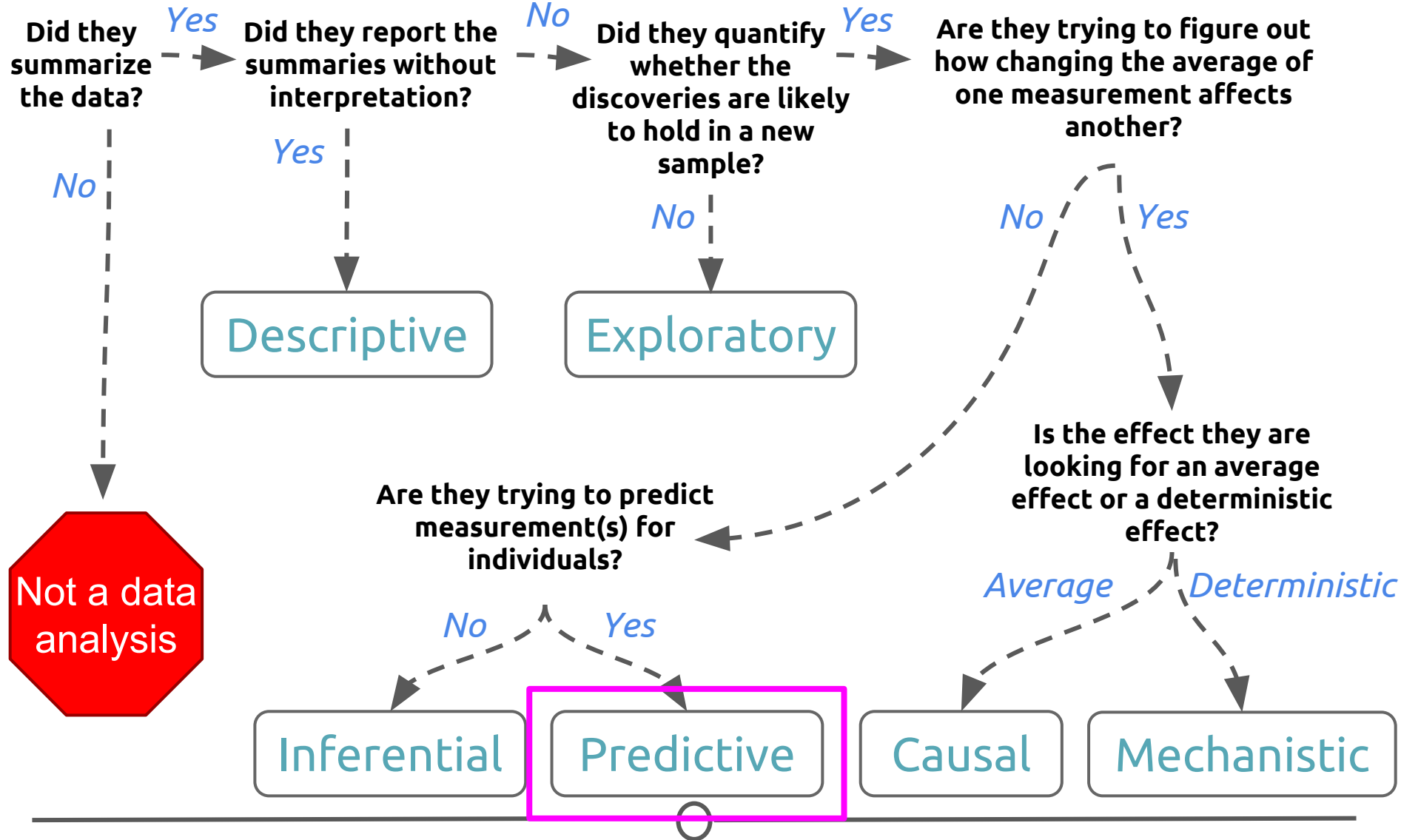
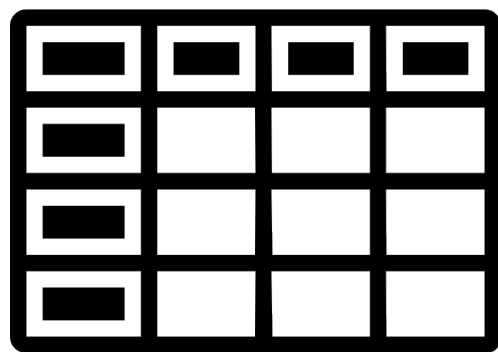


Prediction & Machine Learning



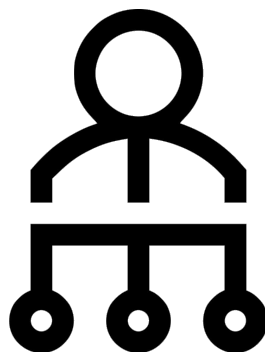
Data Analysis





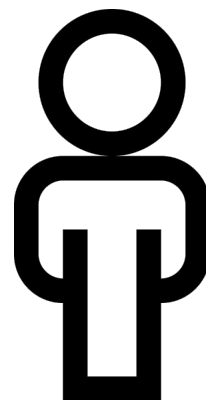
data

train →



model

→ predict





THE LATEST

8:57 AM

**The Rockets Are
Melo's Best, Last
Hope**

7:20 AM

**Significant Digits For
Tuesday, July 24,
2018**

6:00 AM

**What The Rise Of
Kamala Harris Tells
Us About The
Democratic Party**

INTERACTIVES

How Popular Is Donald Trump?

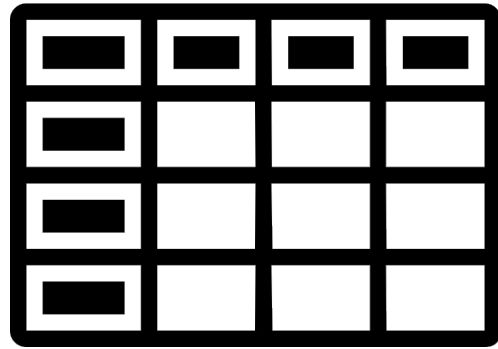
UPDATED 15 HOURS AGO

52.9%
Disapprove

41.8%
Approve

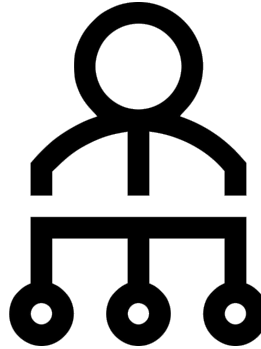
See all approval polls

predictive analysis uses
data you have now to make
predictions in the future



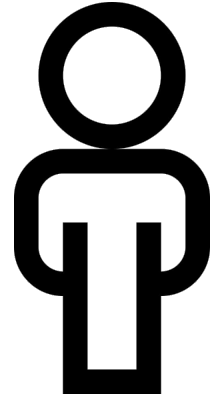
data

train →



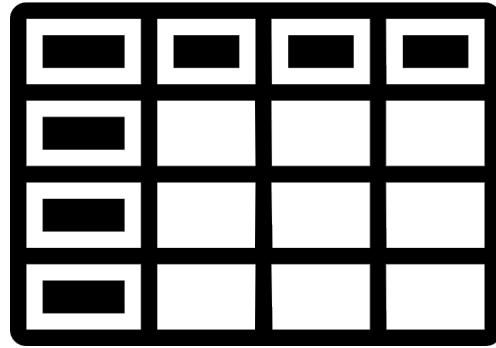
model

→ predict



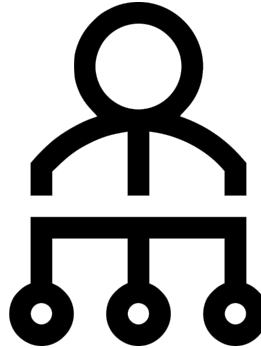
predictive analysis uses
data you have now to make
predictions in the future

machine learning is another
term for this!



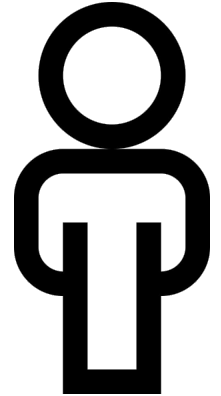
data

train →

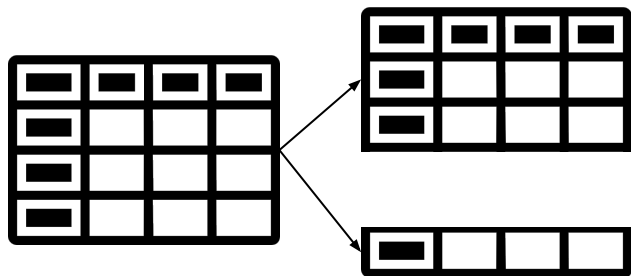


model

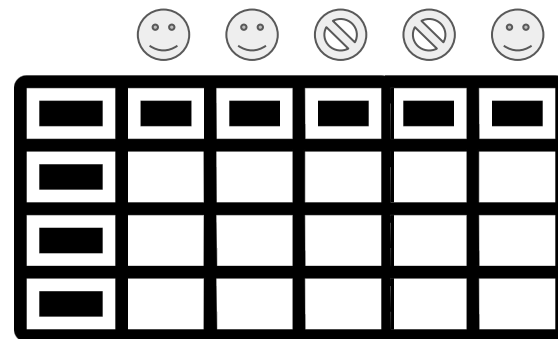
→ predict



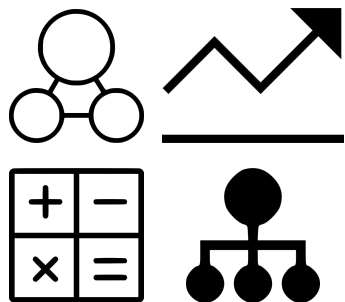
Basic Steps to Prediction



data splitting



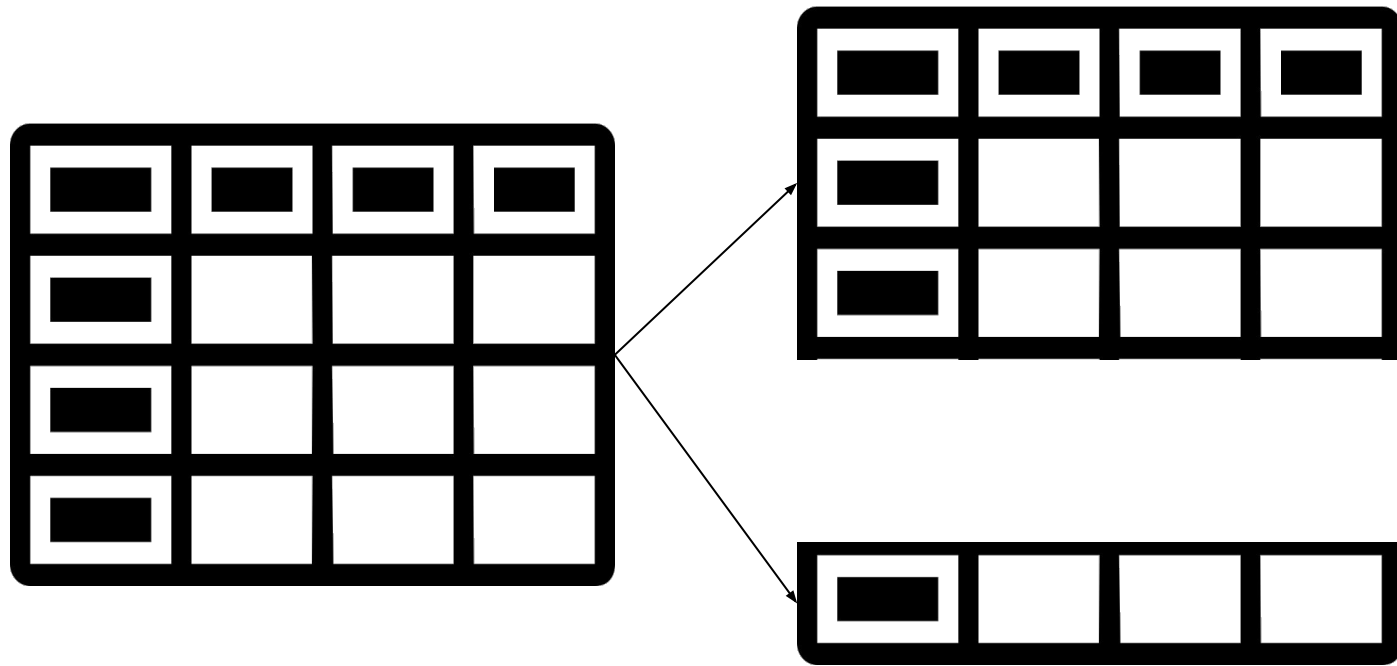
variable selection



model selection



accuracy assessment



data splitting





Michael Hoffman

@michaelhoffman

Following



What do you call the datasets you use for (1) training, (2) feature selection and hyperparameter tuning, and (3) quantifying performance. Please share your reasoning and disciplinary background too.

32% train, test, validate

37% train, validate, test

3% other (specify)

28% Just show me the results

pretty even split
between the two
options...

244 votes • Final results

5:15 PM - 25 Apr 2018

<https://twitter.com/michaelhoffman/status/989251677646704641>



Michael Hoffman @michaelhoffman · Apr 27



@CarldeBoerPhD suggests train, tune, test as an alternative. I think I like that. "Tune" is a better description for what goes on in the second part and it avoids the contentious and multisyllabic "validate".

Carl de Boer @CarldeBoerPhD

Let's all switch to **train, tune, test**. Alliterative and descriptive.
Alliterscriptive.

we'll go with **train,**
tune, test instead



2



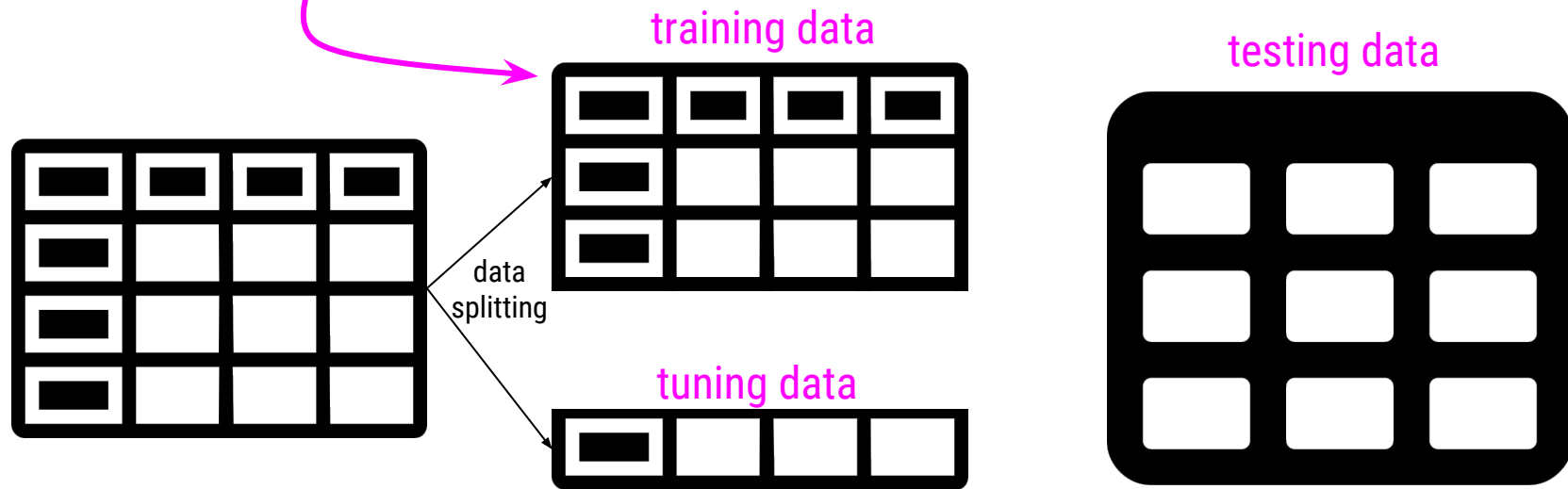
4

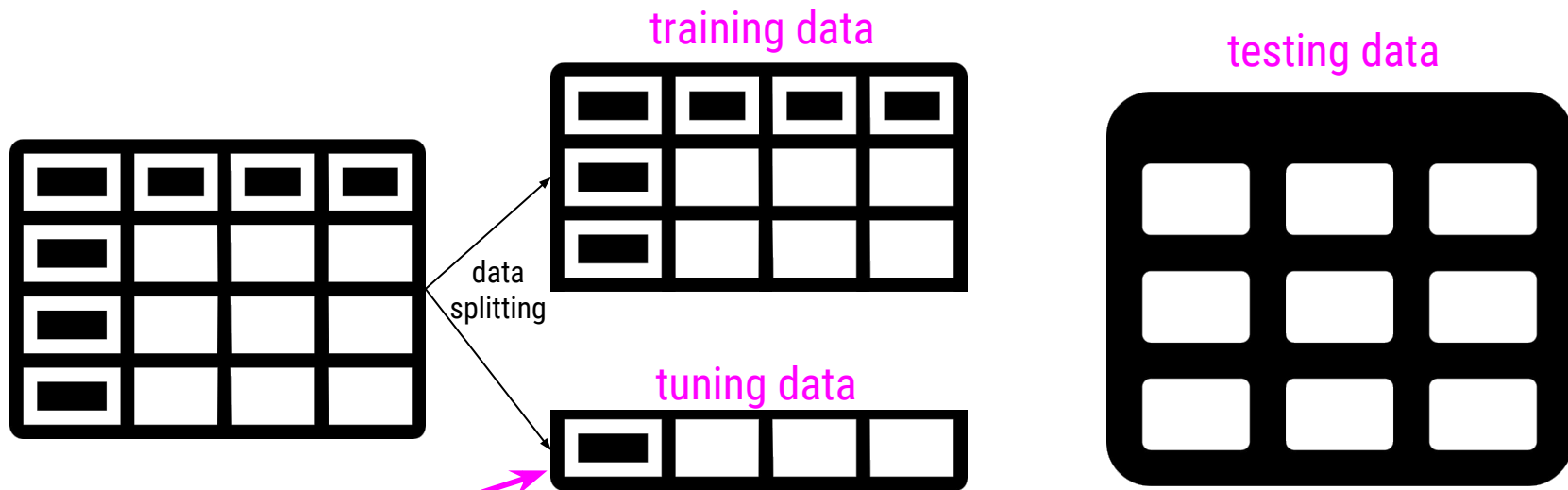


14



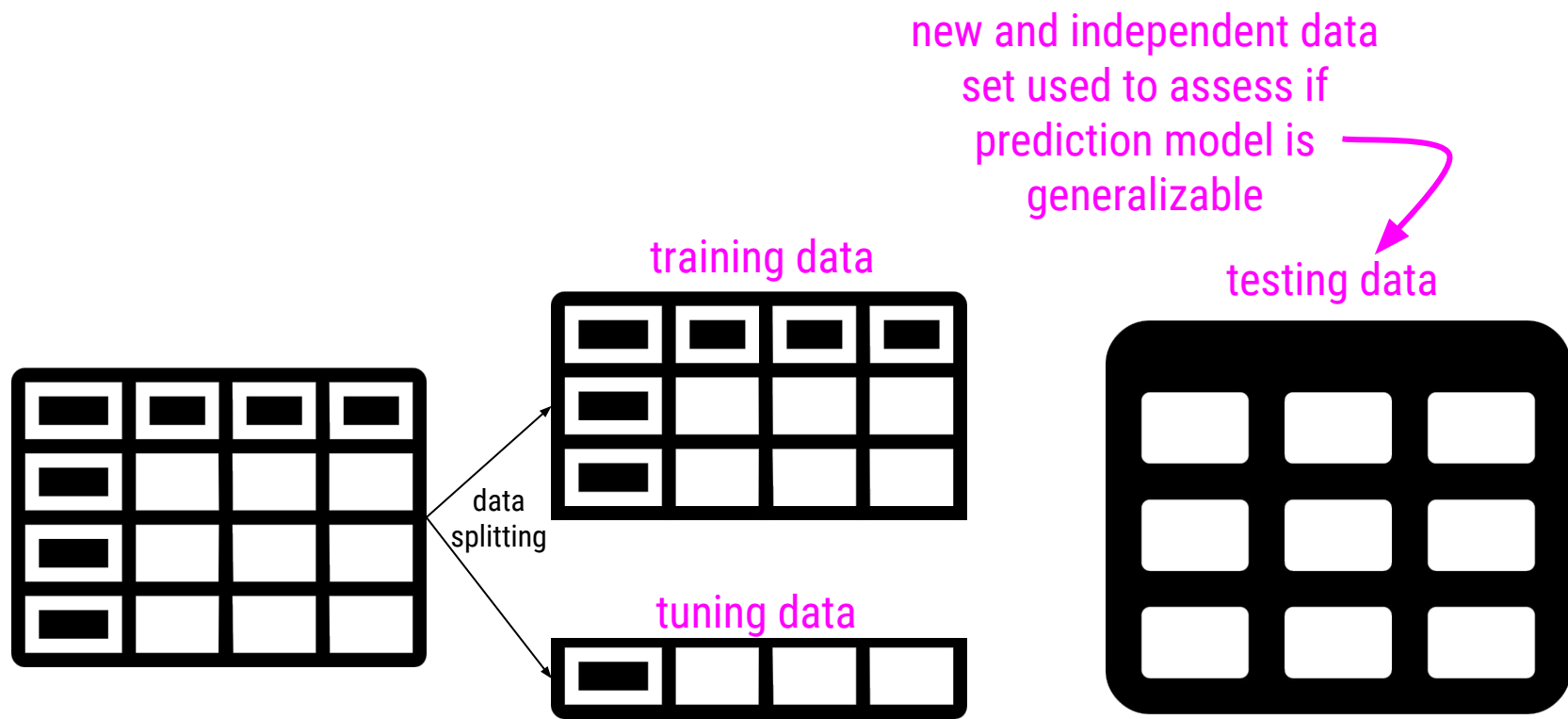
the data used to
build your predictive
model

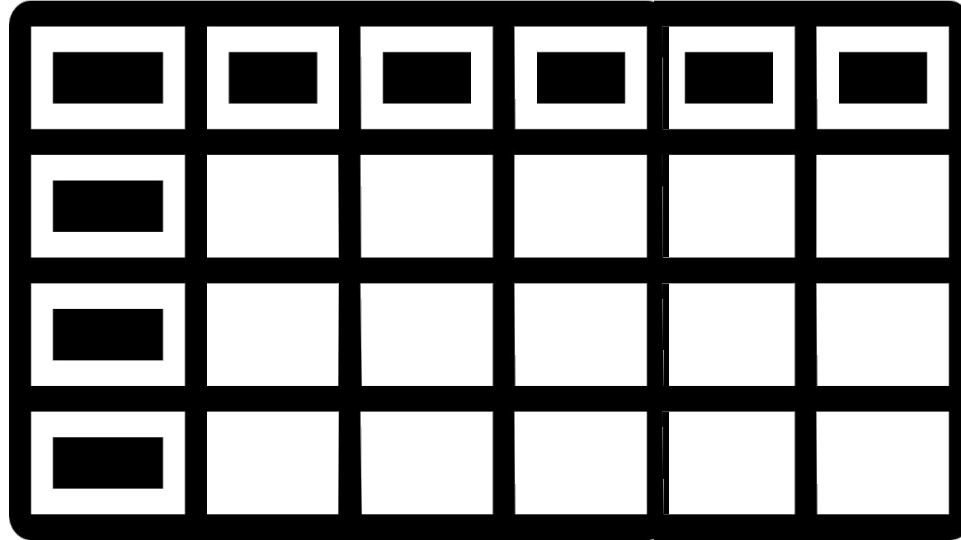




Data from original dataset that was held out and not used in training the model ; helpful in fine-tuning prediction accuracy



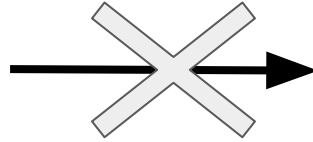
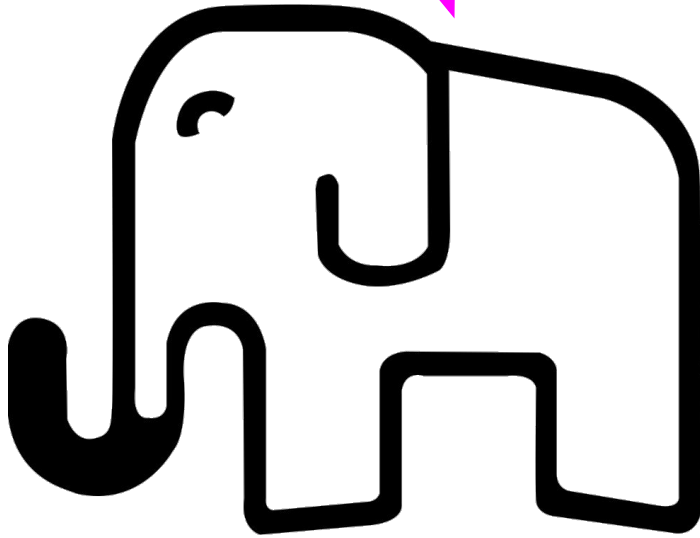


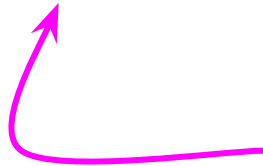
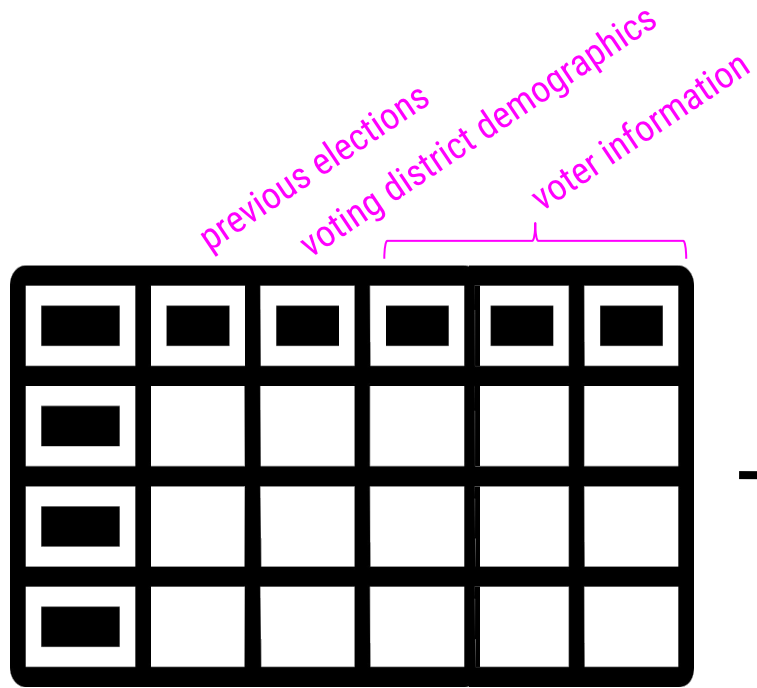


variable selection



elephant height data are
likely not predictive of US
elections

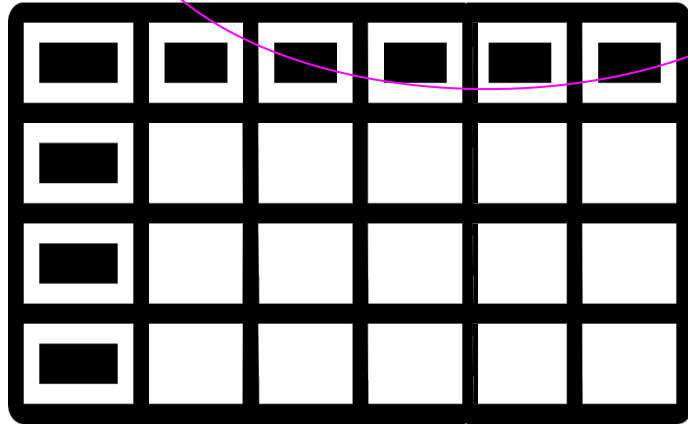




these data are likely
predictive of US election
outcomes



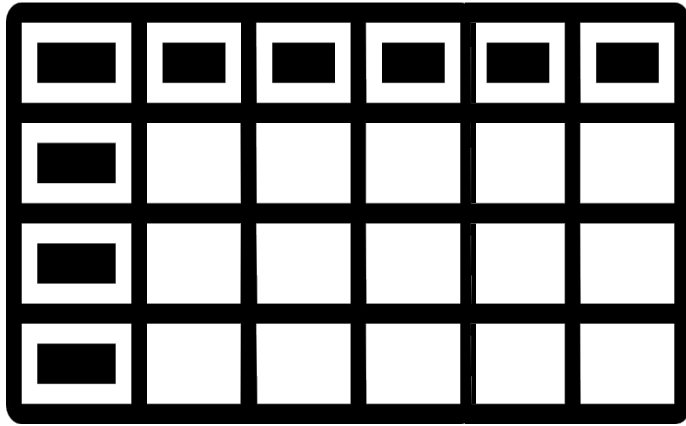
variable selection determines
which variables are most predictive
and includes them in the model



■	■	■	■	■	■
■	■	■	■	■	■
■	■	■	■	■	■
■	■	■	■	■	■

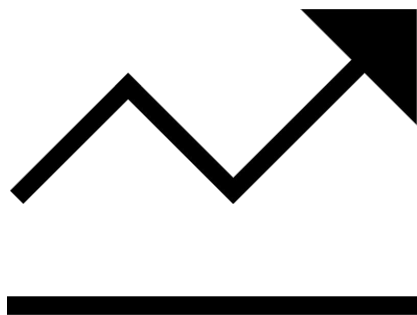
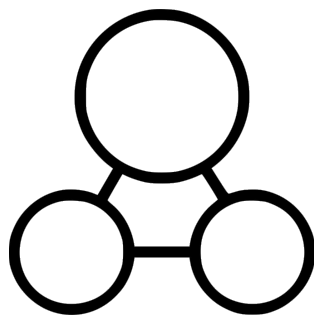
these data are likely
predictive of US election
outcomes



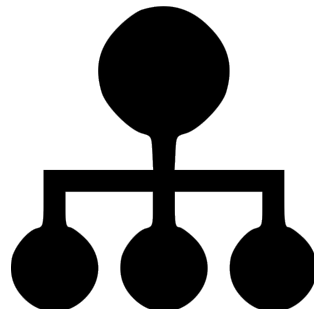


variables that can be used for accurate
prediction exploit the relationship
between the variables but do NOT mean
that one causes the other

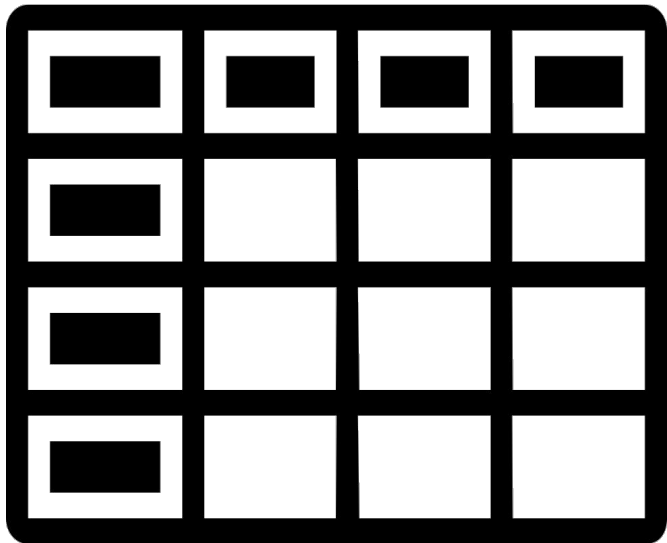




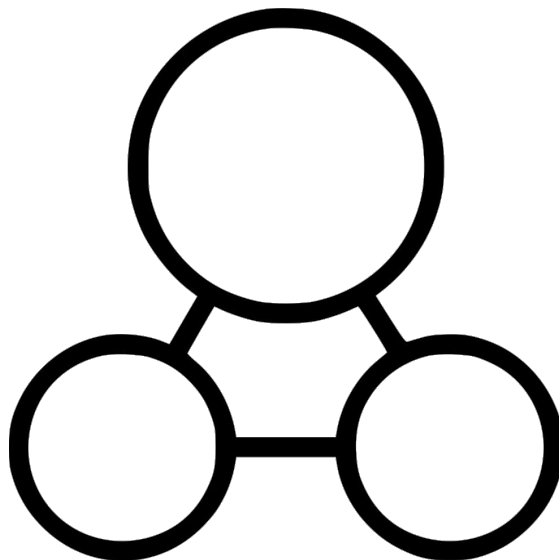
+	-
×	=



model selection

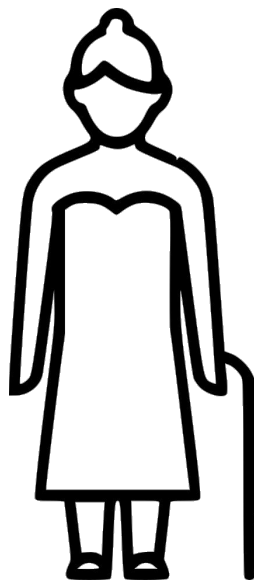


big
datasets



simple
models



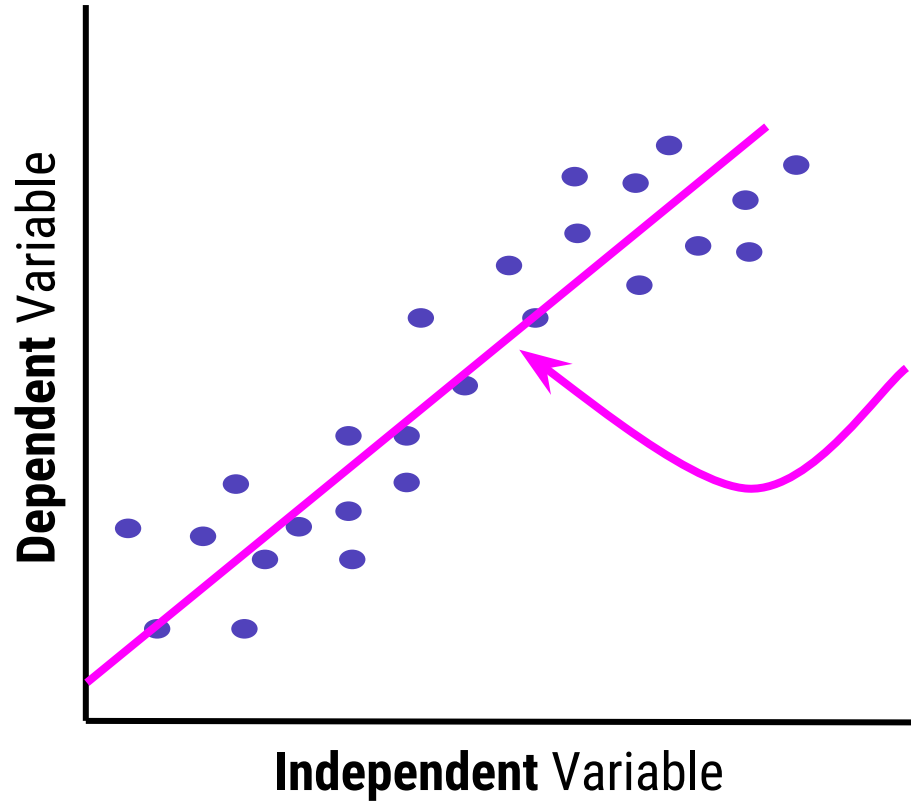


Regression:
predicting continuous
variables
(i.e. Age)



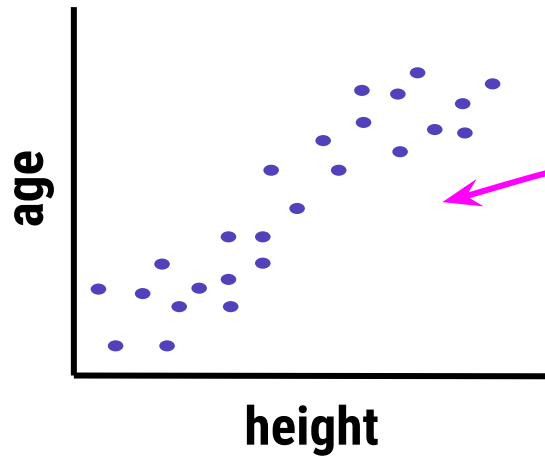
Classification:
predicting categorical
variables
(i.e. education level)





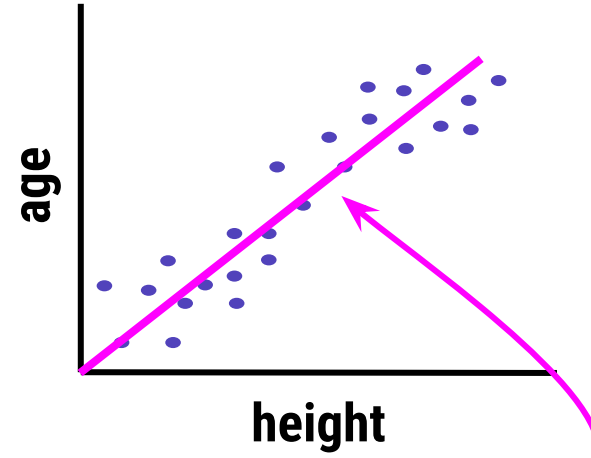
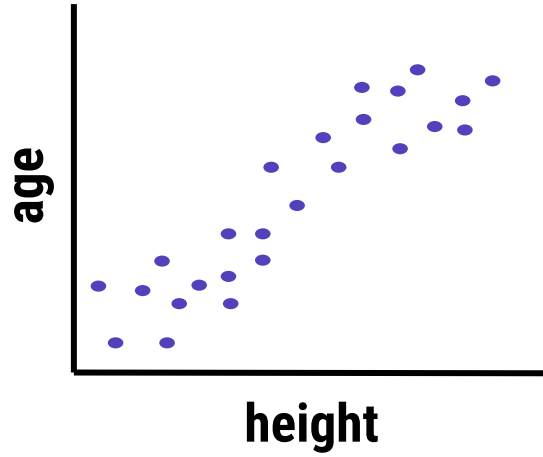
We'll use the
linear relationship
between variables
to generate a
predictive model!





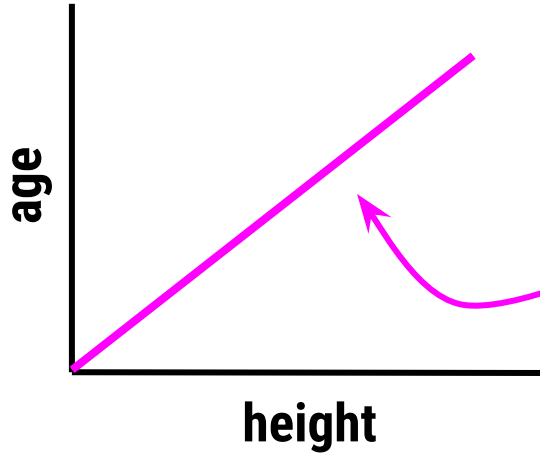
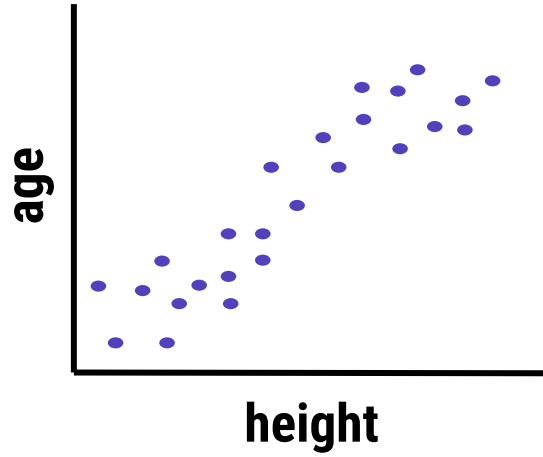
the training data
will be used to
build the
predictive model





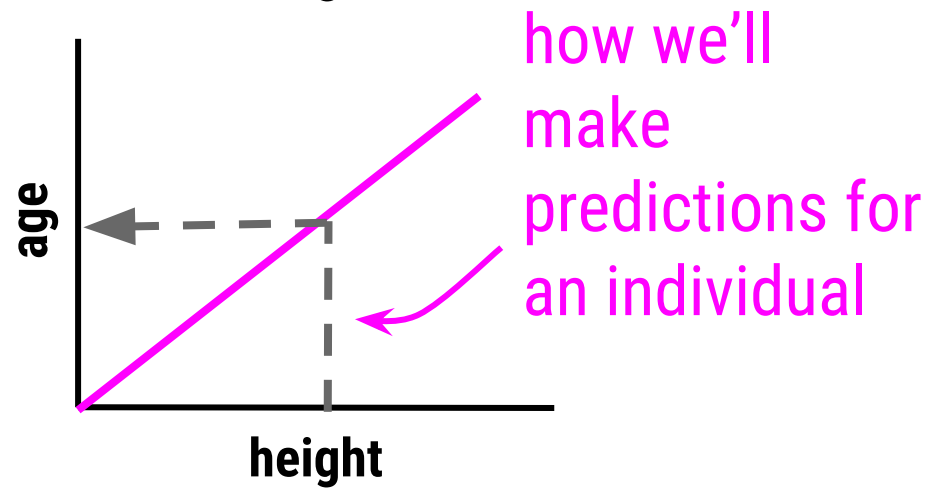
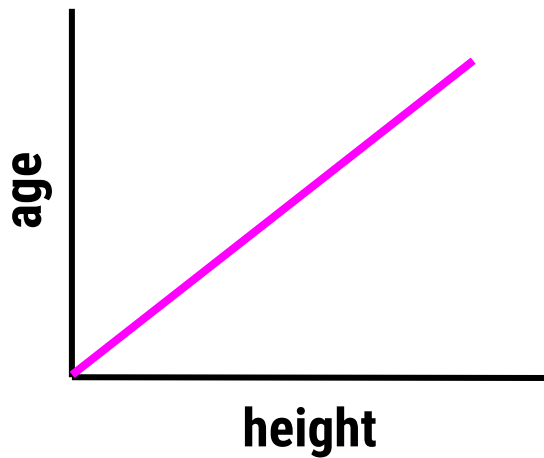
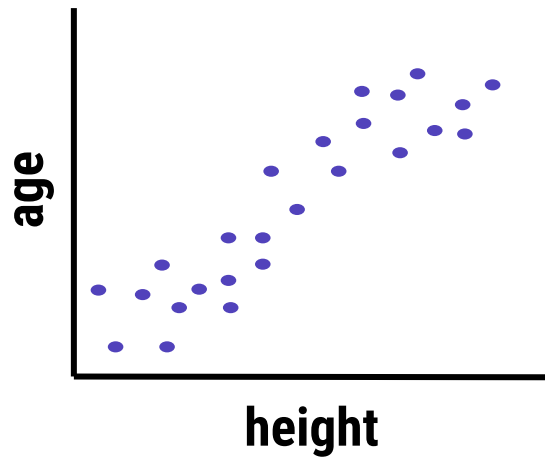
use **linear**
regression to
model the
relationship

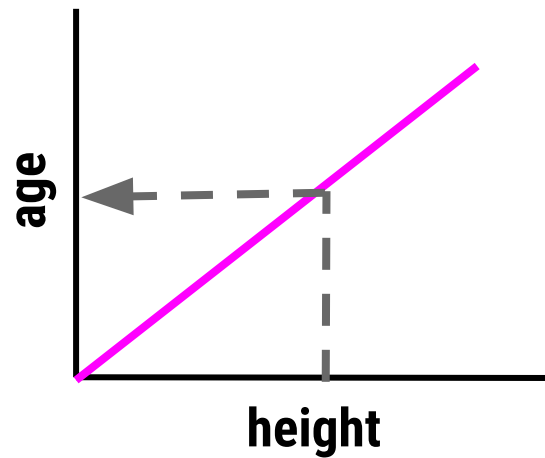
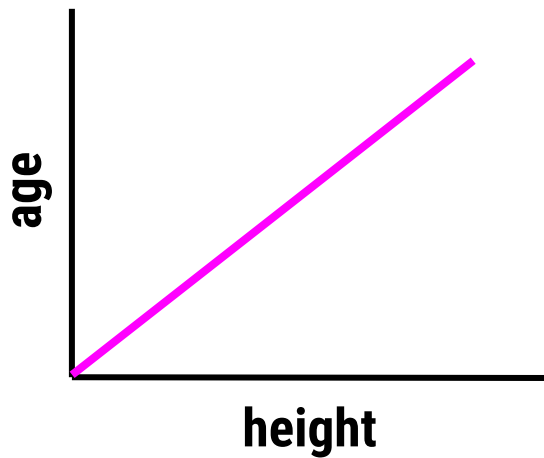
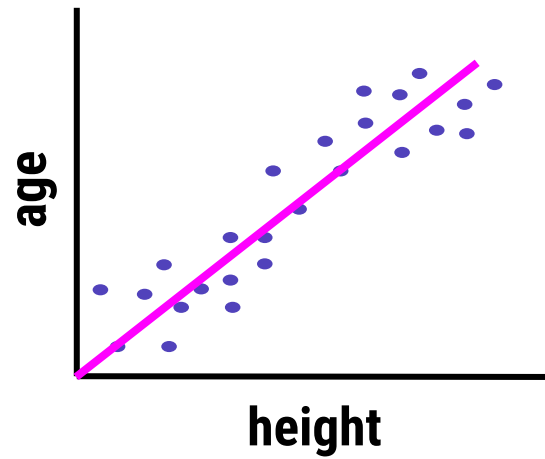
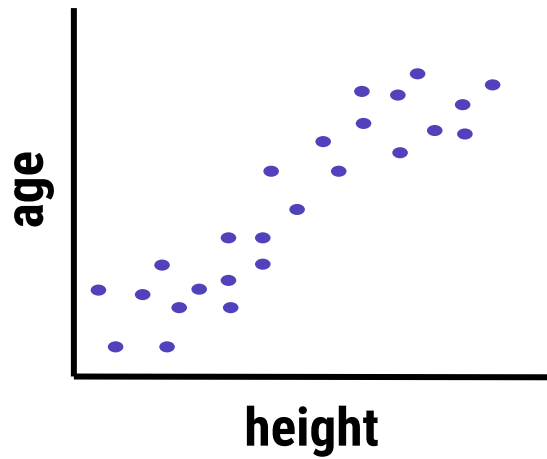




For prediction, the individual values in the training data are *not* important. We only need the model.







training data

Y

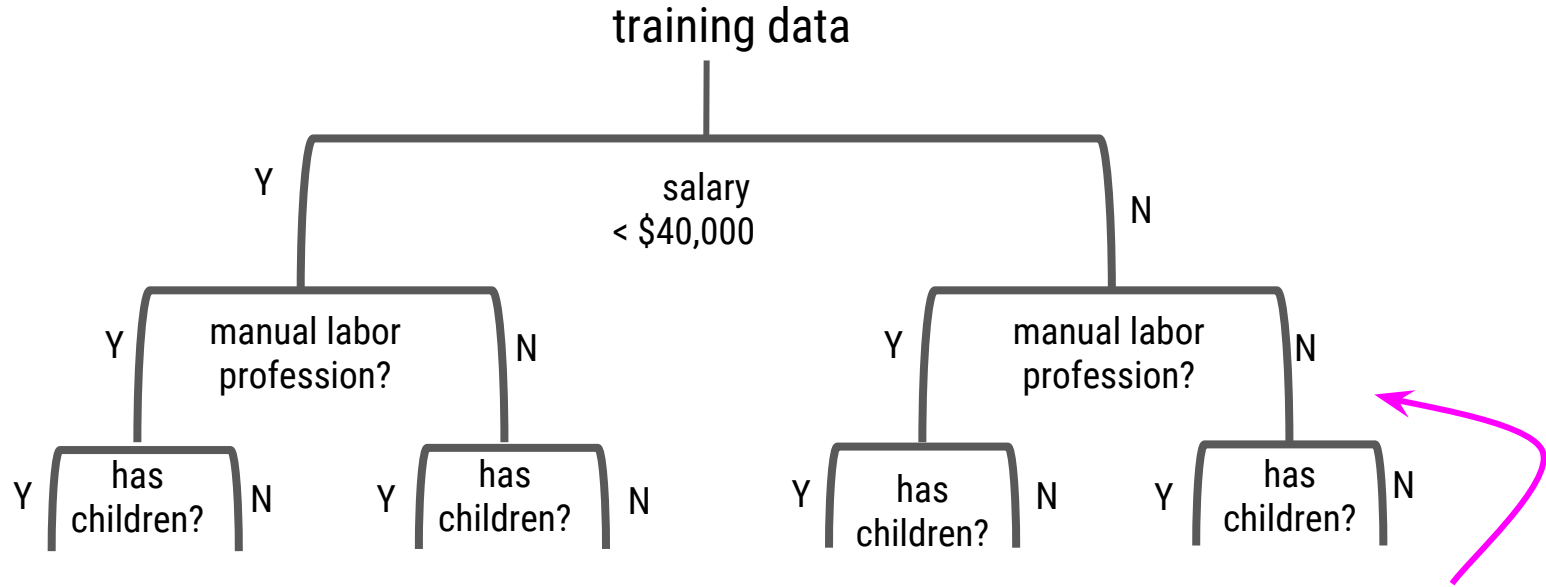
salary
< \$40,000

N

All the people
who make
less than 40K
over here

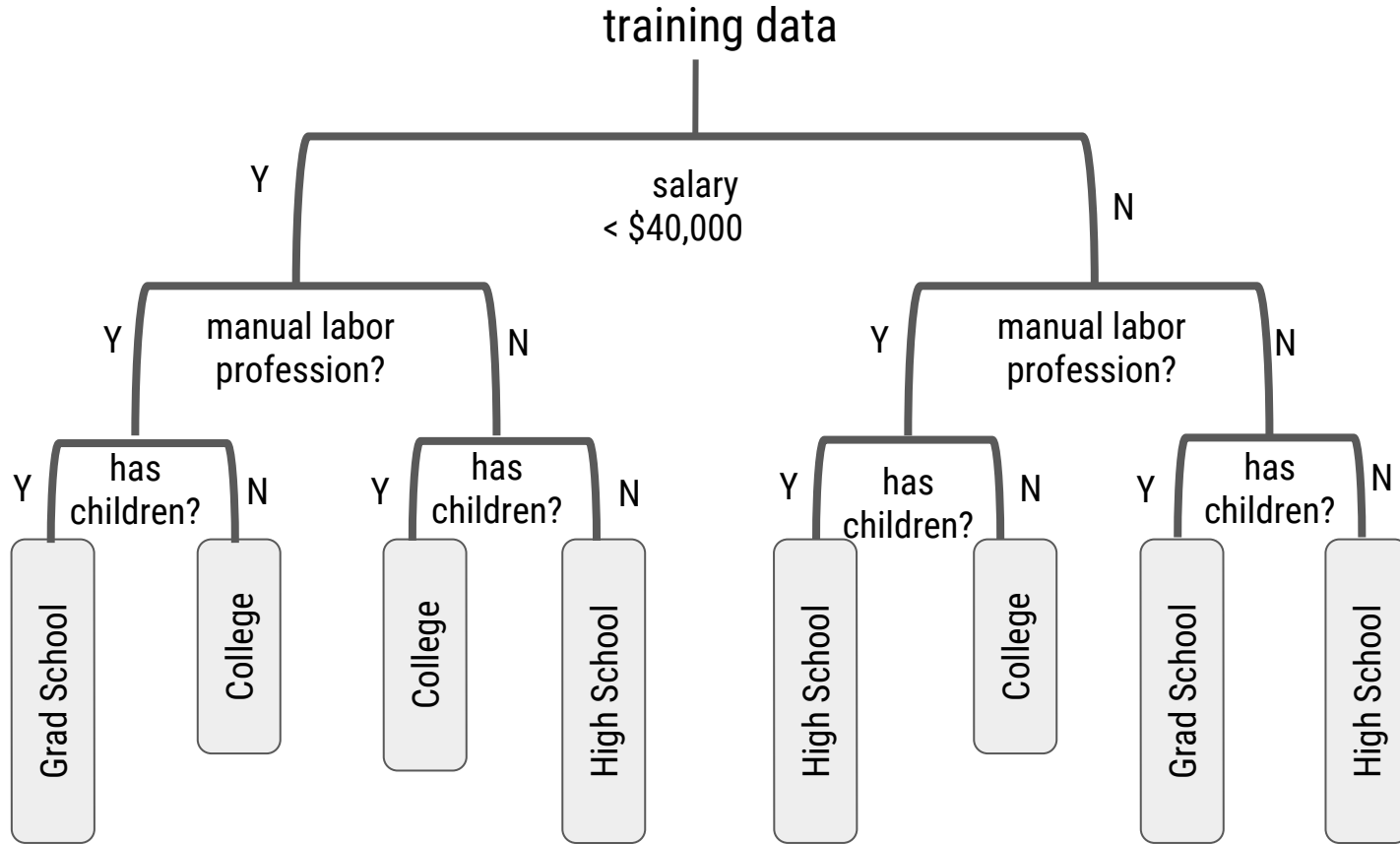
All the people
who make
more than 40K
over here



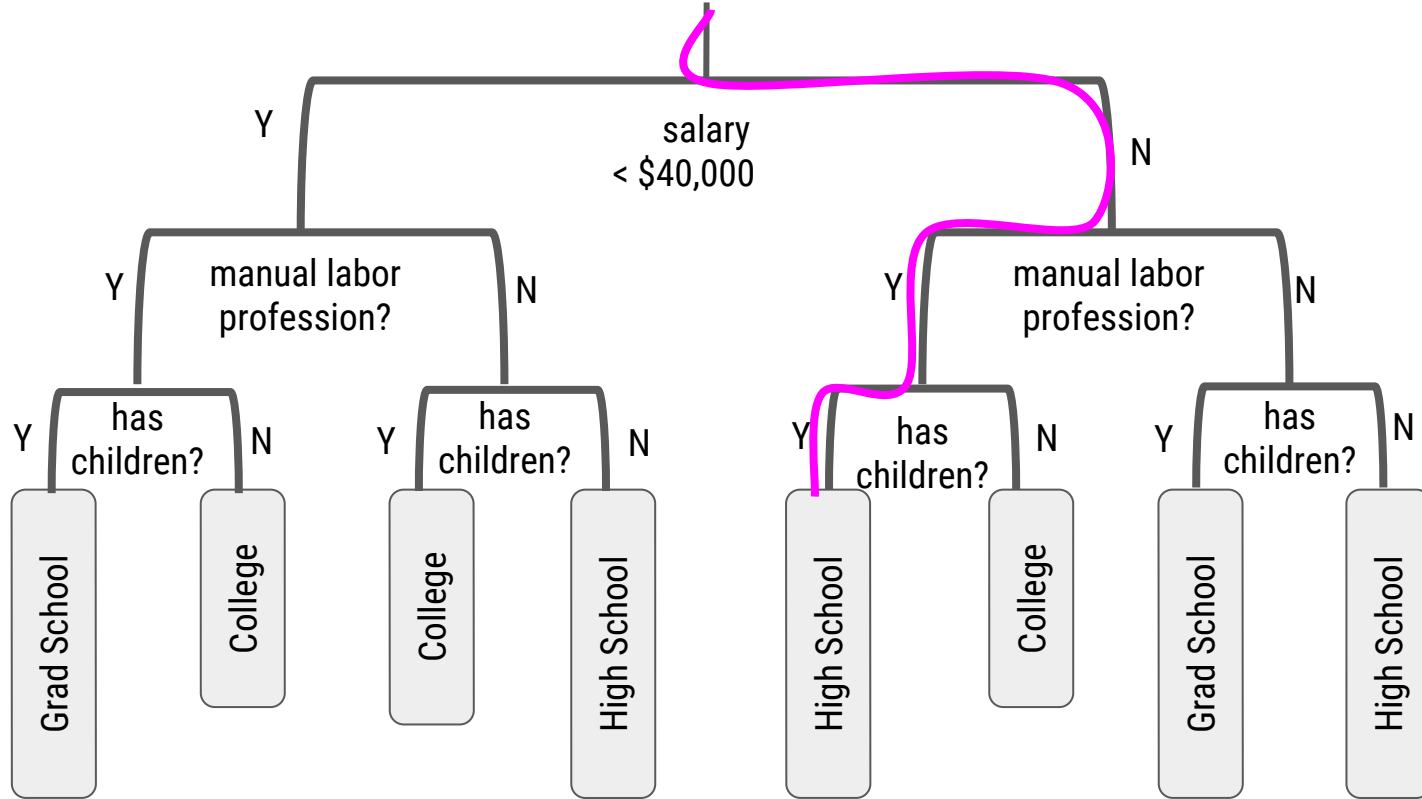


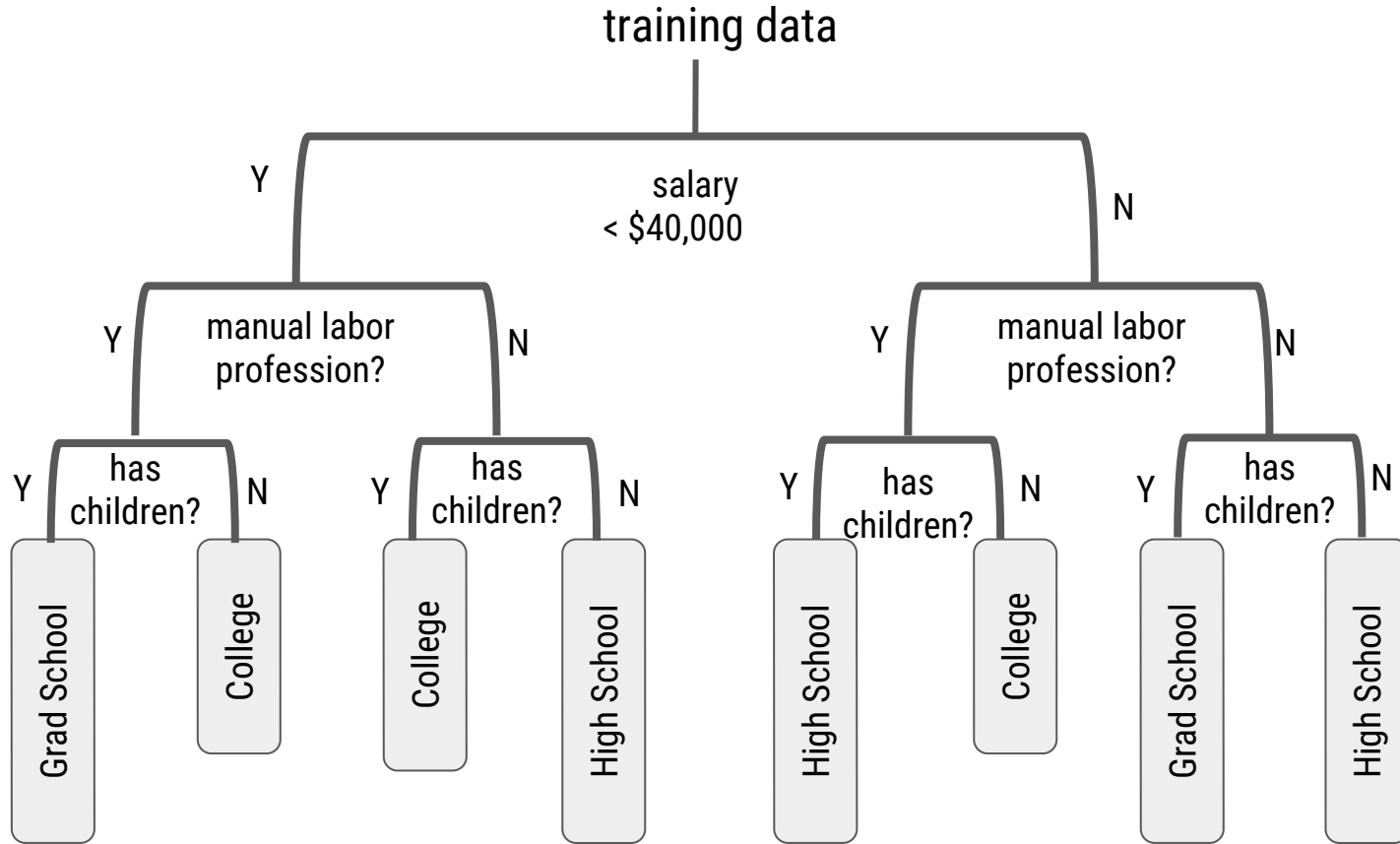
Continue building the decision tree where the variables and information in the training data decide who goes down which branch





training data







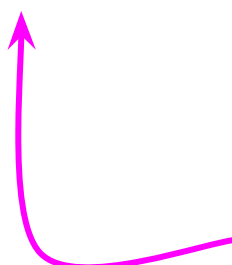
accuracy assessment



$$RMSE = \sqrt{\frac{\sum_{i=1}^N (\text{Predicted}_i - \text{Actual}_i)^2}{N}}$$



$$RMSE = \sqrt{\frac{\sum_{i=1}^N (\text{Predicted}_i - \text{Actual}_i)^2}{N}}$$



A few outliers can lead to a big increase in RMSE, even if all the other predictions are pretty good



$$\text{Accuracy} = \frac{\# \text{ of samples predicted correctly}}{\# \text{ of samples predicted}} * 100$$



1 Introduction

2 Visualizations

3 Pre-Processing

3.1 Creating Dummy Variables

3.2 Zero- and Near Zero-Variance Pr...

3.3 Identifying Correlated Predictors

3.4 Linear Dependencies

3.5 The `preProcess` Function

3.6 Centering and Scaling

3.7 Imputation

3.8 Transforming Predictors

3.9 Putting It All Together

3.10 Class Distance Calculations

4 Data Splitting

4.1 Simple Splitting Based on the O...

4.2 Splitting Based on the Predictors

4.3 Data Splitting for Time Series

4.4 Simple Splitting with Important ...

5 Model Training and Tuning

5.1 Model Training and Parameter T...



The `caret` Package

Max Kuhn

2018-05-26

1 Introduction

The `caret` package (short for `_C_lassification_A_nd_RE_gression_T_raining`) is a set of functions that attempt to streamline the process for creating predictive models. The package contains tools for:

- data splitting
- pre-processing
- feature selection
- model tuning using resampling
- variable importance estimation

as well as other functionality.

There are many different modeling functions in R. Some have different syntax for model training and/or prediction. The package started off as a way to provide a uniform interface the functions themselves, as well as a way to standardize common tasks (such parameter tuning and variable importance).

Edgar Anderson's Iris Data

Description

This famous (Fisher's or Anderson's) iris data set gives the measurements in centimeters of the variables sepal length and width and petal length and width, respectively, for 50 flowers from each of 3 species of iris. The species are *Iris setosa*, *versicolor*, and *virginica*.

Usage

```
iris  
iris3
```

Format

`iris` is a data frame with 150 cases (rows) and 5 variables (columns) named `Sepal.Length`, `Sepal.Width`, `Petal.Length`, `Petal.Width`, and `Species`.

`iris3` gives the same data arranged as a 3-dimensional array of size 50 by 4 by 3, as represented by S-PLUS. The first dimension gives the case number within the species subsample, the second the measurements with names `Sepal L.`, `Sepal W.`, `Petal L.`, and `Petal W.`, and the third the species.

Source

Fisher, R. A. (1936) The use of multiple measurements in taxonomic problems. *Annals of Eugenics*, **7**, Part II, 179–188.

The data were collected by Anderson, Edgar (1935). The irises of the Gaspe Peninsula, *Bulletin of the American Iris Society*, **59**, 2–5.

References

Becker, R. A., Chambers, J. M. and Wilks, A. R. (1988) *The New S Language*. Wadsworth & Brooks/Cole. (has `iris3` as `iris`.)



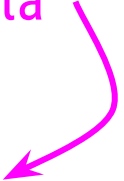
```
## install and load packages
```

```
install.packages("caret")
```

```
library(caret)
```

```
library(dplyr)
```

Specify to include 70%
of the observations in
the training data



```
## get Index for training set
```

```
set.seed(123)
```

```
trainIndex <- createDataPartition(iris$Species, p = .7,  
                                   list = FALSE,  
                                   times = 1)
```

```
## split into training and tuning set
```

```
iris_train <- iris %>% slice(trainIndex)
```

```
iris_tune <- iris %>% slice(-trainIndex)
```

```
## take a look
```

```
str(iris_train)
```

```
str(iris_tune)
```



70% of the observations
are in the *training* data

```
> str(iris_train)
```

```
'data.frame':  105 obs. of  5 variables:
 $ Sepal.Length: num  5.1 4.9 4.7 4.6 4.6 4.4 5.4 4.8 4.3 5.8 ...
 $ Sepal.Width : num  3.5 3 3.2 3.1 3.4 2.9 3.7 3 3 4 ...
 $ Petal.Length: num  1.4 1.4 1.3 1.5 1.4 1.4 1.5 1.4 1.1 1.2 ...
 $ Petal.Width : num  0.2 0.2 0.2 0.2 0.3 0.2 0.2 0.1 0.1 0.2 ...
 $ Species      : Factor w/ 3 levels "setosa","versicolor",...: 1 1 1 1 1 1 1 1 1 1 ...
```

```
> str(iris_tune)
```

```
'data.frame':  45 obs. of  5 variables:
 $ Sepal.Length: num  5 5.4 5 4.9 4.8 5.7 5.4 5.2 5.2 5.5 ...
 $ Sepal.Width : num  3.6 3.9 3.4 3.1 3.4 4.4 3.9 3.4 4.1 4.2 ...
 $ Petal.Length: num  1.4 1.7 1.5 1.5 1.6 1.5 1.3 1.4 1.5 1.4 ...
 $ Petal.Width : num  0.2 0.4 0.2 0.1 0.2 0.4 0.4 0.2 0.1 0.2 ...
 $ Species      : Factor w/ 3 levels "setosa","versicolor",...: 1 1 1 1 1 1 1 1 1 1 ...
```

30% of the observations
are in the *tuning* data




```
## train regression model  
set.seed(123)  
fit.lm <- train(Sepal.Length ~  
Sepal.Width,  
                data = iris,  
                method = "lm",  
                metric = "RMSE")
```



```
> ## look at RMSE
```

```
> fit.lm$results
```

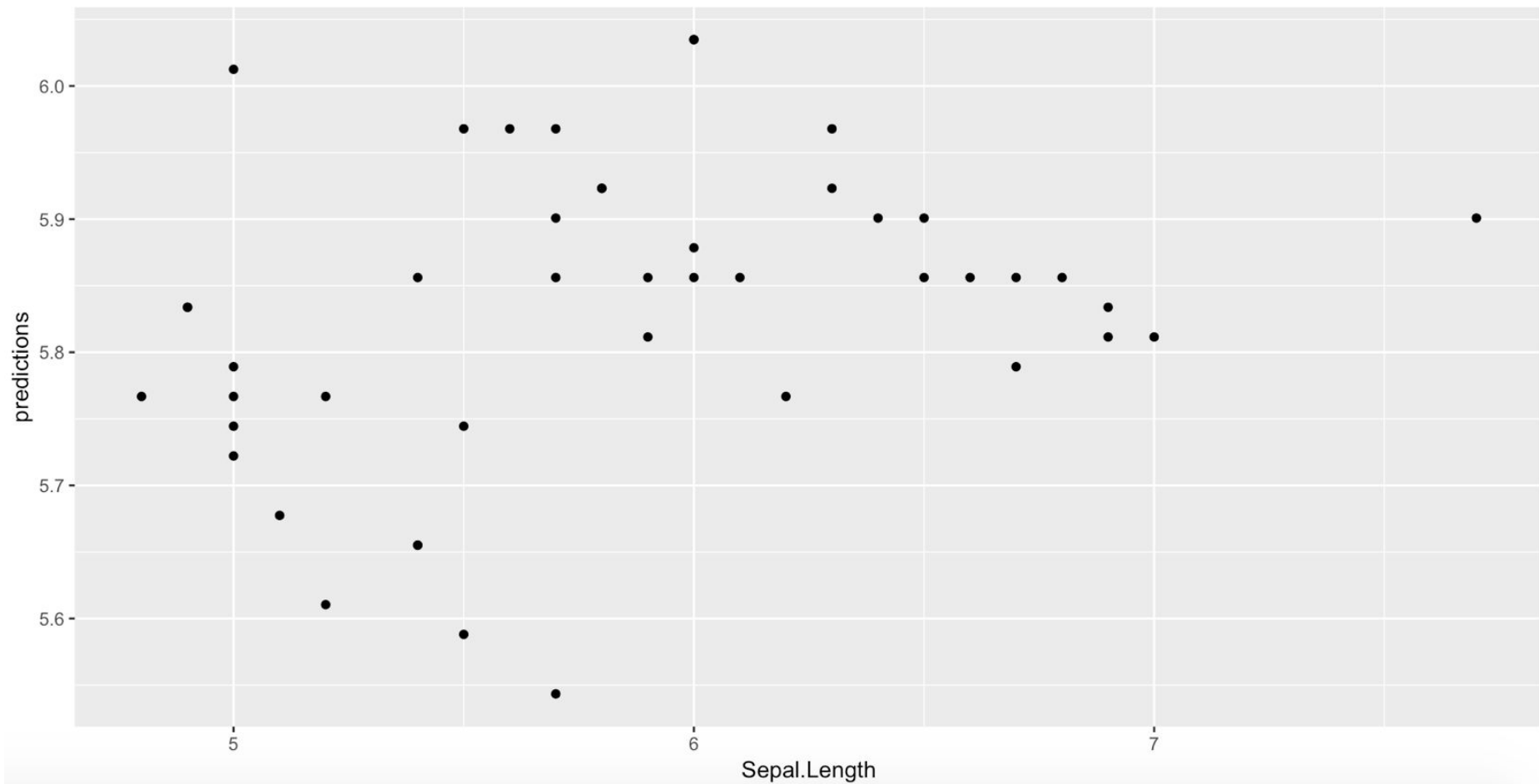
	intercept	RMSE	Rsquared	MAE	RMSESD	RsquaredSD	MAESD
1	TRUE	0.8206736	0.02384196	0.6755489	0.04703881	0.0306969	0.04749583



```
## make predictions in tuning data set
predictions <- predict(fit.lm, iris_tune)

## visualize results
iris_tune %>%
  mutate(predictions = predictions) %>%
  ggplot() +
  geom_point(aes(Sepal.Length, predictions))
```





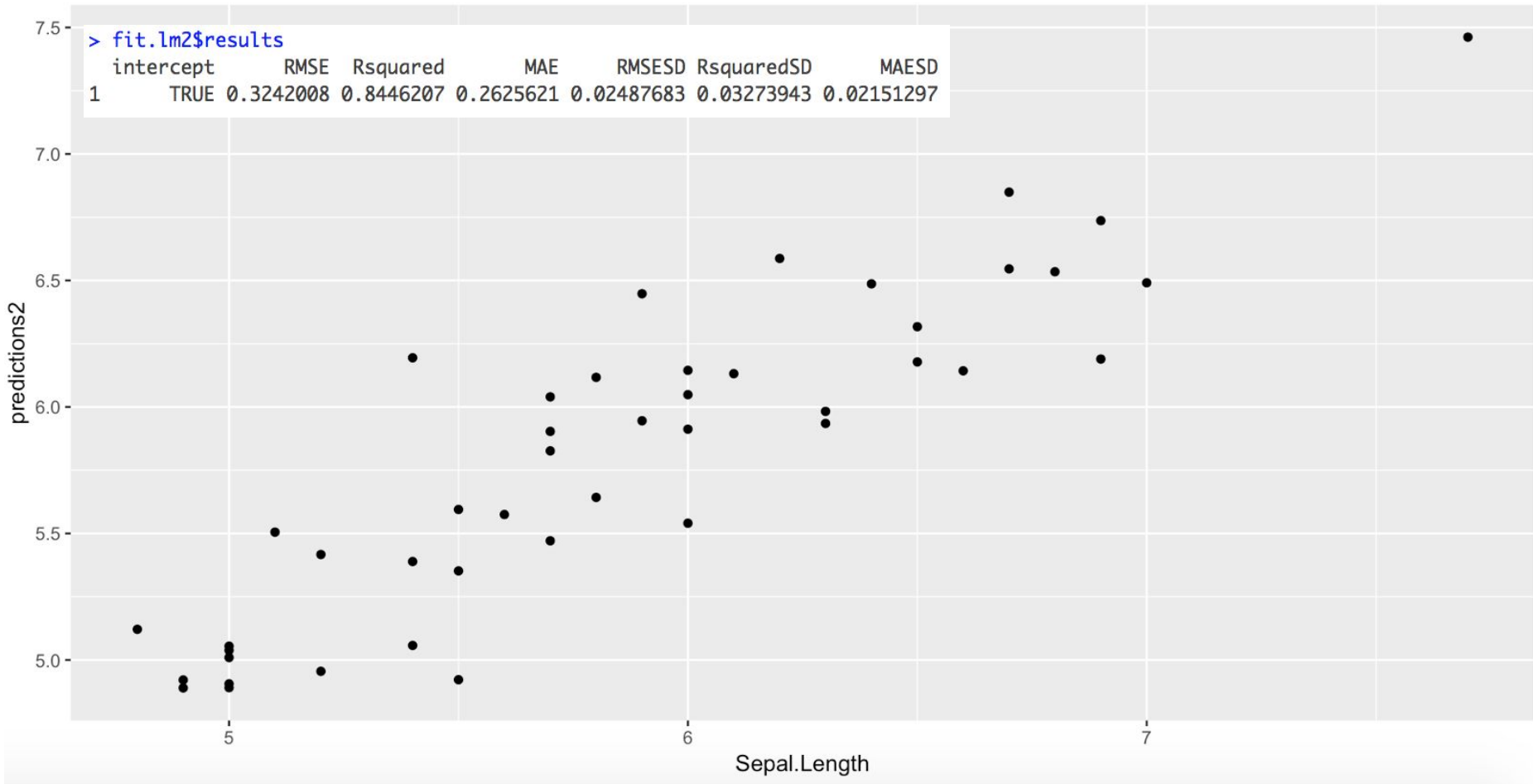
```
## train regression model
set.seed(123)
fit.lm <- train(Sepal.Length ~ .,
               data = iris,
               method = "lm",
               metric = "RMSE")

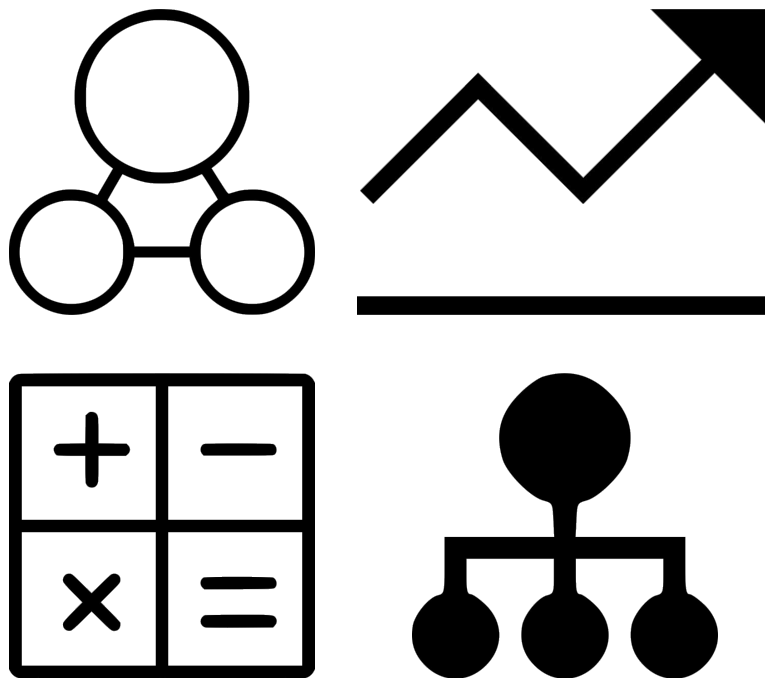
## look at RMSE
fit.lm2$results

## make predictions in tuning data set
predictions2 <- predict(fit.lm2, iris_tune)

## visualize results
iris_tune %>%
  mutate(predictions2 = predictions2) %>%
  ggplot() +
  geom_point(aes(Sepal.Length, predictions2))
```







model selection

```
## CART
```

```
set.seed(7)
```

```
fit.cart <- train(Species~.,  
                  data = iris,  
                  method = "rpart",  
                  metric = "Accuracy")
```

rpart specifies
to use a CART for
classification



```
## look at Accuracy
```

```
fit.cart$results
```

```
## make predictions in tuning data set
```

```
predictions_cart <- predict(fit.cart, iris_tune)
```



predictions

```
> table(iris_tune$Species, predictions_cart)
```

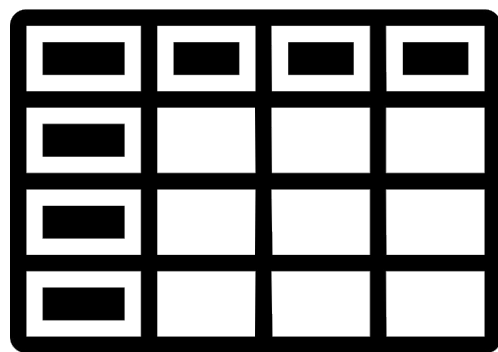
predictions_cart

setosa versicolor virginica

setosa	15	0	0
versicolor	0	14	1
virginica	0	1	14

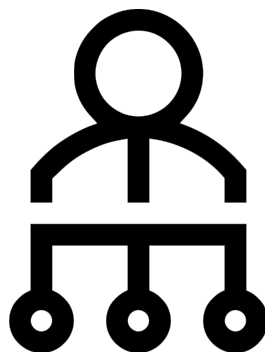
actual





data

train →



model

→ predict

