Overview and linear regression

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Overview. What is Machine Learning?

Example of problem/task *not* well suited for machine learning: multiply two 5-digit numbers

- A human can write a computer program (teach the computer/machine) exact steps/algorithm to follow
- Computers excel at this kind of mechanical task – humans no so much

Overview. What is Machine Learning?

- Example of problem well suited for ML: Spam email recognition
  - Very easy for a human to do
  - But very hard for a human to translate into a well-defined sequence of steps/algorithm
- Idea behind ML: ‘feed’ the computer many examples (data) of spam and non-spam emails
  - Let the machine/computer come up with its own set of ‘rules’
- ‘Feeding’ **features** extracted from the emails and **labels** indicating spam/no-spam

Features and Labels

- Features: Characteristics of the emails human believes relevant to determining spam/no-spam
    - Total number of words (numeric feature)
    - Appearance of keywords/phrases (e.g. ‘act now’, ‘for free’, ‘save $’) (yes/no) (binary feature)
    - Single word frequencies (numeric features)
    - Pairs of words frequencies (numeric features)
    - Email sender in your contact list (yes/no)?
    - Time of day email was sent 0-24 (numeric)
    - Day of week email wass sent (categorical)
- Label: spam/no-spam (binary)

Algorithms

- How does a machine learn by example?
- Need a algorithm to train a model/label generator (e.g. classify a new email as spam/no-spam)
    - Input: features and labels of the training data/examples
    - Output: ‘label generator’ for new instances (without label)
- Example algorithms/method for the spam problem: Naive Bayes Classifier, Support Vector Machines, Discriminant Analysis, logistic regression
- Need a training method to ‘fit’ the model (e.g. gradient descent)

Machine Learning vs. Statistics

- Lots of overlap - they share many techniques/models (e.g. linear and logistic regression, principal components)
- But goals are different
- Statistics focuses on inference:
  - estimation and hypothesis testing of parameters of interest (e.g. odds ratio, regression slope)
  - Establishing association/causation (e.g. is smoking a risk factor for lung cancer?)
- Machine learning focuses on prediction and detection (e.g. does this patient have lung cancer? Is this patient likely to have a relapse?)
- We'll refer to both as 'prediction'

Machine Learning vs. Statistics

- ML Theory makes very few distributional assumptions: independent, identically distributed instances/samples
- Statistics (typically but not always) makes lots of distributional assumptions (e.g. data is normally distributed)
- ML assumes less but has the 'simpler' goal of prediction
- Statistics assumes more but has the more complex goal of establishing association/causation

Prediction

- Machine Learning emphasizes prediction
- But, why do we want to ‘predict/detect’?
  - to anticipate/predict future (e.g. patient likely to die within 5 years)
  - to avoid costly/unfeasible measure (e.g. estimate body-fat from BMI, detect whether a woman has ovarian cancer based on methylation measurements)
  - to automate/eliminate need for human intervention (e.g. spam detector)
- Two really different meanings of ‘prediction’:
  - prediction of future outcome
  - estimation of unmeasured variable/detection

Artificial Intelligence vs. Machine Learning

- Artificial Intelligence: “The effort to automate intellectual tasks normally performed by humans”*
- Machine Learning is a sub-field AI
- Route finding algorithms (e.g. Waze app) are AI but not ML

* “Deep Learning with R” by Allaire and Chollet

Example of Biomedical applications

Example applications from Health, Medicine, Biology, and related fields

- Predict whether a prostate cancer patient will have a recurrence based on gene expression profiles of the tumor
- Early detection of ovarian vancer patients using methylation patterns
- Identify population structure/ancestry based on millions of single nucleotide polymorphism (SNP) genotypes
- Diagnose cancer subtype based on gene expression or methylation profiles
- Predict lung cancer based on exposure to asbestos, smoking, etc.
- Predict patient length of stay in hospital based on health records
- Early prediction (years before any symptoms) of likelihood of developing Alzheimer's disease based on MRI
- Predicting body fat percent based on BMI, gender, and age
- Predict age based on genomewide methylation patterns

Supervised vs. Unsupervised Learning

- In supervised learning the instances have labels/variables we want to predict based on their features
  - Spam detection is a typical example of a supervised learning problem
  - Analogy with learning under the supervision of a teacher that knows the correct answer (labels)
- In unsupervised learning there are features but no labels
  - Goal is to find structure (groups, clusters) in the instances and/or the features
  - Learning is unsupervised because there is 'no teacher'
  - Cluster analysis and Principal component analysis are typical unsupervised learning techniques

Classification vs. regression

- Supervised learning problems often are of one of two types depending on the type of label
- Classification: when label is binary (spam vs. non-spam) or categorical (3 breast cancer subtypes)
    - e.g. discriminant analysis, logistic regression, support vector machines
- Regression: when label is quantitative/numeric (% body fat, age, survival time)
    - Linear regression, Cox proportional hazards model

Glossary—Machine Learning vs. Statistics

- feature = predictor = independent variable = covariate = regressor = exogenous variable (economics)
- label = outcome = dependent variable
- instance = observation (for us usually subject, patient)
- algorithm = model
- train = fit model

Linear Regression

- Linear regression is a simple supervised regression (quantitative response/label) method
- Very useful despite simplicity
- More flexible than appears (can include higher order terms, interactions, splines, etc.)
- Starting point for other methods/algorithms: Discriminant analysis, logistic regression, ridge regression, LASSO, etc.

Example: predicting brain weight from head size

Data from brain weight (grams) and head size (cubic cm) for 237 adults aged 20 or above and classified by gender and age group from Middlesex Hospital, London

One of the main objects of the investigation which forms the subject of this paper, has been to obtain a series of reconstruction formulae, by which it will be possible, when in possession of certain chief measurements of the head, to predict within the limits of normal variation, the approximate weight of the brain

A Study of the Relations of the Brain to the Size of the Head Biometrika (1905)

The subject of brain-weight in man has for a long time been given considerable attention by anatomists and anthropologists. The reason for this is obvious. Since the brain is the organ of the mind it appeared to earlier workers that size of brain ought to be an index of intellectual capacity.

Biometrical Studies on Man: I. Variation and Correlation in Brain-Weight Biometrika (1905)

Brain weight example

```
setwd("/Users/jp/Google Drive/Teaching/Machine Learning/2021/Lectures/Lecture 2 - Linear regres
brain = read.table("brain.txt", header=T)
head(brain)
```

```
##   Sex Age Head.size Brain.weight
## 1   1   1      4512         1530
## 2   1   1      3738         1297
## 3   1   1      4261         1335
## 4   1   1      3777         1282
## 5   1   1      4177         1590
## 6   1   1      3585         1300
```

Brain weight example

```
str(brain)
```

```
## 'data.frame':    237 obs. of  4 variables:
##  $ Sex         : int  1 1 1 1 1 1 1 1 1 1 ...
##  $ Age         : int  1 1 1 1 1 1 1 1 1 1 ...
##  $ Head.size   : int  4512 3738 4261 3777 4177 3585 3785 3559 3613 3982 ...
##  $ Brain.weight: int  1530 1297 1335 1282 1590 1300 1400 1255 1355 1375 ...
```

```
summary(brain)
```

```
##       Sex             Age          Head.size     Brain.weight
##  Min.   :1.000   Min.   :1.000   Min.   :2720   Min.   : 955
##  1st Qu.:1.000   1st Qu.:1.000   1st Qu.:3389   1st Qu.:1207
##  Median :1.000   Median :2.000   Median :3614   Median :1280
##  Mean   :1.435   Mean   :1.536   Mean   :3634   Mean   :1283
##  3rd Qu.:2.000   3rd Qu.:2.000   3rd Qu.:3876   3rd Qu.:1350
##  Max.   :2.000   Max.   :2.000   Max.   :4747   Max.   :1635
```

Brain weight example

```
table(brain$Sex)
```

```
##
##   1   2
## 134 103
```

```
table(brain$Age)
```

```
##
##   1   2
## 110 127
```

- Need to convert `Sex` and `Age` to categorical variables before running `lm`

```
brain$Sex = factor(brain$Sex, levels=1:2, labels=c("Male", "Female"))
brain$Age = factor(brain$Age, levels=1:2, labels=c("20-46", "46+"))
```

Linear Regression in R

```
table(brain$Sex)
```

```
##
##   Male Female
##    134    103
```

```
table(brain$Age)
```

```
##
## 20-46   46+
##   110   127
```

- By converting to factor `lm` will properly treat `Sex` and `Age` :
  - `lm` will automatically create dummy variables

Brain weight example

Split data into training (70%) and test (30%) data

```
set.seed(301)
n = nrow(brain)
n
```

```
## [1] 237
```

```
trainset = sample(1:n, floor(0.7*n))
head(trainset, 10)
```

```
##  [1] 220 218 141   5  57 234  47  26  52   9
```

Brain weight example

Split data into training (70%) and test (30%) data

```
brain_train = brain[trainset,]; n_train = nrow(brain_train)
brain_test = brain[-trainset,]; n_test = nrow(brain_test)
dim(brain_train)
```

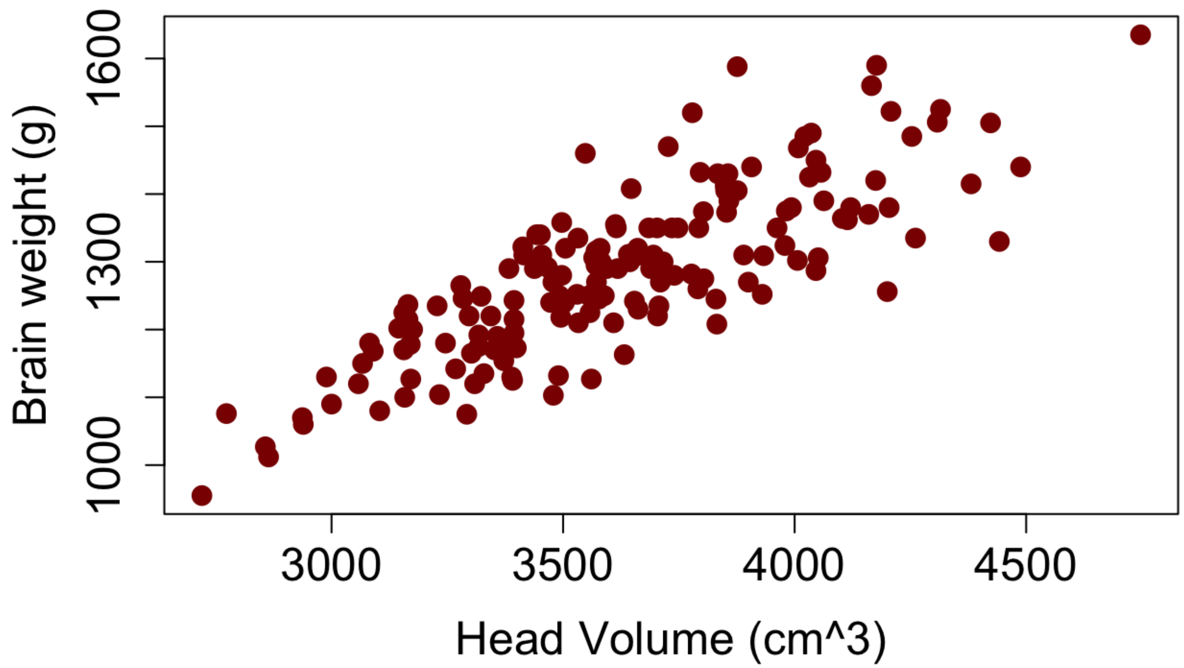
```
## [1] 165   4
```

```
dim(brain_test)
```

```
## [1] 72  4
```

Clear positive relationship between head volume and brain weight

```
par(mar=c(8,9,1,1))
plot(brain_train$Brain.weight ~ brain_train$Head.size,
     pch=16, cex=1.5, col='red4', xlab='Head Volume (cm^3)',
     ylab='Brain weight (g)', cex.lab=1.5, cex.axis=1.5, cex.main=1.5)
```



Linear Regression in R

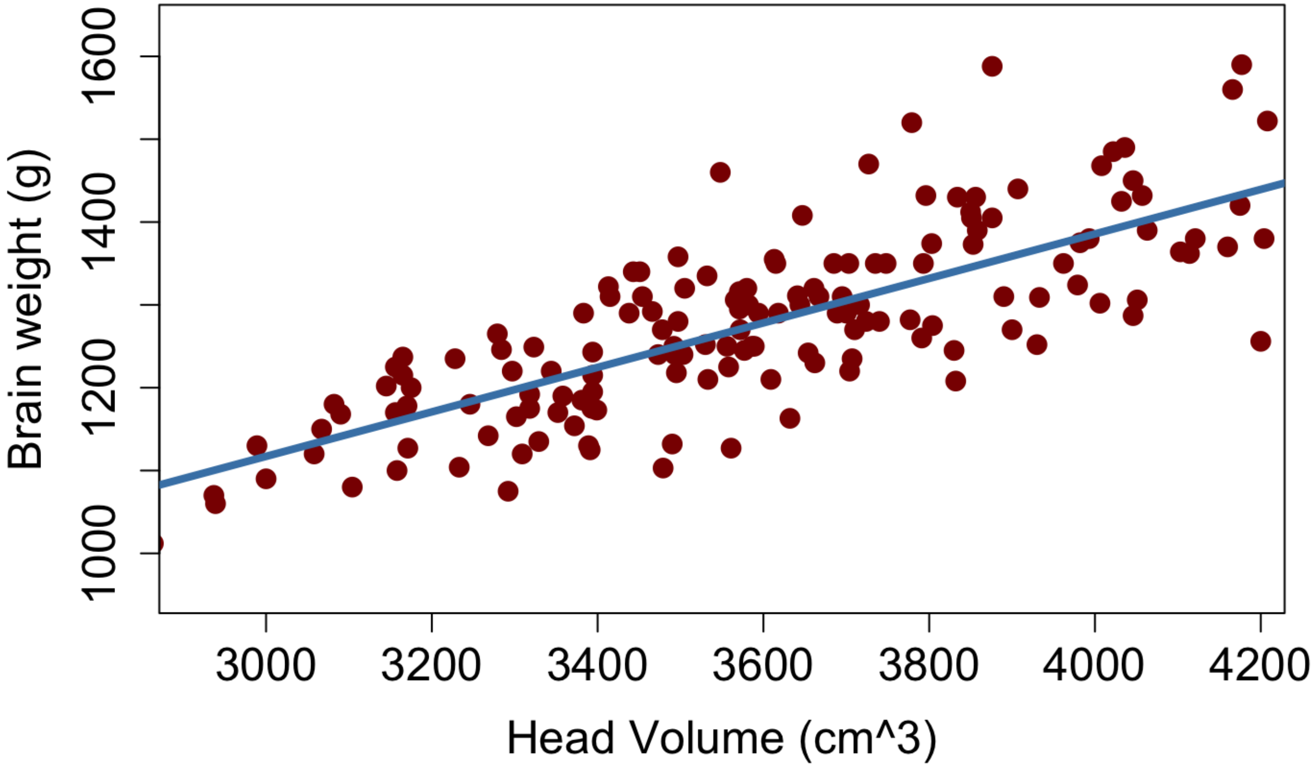
Will use only the training portion of the brain weight data to train the SLR model

```
brain_lm0 = lm(Brain.weight ~ Head.size, data = brain_train)
```

```
summary(brain_lm0)
```

```
##
## Call:
## lm(formula = Brain.weight ~ Head.size, data = brain_train)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -183.437  -50.277   -3.188   47.098  235.591
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 311.29654   54.67694   5.693 5.67e-08 ***
## Head.size     0.26860    0.01501  17.891  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 71.58 on 163 degrees of freedom
## Multiple R-squared:  0.6626, Adjusted R-squared:  0.6605
## F-statistic: 320.1 on 1 and 163 DF,  p-value: < 2.2e-16
```

Linear Regression in R



Prediction

- Using linear regression we constructed a model that approximates brain weight based on head size in our (training) data
- But our goal is to predict brain weight based on head size in the population
- What population? **A population the training data can be considered a random sample of**

   1. Patients aged 20+ in London's Middlesex Hospital in 1905
   2. Population of London inhabitants aged 20 or older in 1905
   3. Population of London inhabitants aged 20 or older today

- If the model predicts in the population the training data was sampled from we say that the model *generalizes*

How do we know if the model generalizes?

- Ideally we'd need to compare the brain weight predicted by the model with the true brain weight in the entire target population to *compute the average error* incurred by the model.
- Obviously we can't do that. Next best thing is to take a 'test' sample from the target population and use it to estimate the average error by the *sample average error*
- How do I get such a sample? We set aside part of the original data for this purpose before building our model.
- We split the data into training and testing
  - Use training data for fitting the model
  - Use test data to evaluate/estimate how well the model performs

Prediction performance metrics

y_i is the true observed outcome (e.g. brain weight) and

$\widehat{y_i} = \widehat{\beta_0} + \widehat{\beta_1}x_i$ is the outcome predicted by the linear model for observation i

$y_i - \widehat{y_i}$ is the error in prediction for observation i

- Mean Square error:

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{y_i})^2$$

- Root Mean Square error:

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \widehat{y_i})^2}$$

- Root Mean Square error is perhaps easier to interpret as it's on the same scale as the outcome (e.g. grams instead of square grams)

Prediction performance metrics in R

```
# Residual standard error - same as reported by lm
sqrt(sum((residuals(brain_lm0))^2)/(nrow(brain_train)-2))
```

```
## [1] 71.58431
```

```
# RMSE
RMSE_train0 = sqrt(sum((residuals(brain_lm0))^2)/nrow(brain_train))

RMSE_train0
```

```
## [1] 71.14914
```

Prediction performance metrics

R^2, proportion of variance explained

$\text{RSS} = \sum_{i=1}^{n} (y_i - \widehat{y_i})^2$

$\text{TSS} = \sum_{i=1}^{n} (y_i - \bar{y})^2$

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

```
RSS <- sum((residuals(brain_lm0))^2)
TSS <- sum((brain_train$Brain.weight - mean(brain_train$Brain.weight))^2)
R2_train0 = 1 - RSS/TSS
R2_train0
```

```
## [1] 0.662597
```

Which coincides with R^2 value in `lm` results above

Discussion Question

Can we evaluate prediction performance on the same data set used for building the model, i.e. the training data?

Evaluating (estimating) prediction performance

- Evaluating performance using training data **overestimates performance**
- We'd get an underestimate of true population prediction performance
- Why? Model was chosen so as to make MSE as small as possible in the training data.
- Analogous to using a practice exam to assess students
- Need to assess performance in yet **unseen/unused data**
- We **reserved test data** only for assessing performance
- Trade-off between:
  - better model (more training data) and
  - more accurate performance evaluation (more test data)
- Common split is **train=70-80%** and **test=20-30%** of data
- We will see next class that we can do better by using multiple training/testing splits

Prediction performance in weight data

```
pred0 = predict(brain_lm0, newdata=brain_test)
head(pred0)
```

```
##        1        2        6        7        8       13
## 1523.241 1315.341 1274.245 1327.966 1267.261 1289.018
```

```
head(cbind(brain_test, predicted=pred0))
```

```
##     Sex   Age Head.size Brain.weight predicted
## 1  Male 20-46      4512         1530  1523.241
## 2  Male 20-46      3738         1297  1315.341
## 6  Male 20-46      3585         1300  1274.245
## 7  Male 20-46      3785         1400  1327.966
## 8  Male 20-46      3559         1255  1267.261
## 13 Male 20-46      3640         1355  1289.018
```

Prediction performance in weight data

```
n_test = nrow(brain_test)

RMSE_test0 =
  sqrt(sum((brain_test$Brain.weight - pred0)^2)/n_test)

RMSE_test0
```

```
## [1] 74.83068
```

```
RMSE_train0
```

```
## [1] 71.14914
```

As expected, $RMSE_{test} > RMSE_{train}$

Prediction performance in weight data

```
R2_test0 = 1 -
  sum((brain_test$Brain.weight - pred0)^2)/
  sum((brain_test$Brain.weight - mean(brain_test$Brain.weight))^2)

R2_test0
```

```
## [1] 0.571456
```

```
R2_train0
```

```
## [1] 0.662597
```

As expected, $R^2_{test} < R^2_{train}$

Warning on R squared

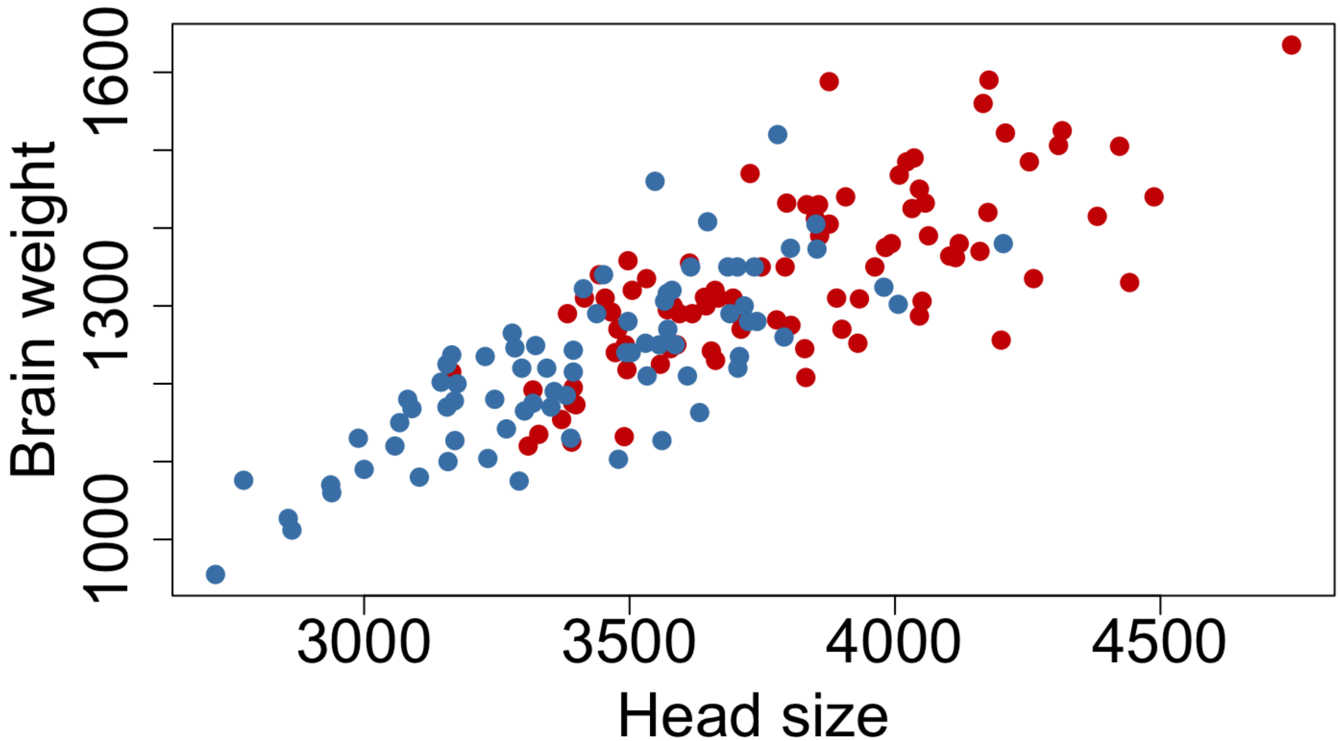
- For training set $R^2 = corr(y, \hat{y})^2$
- **Not true** in test set: $R^2 \neq corr(y, \hat{y})^2$
- In **training set** $0 \leq R^2 \leq 1$
- In **test set** R^2 can be negative!
- Negative R^2 in test set indicates extremely poor prediction!

Linear Regression for machine learning

- Want to predict the outcome using a linear function of the features
- $\widehat{Y} = f(X) = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p$
- Model is $Y = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p + \epsilon$
- where $\epsilon = Y - \widehat{Y}$
- The residual/error term simply captures the discrepancy between the outcome and the predicted value due to:
  - noise
  - predictive variables not included the model
  - true relationship not being linear
- BUT, **we will not assume linearity or that ϵ is normally distributed or that it has the same variance across observations**

Fitting a more complex model

- Plot by `Sex`, distinguishing Males (red) and Females (blue)



- Separate intercepts may improve prediction

Multiple Linear Regression in R

```
brain_lm1 = lm(Brain.weight ~ Head.size + Sex, data = brain_train)
summary(brain_lm1)
```

```
##
## Call:
## lm(formula = Brain.weight ~ Head.size + Sex, data = brain_train)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -183.796  -50.258   -3.397   48.411  233.505
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 334.03647   68.47214   4.878 2.54e-06 ***
## Head.size     0.26328    0.01786  14.742  < 2e-16 ***
## SexFemale    -7.35880   13.28798  -0.554     0.58
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 71.74 on 162 degrees of freedom
## Multiple R-squared:  0.6632, Adjusted R-squared:  0.6591
## F-statistic: 159.5 on 2 and 162 DF,  p-value: < 2.2e-16
```

Multiple Linear Regression in R

Computed train and test RMSE and R^2 for this modes (code not shown):

```
## RMSE_train0  RMSE_test0 RMSE_train1  RMSE_test1
##       71.15       74.83       71.08       74.17
```

- Adding `Sex` to the linear regression model yields only a marginal improvement in prediction performance