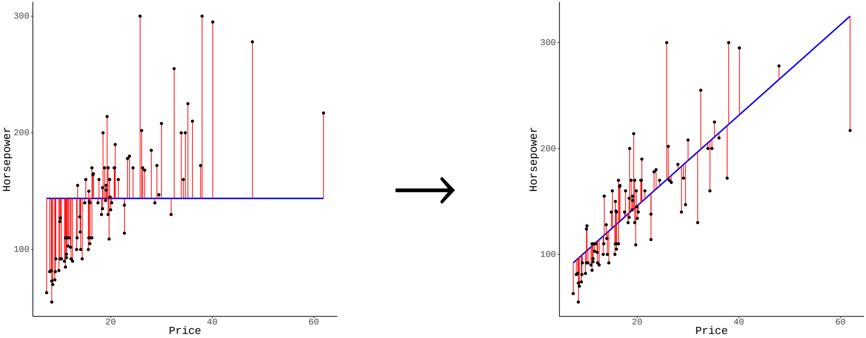

Model Fit

We quantify the proportion of the outcome's variance that is explained by our model using the R^2 statistic:

$$R^2 = \frac{TSS - RSS}{TSS} = 1 - \frac{RSS}{TSS}$$

where

$$TSS = \sum_{n=1}^{N} \left(Y_n - \bar{Y}\right)^2 = \mathrm{Var}(Y) \times (N-1)$$

For our example problem, we get:

$$R^2 = 1 - \frac{95573}{252363} \approx 0.62$$

Indicating that car price explains 62% of the variability in horsepower.

Model Fit for Prediction

When assessing predictive performance, we will most often use the *mean squared error* (MSE) as our criterion.

$$
\begin{aligned}
MSE &= \frac{1}{N} \sum_{n=1}^{N} \left(Y_n - \hat{Y}_n \right)^2 \\
&= \frac{1}{N} \sum_{n=1}^{N} \left(Y_n - \hat{\beta}_0 - \sum_{p=1}^{P} \hat{\beta}_p X_{np} \right)^2 \\
&= \frac{RSS}{N}
\end{aligned}
$$

For our example problem, we get:

$$
MSE = \frac{95573}{93} \approx 1027.67
$$

Interpreting MSE

The MSE quantifies the average squared prediction error.

- Taking the square root improves interpretation.

$$RMSE = \sqrt{MSE}$$

The RMSE estimates the magnitude of the expected prediction error.

- For our example problem, we get:

$$RMSE = \sqrt{\frac{95573}{93}} \approx 32.06$$

- When using price as the only predictor of horsepower, we expect prediction errors with magnitudes of 32.06 horsepower.

Information Criteria

We can use *information criteria* to quickly compare *non-nested* models while accounting for model complexity.

- Akaike's Information Criterion (AIC)

$$AIC = 2K - 2\hat{\ell}(\theta|X)$$

- Bayesian Information Criterion (BIC)

$$BIC = K\ln(N) - 2\hat{\ell}(\theta|X)$$

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$$BIC = K\ln(N) - 2\hat{\ell}(\theta|X)$$

Information criteria balance two competing forces.

- The optimized loglikelihood quantifies fit to the data.
- The penalty term corrects for model complexity.

Information Criteria

For our example, we get the following estimates of AIC and BIC:

$$\begin{aligned} AIC &= 2(3) - 2(-454.44) \\ &= 914.88 \end{aligned}$$

$$\begin{aligned} BIC &= 3\ln(93) - 2(-454.44) \\ &= 922.48 \end{aligned}$$

To compute the AIC/BIC from a fitted `lm()` object in R:

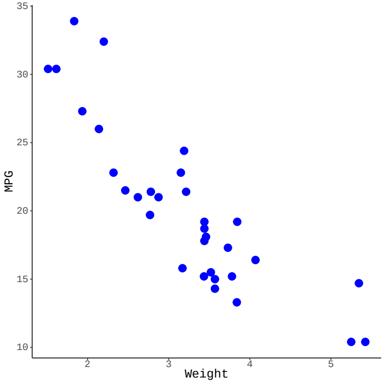
```
AIC(out1)

[1] 914.8821

BIC(out1)

[1] 922.4799
```

Multiple Linear Regression

Graphical Representations of Regression Models

A regression of two variables can be represented on a 2D scatterplot.

- Simple linear regression implies a 1D line in 2D space.



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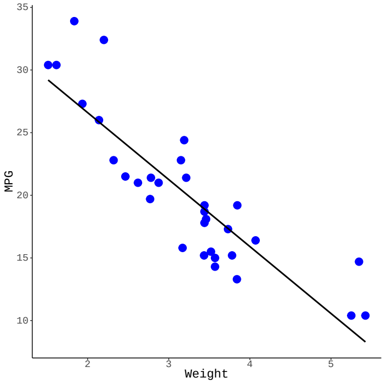
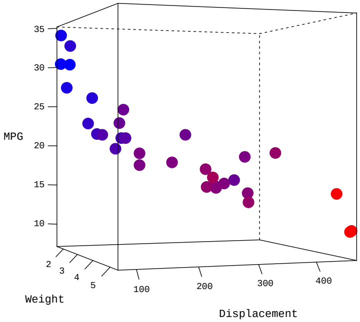


Graphical Representations of Regression Models

Adding an additional predictor leads to a 3D point cloud.

- A regression model with two IVs implies a 2D plane in 3D space.



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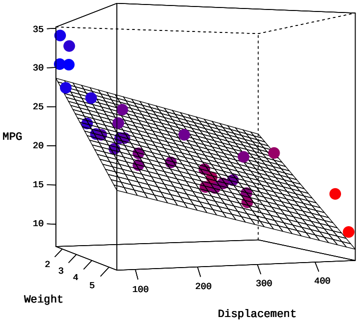

Partial Effects

In MLR, we want to examine the *partial effects* of the predictors.

- What is the effect of a predictor after controlling for some other set of variables?

This approach is crucial to controlling confounds and adequately modeling real-world phenomena.

Example

```r
## Read in the 'diabetes' dataset:
dataDir <- "../../../data/"
dDat    <- readRDS(paste0(dataDir, "diabetes.rds"))

## Simple regression with which we're familiar:
out1 <- lm(bp ~ age, data = dDat)
```

Asking: What is the effect of age on average blood pressure?

Example

```
partSummary(out1, -1)

Residuals:
    Min      1Q  Median      3Q     Max 
-31.188  -8.897  -1.209   8.612  39.952 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 77.47605    2.38132  32.535  < 2e-16
age          0.35391    0.04739   7.469 4.39e-13

Residual standard error: 13.04 on 440 degrees of freedom
Multiple R-squared:  0.1125, Adjusted R-squared:  0.1105
F-statistic: 55.78 on 1 and 440 DF,  p-value: 4.393e-13
```

Example

```r
## Add in another predictor:
out2 <- lm(bp ~ age + bmi, data = dDat)
```

Asking: What is the effect of BMI on average blood pressure, *after controlling for age?*

- We're partialing age out of the effect of BMI on blood pressure.

Example

```
partSummary(out2, -1)

Residuals:
    Min      1Q  Median      3Q     Max 
-29.287  -8.198  -0.178   8.413  41.026 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 52.24654    3.83168  13.635  < 2e-16
age          0.28651    0.04504   6.362 5.02e-10
bmi          1.08053    0.13363   8.086 6.06e-15

Residual standard error: 12.18 on 439 degrees of freedom
Multiple R-squared:  0.2276, Adjusted R-squared:  0.224 
F-statistic: 64.66 on 2 and 439 DF,  p-value: < 2.2e-16
```

Multiple R^2

How much variation in blood pressure is explained by the two models?

- Check the R^2 values.

```
## Extract R^2 values:
r2.1 <- summary(out1)$r.squared
r2.2 <- summary(out2)$r.squared

r2.1

[1] 0.1125117

r2.2

[1] 0.2275606
```

F-Statistic

How do we know if the R^2 values are significantly greater than zero?

- We use the F-statistic to test $H_0 : R^2 = 0$ vs. $H_1 : R^2 > 0$.

```
f1 <- summary(out1)$fstatistic
f1

    value     numdf     dendf
 55.78116   1.00000 440.00000

pf(q = f1[1], df1 = f1[2], df2 = f1[3], lower.tail = FALSE)

       value
4.392569e-13
```

F-Statistic

```
f2 <- summary(out2)$fstatistic
f2

   value    numdf    dendf 
 64.6647   2.0000 439.0000 

pf(f2[1], f2[2], f2[3], lower.tail = FALSE)

       value 
2.433518e-25 
```

Comparing Models

How do we quantify the additional variation explained by BMI, above and beyond age?

- Compute the ΔR^2

```
## Compute change in R^2:
r2.2 - r2.1

[1] 0.115049
```

Significance Testing

How do we know if ΔR^2 represents a significantly greater degree of explained variation?

- Use an F-test for $H_0 : \Delta R^2 = 0$ vs. $H_1 : \Delta R^2 > 0$

```
## Is that increase significantly greater than zero?
anova(out1, out2)

Analysis of Variance Table

Model 1: bp ~ age
Model 2: bp ~ age + bmi
  Res.Df   RSS Df Sum of Sq      F    Pr(>F)
1    440 74873
2    439 65167  1    9706.1 65.386 6.057e-15 ***
---
Signif. codes:
0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Model Comparison

We can also compare models based on their prediction errors.

- For OLS regression, we usually compare MSE values.

```
mse1 <- MSE(y_pred = predict(out1), y_true = dDat$bp)
mse2 <- MSE(y_pred = predict(out2), y_true = dDat$bp)

mse1

[1] 169.3963

mse2

[1] 147.4367
```

In this case, the MSE for the model with BMI included is smaller.

- We should prefer the the larger model.

Model Comparison

Finally, we can compare models based on information criteria.

```
AIC(out1, out2)

     df      AIC
out1  3 3528.792
out2  4 3469.424

BIC(out1, out2)

     df      BIC
out1  3 3541.066
out2  4 3485.789
```

In this case, both the AIC and the BIC for the model with BMI included are smaller.

- We should prefer the the larger model.