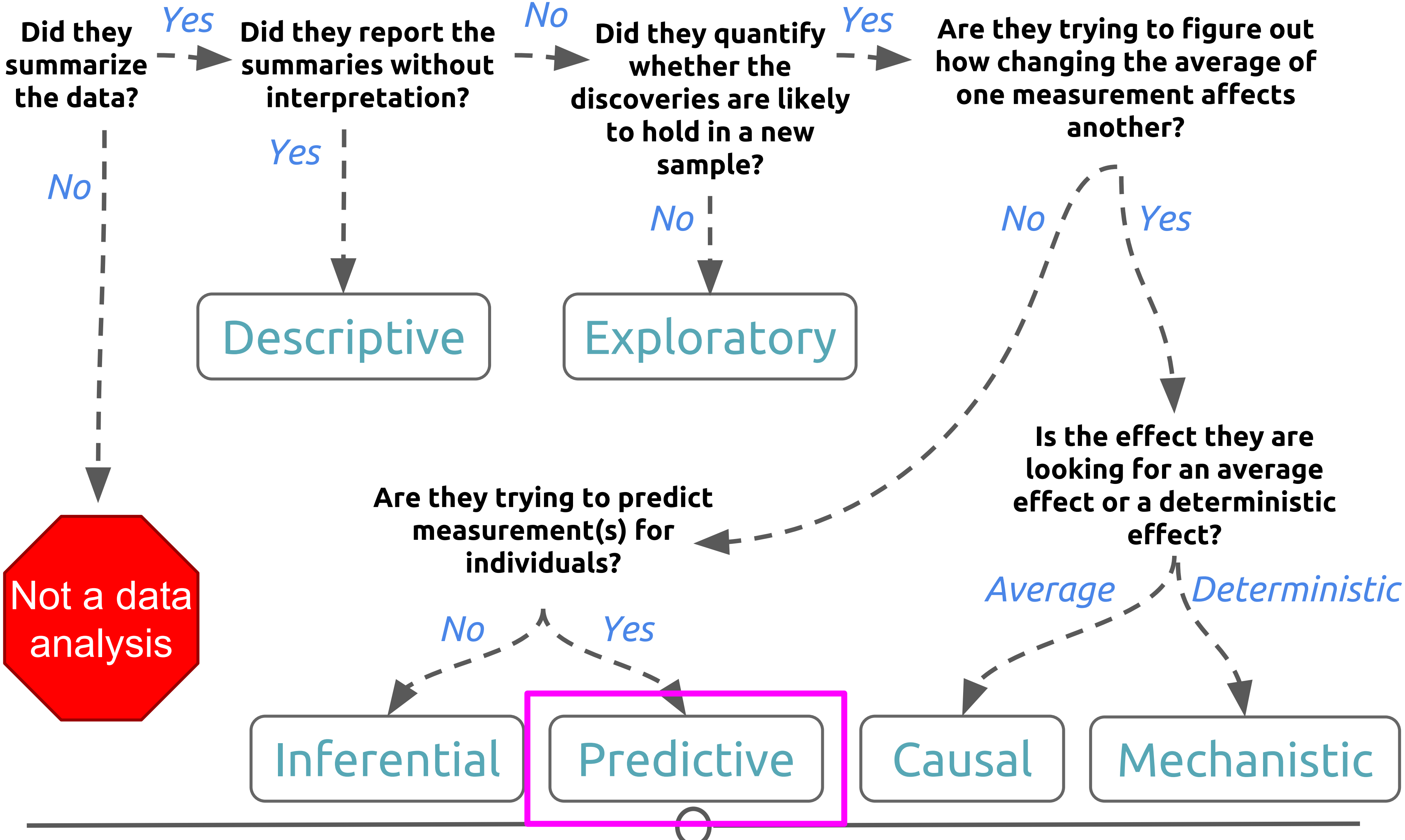
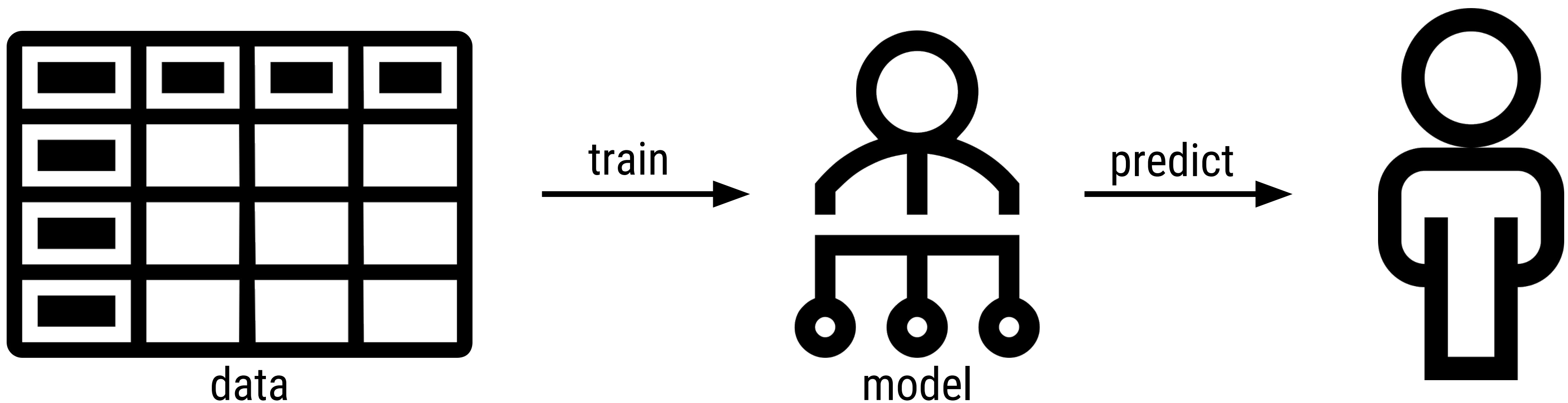
Prediction & Machine Learning

Data Analysis



http://science.sciencemag.org/content/347/6228/1314


train
predict
data
model

FiveThirtyEight

abcNEWS

Politics | Sports | Science & Health | Economics | Culture

Politics Podcast: The Far Left And The Democratic Party

THE LATEST

8:57 AM

The Rockets Are Melo's Best, Last Hope

7:20 AM

Significant Digits For Tuesday, July 24, 2018

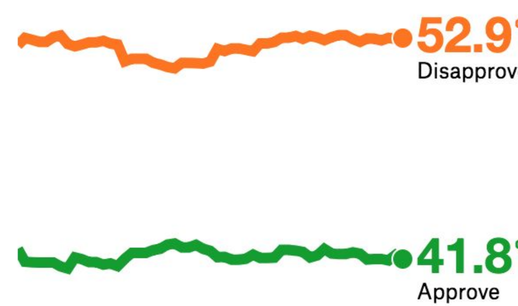
6:00 AM

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

INTERACTIVES

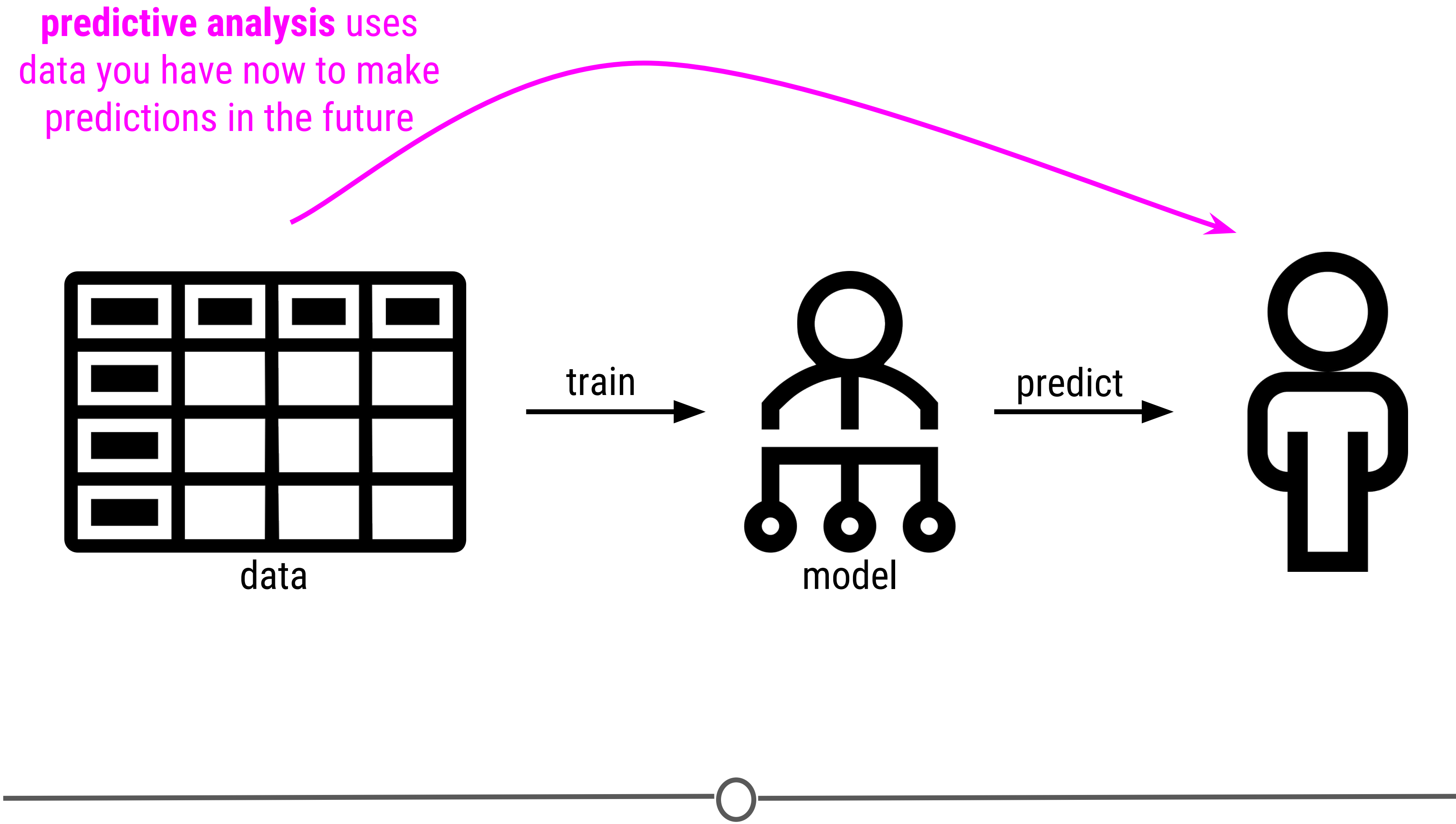
How Popular Is Donald Trump?

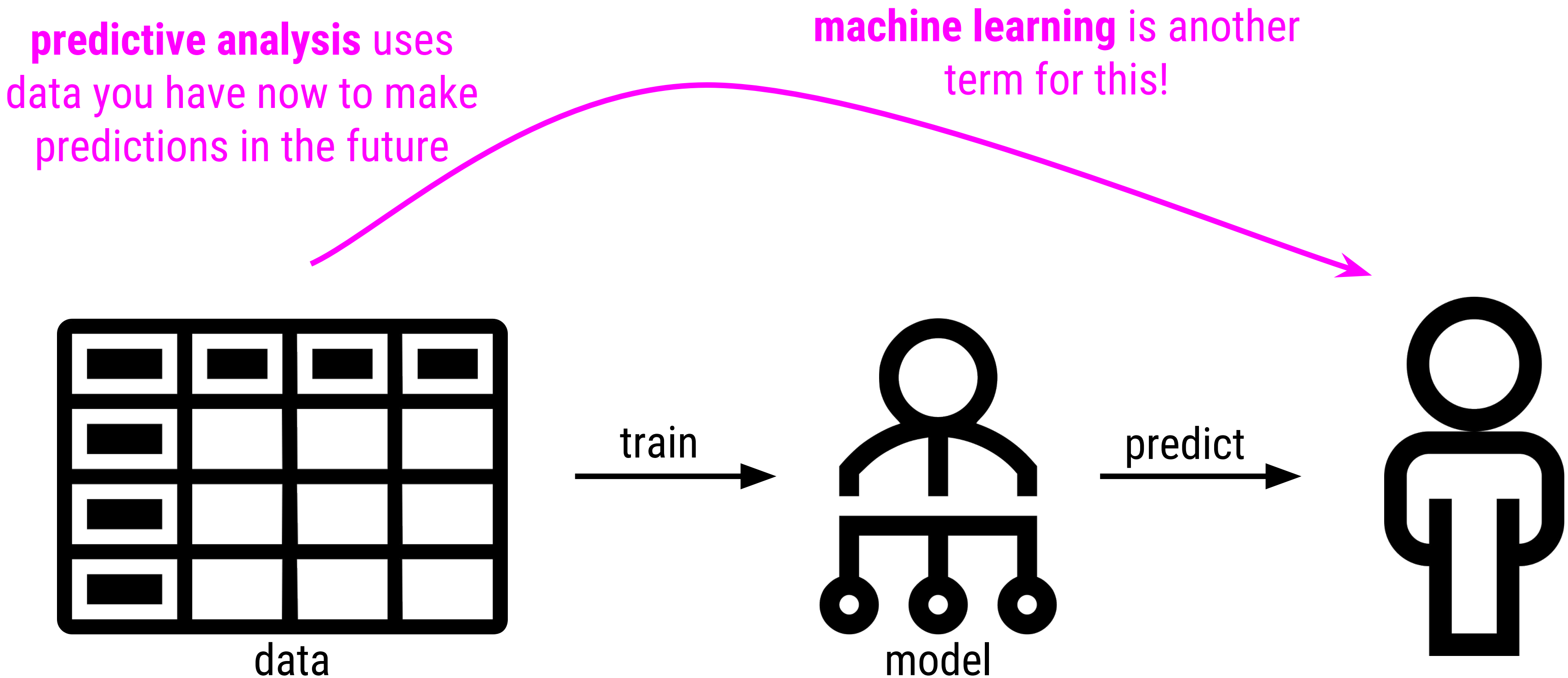
UPDATED 15 HOURS AGO



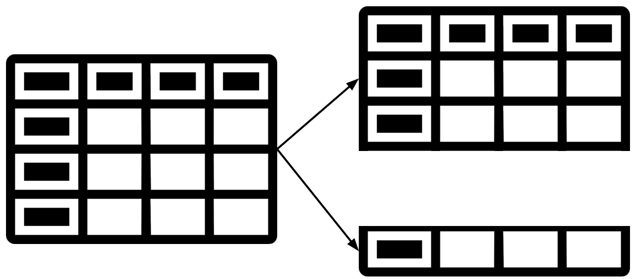
See all approval polls

https://fivethirtyeight.com/

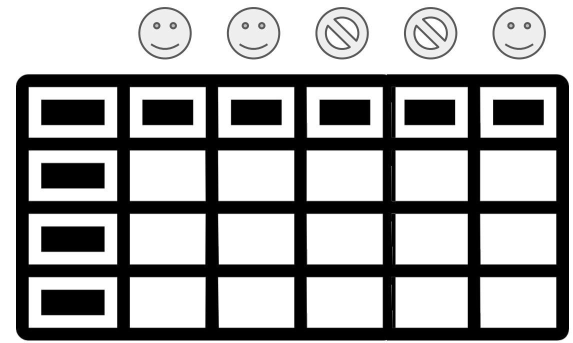

predictive analysis uses data you have now to make predictions in the future
train
predict
data
model


predictive analysis uses data you have now to make predictions in the future
machine learning is another term for this!
train
predict
data
model

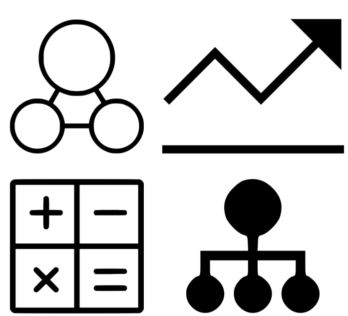
Basic Steps to Prediction



data splitting

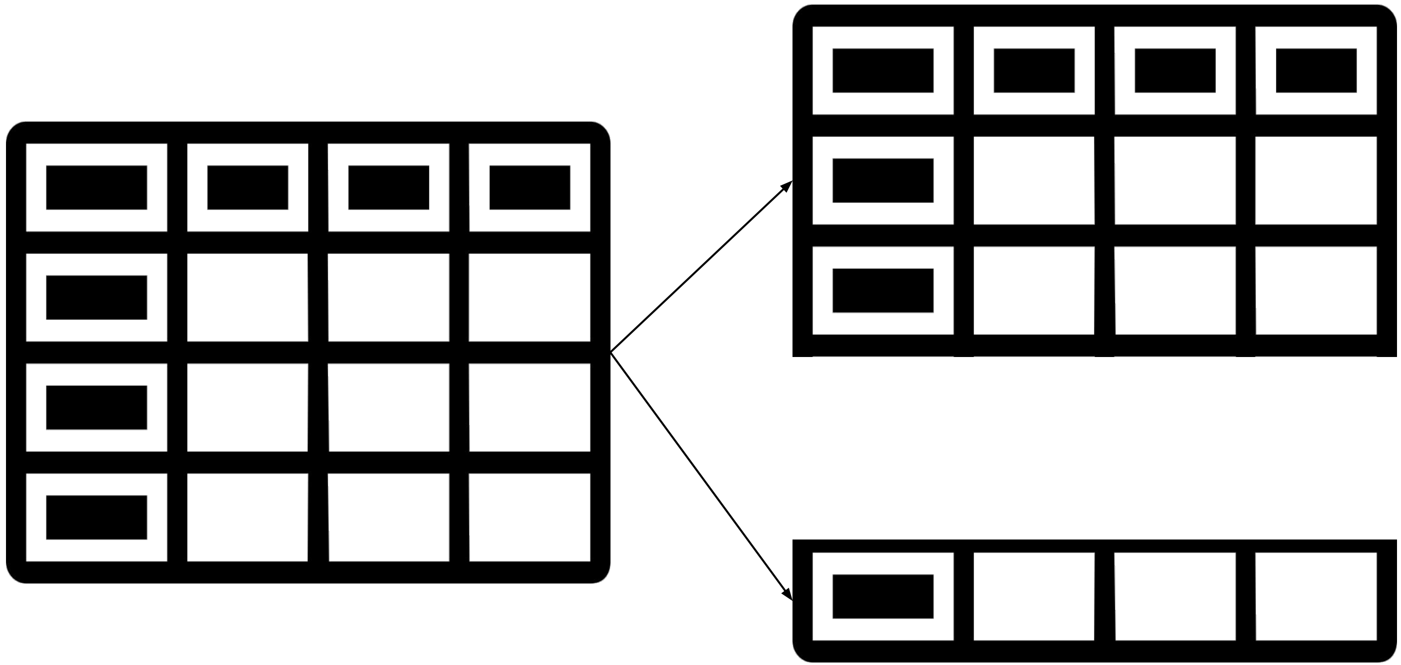


variable selection



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

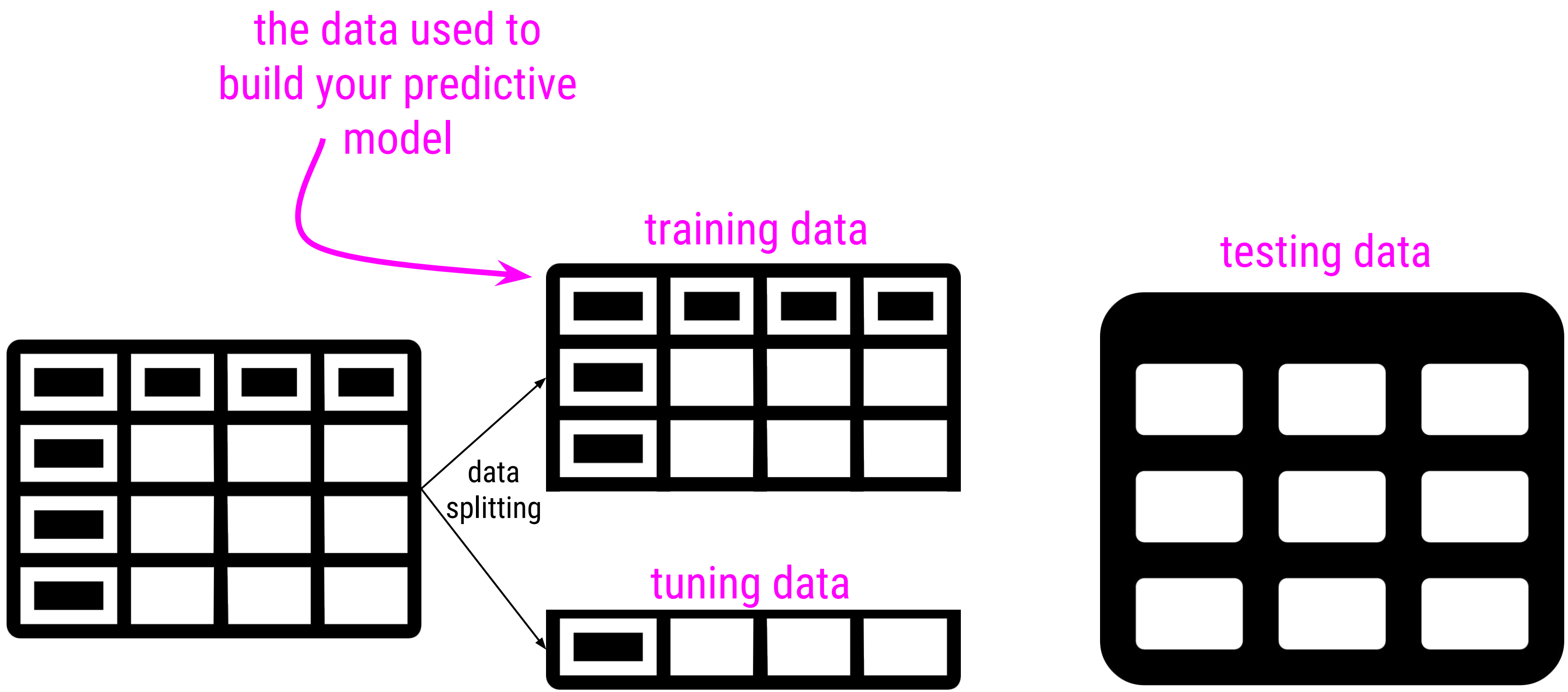
Michael Hoffman @michaelhoffman · Apr 27

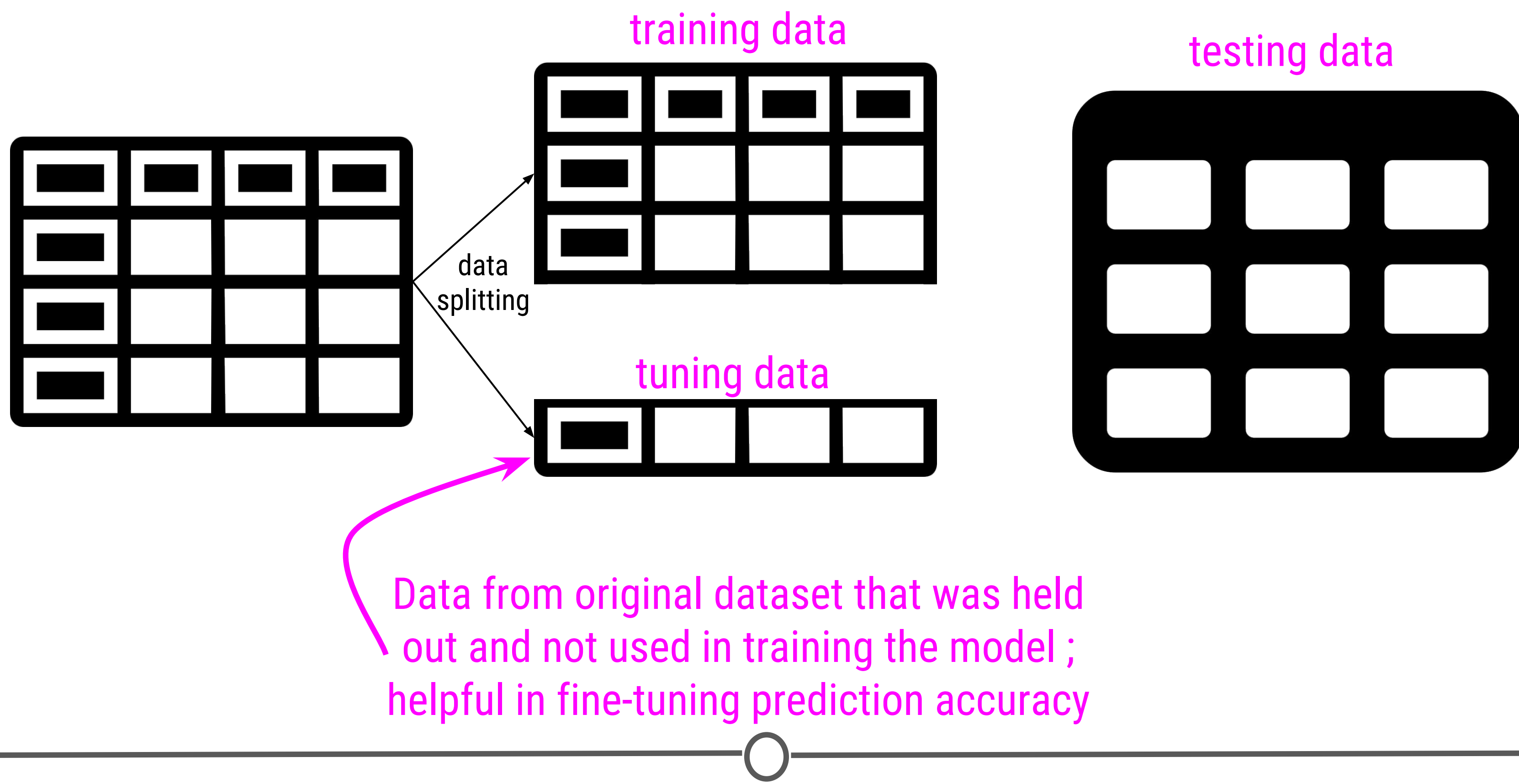
@CarldeBoerPhD suggests train, tune, test as an alternative. I think I like that. "Tune" is a better description for what goes on in the second part and it avoids the contentious and multisyllabic "validate".

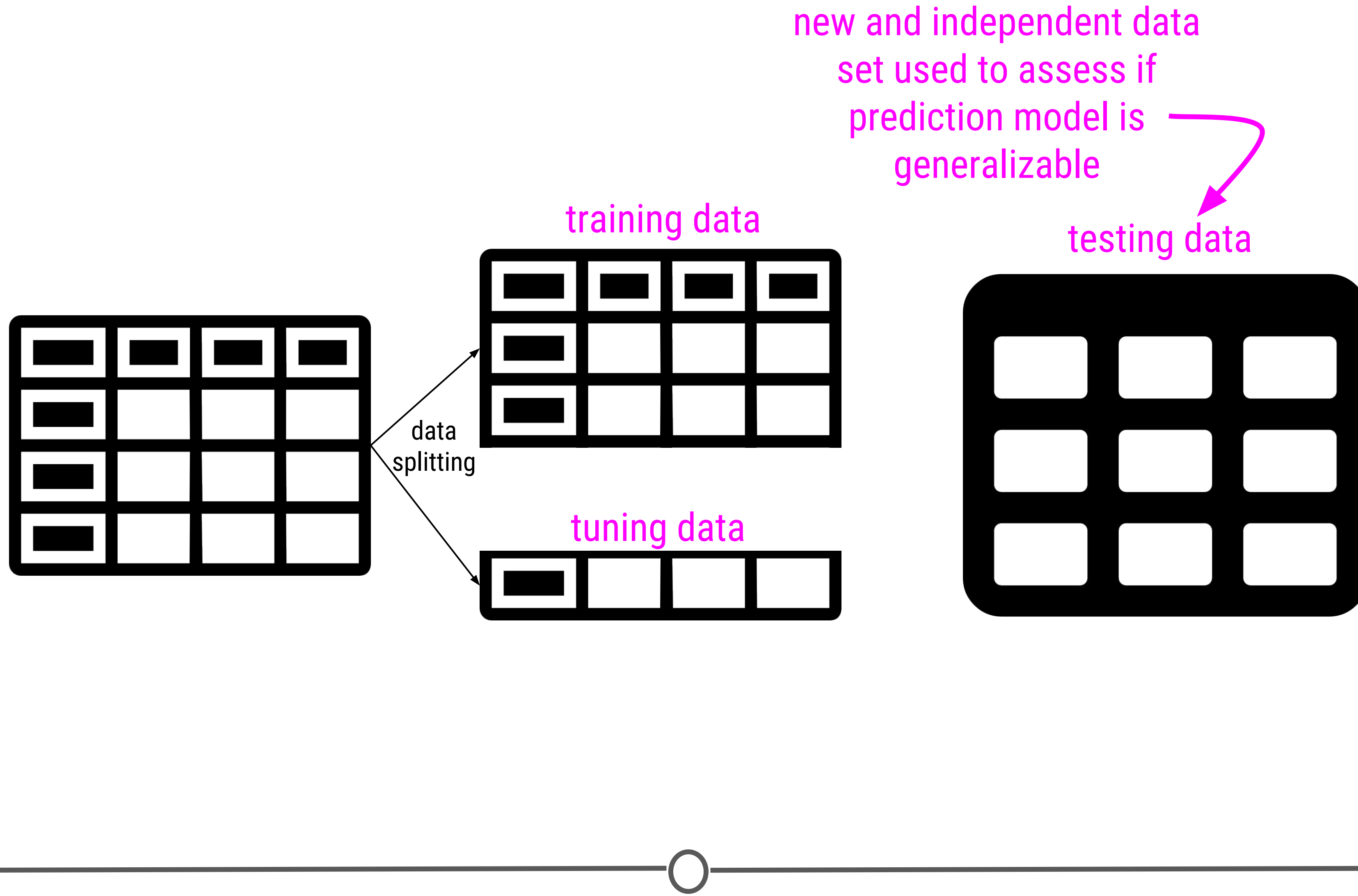
> **Carl de Boer** @CarldeBoerPhD
>
> Let's all switch to train, tune, test. Alliterative and descriptive. Alliterscriptive.

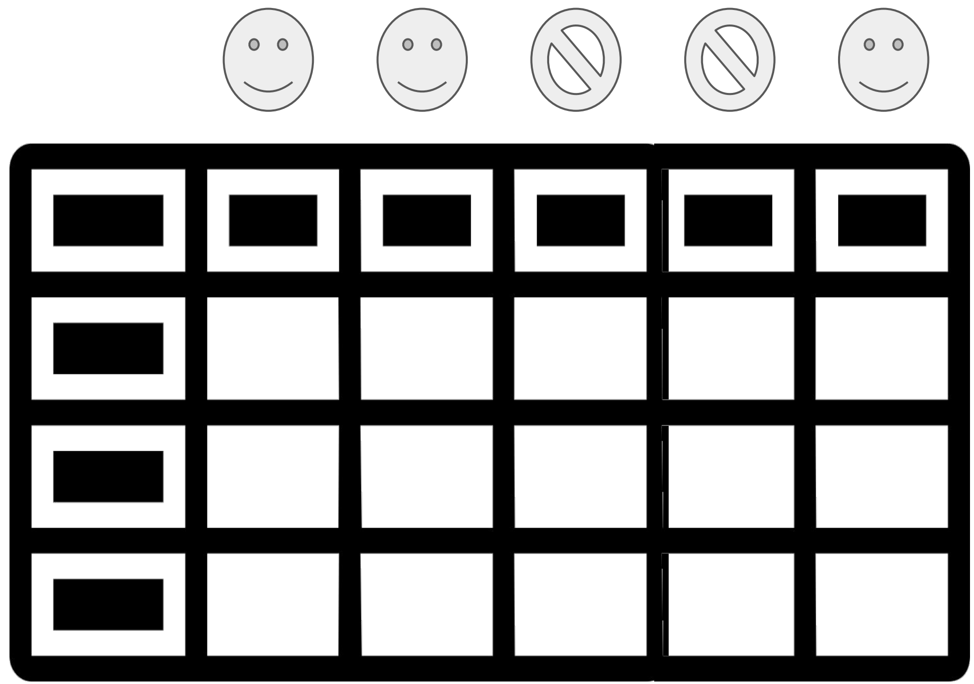
we'll go with **train, tune, test** instead

2 4 14

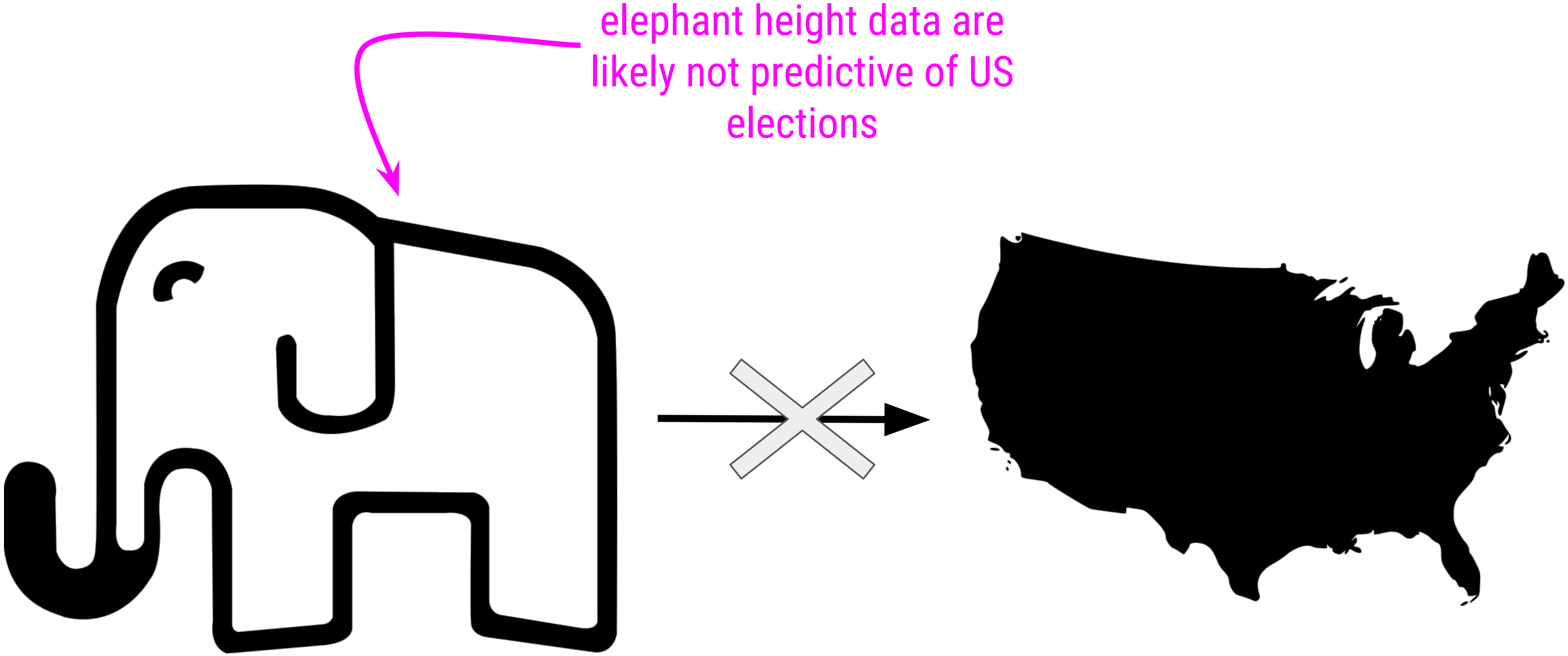

the data used to build your predictive model
training data
data splitting
tuning data
testing data

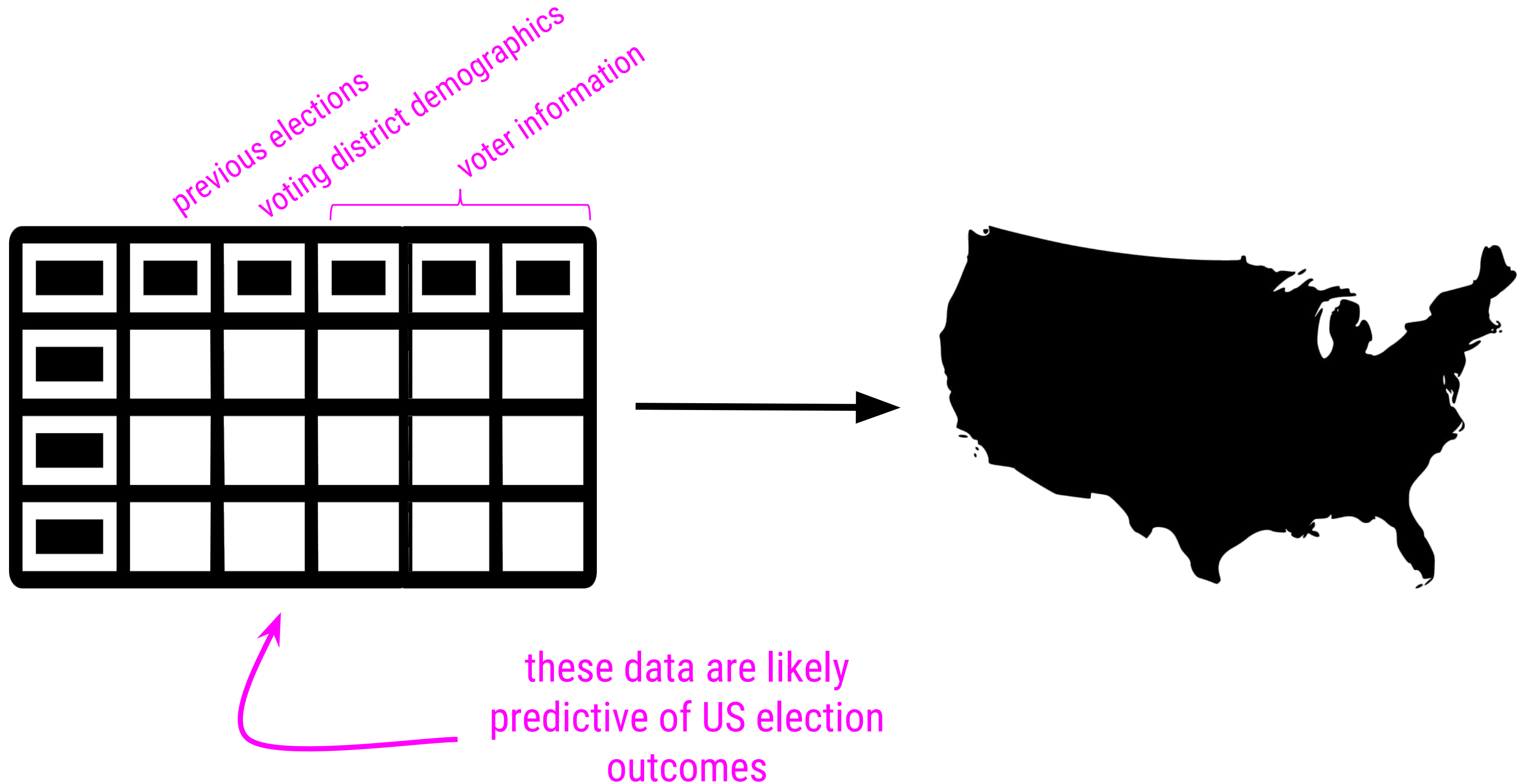

training data
testing data
data
splitting
tuning data
Data from original dataset that was held
out and not used in training the model ;
helpful in fine-tuning prediction accuracy

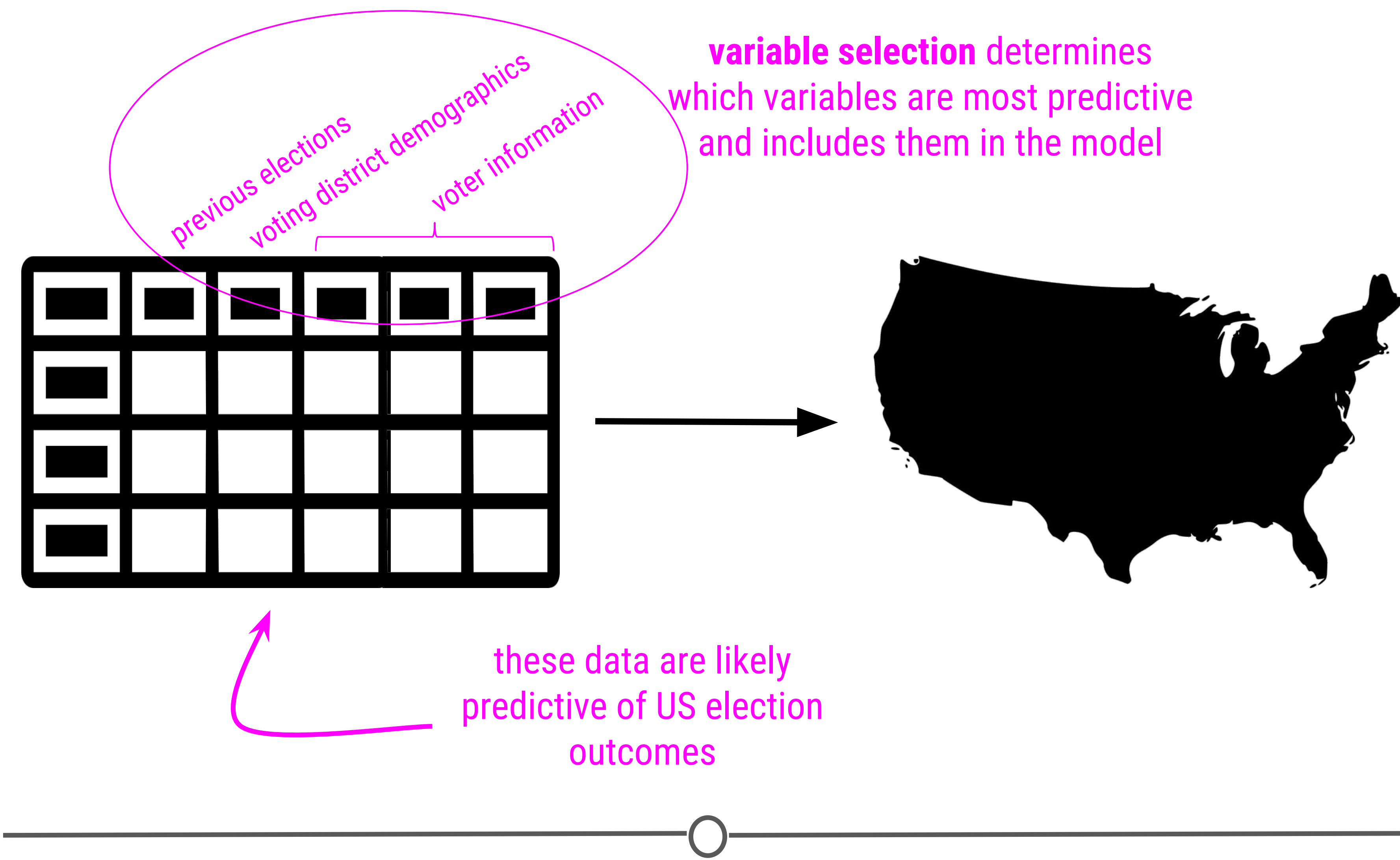

new and independent data set used to assess if prediction model is generalizable
training data
data splitting
tuning data
testing data

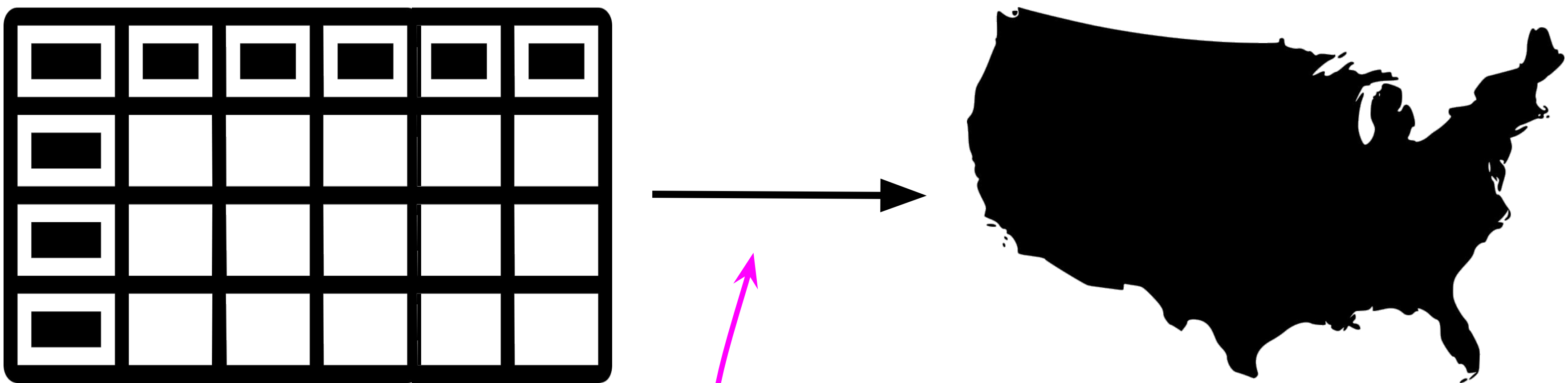


variable selection

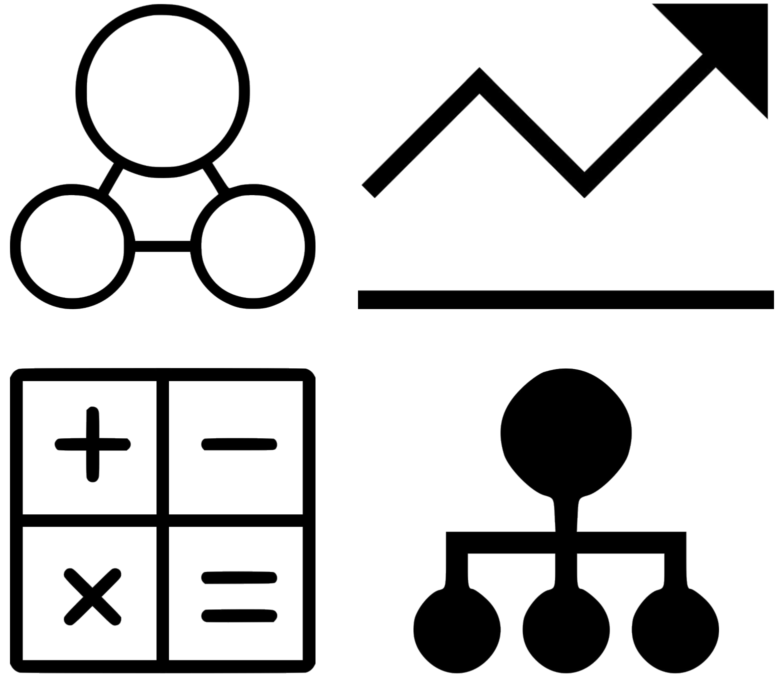

elephant height data are likely not predictive of US elections


previous elections
voting district demographics
voter information
these data are likely predictive of US election outcomes

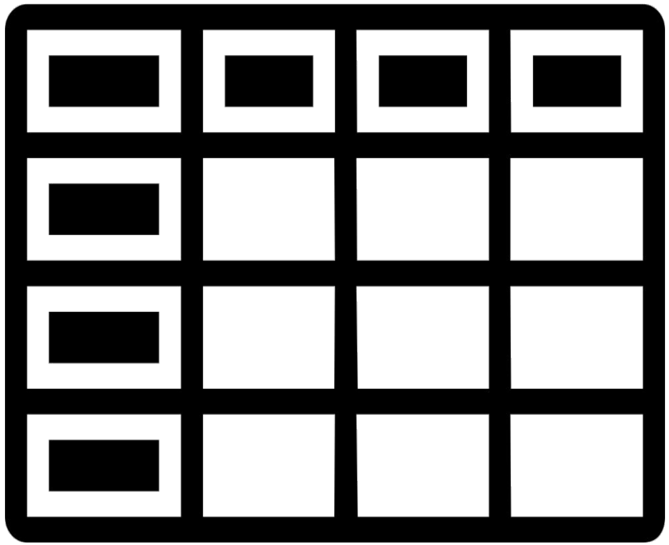

previous elections
voting district demographics
voter information
variable selection determines which variables are most predictive and includes them in the model
these data are likely predictive of US election outcomes



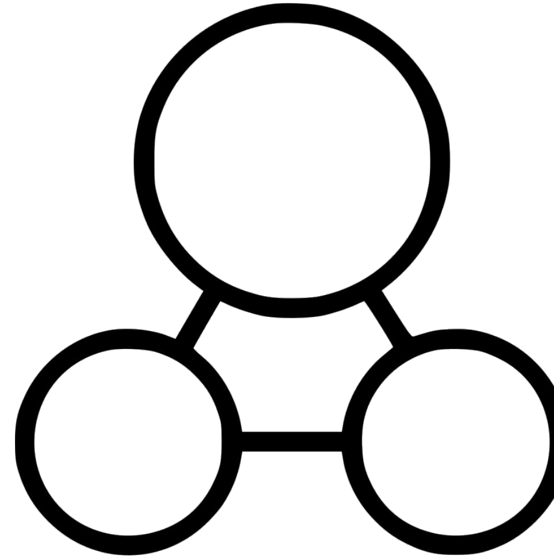
variables that can be used for accurate prediction exploit the relationship between the variables but do NOT mean that one causes the other



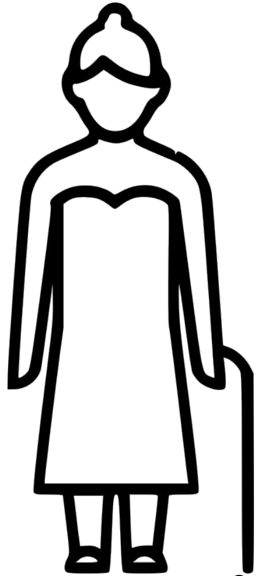
model selection



big
datasets

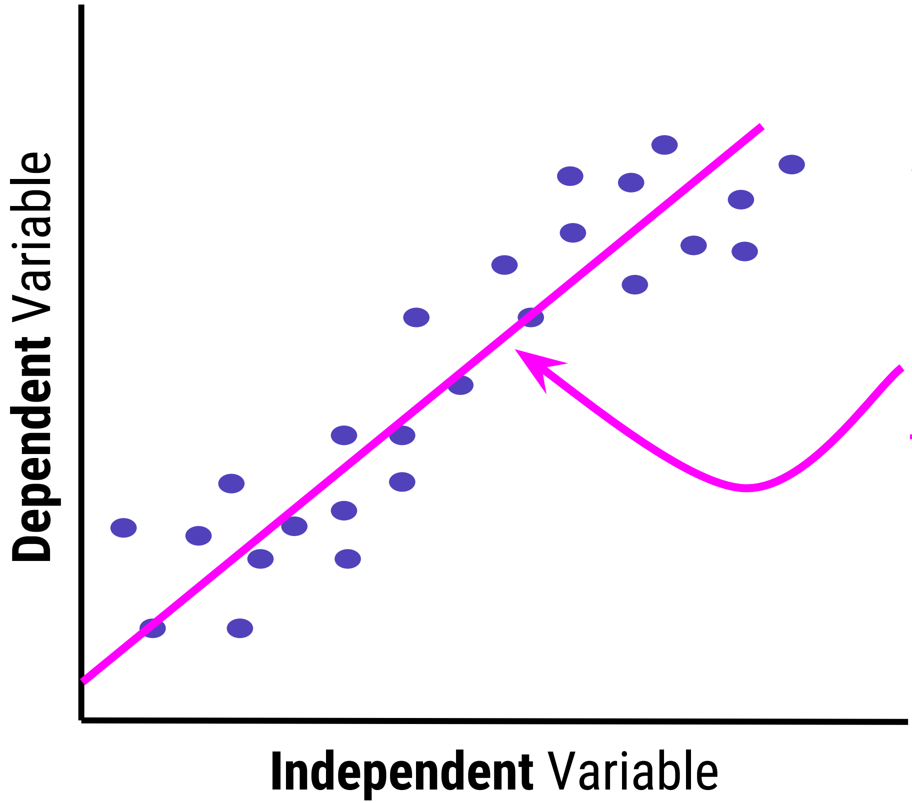


simple
models

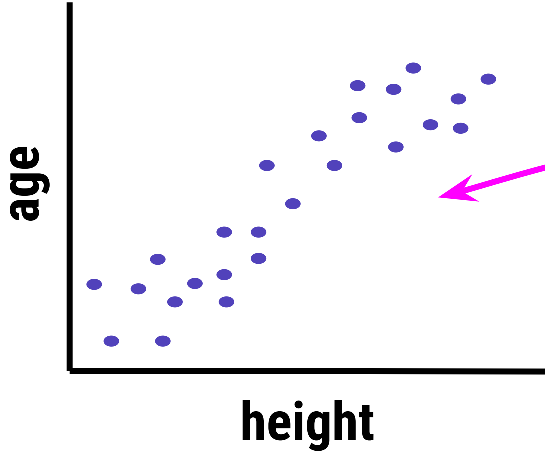


Regression:
predicting continuous variables
(i.e. Age)

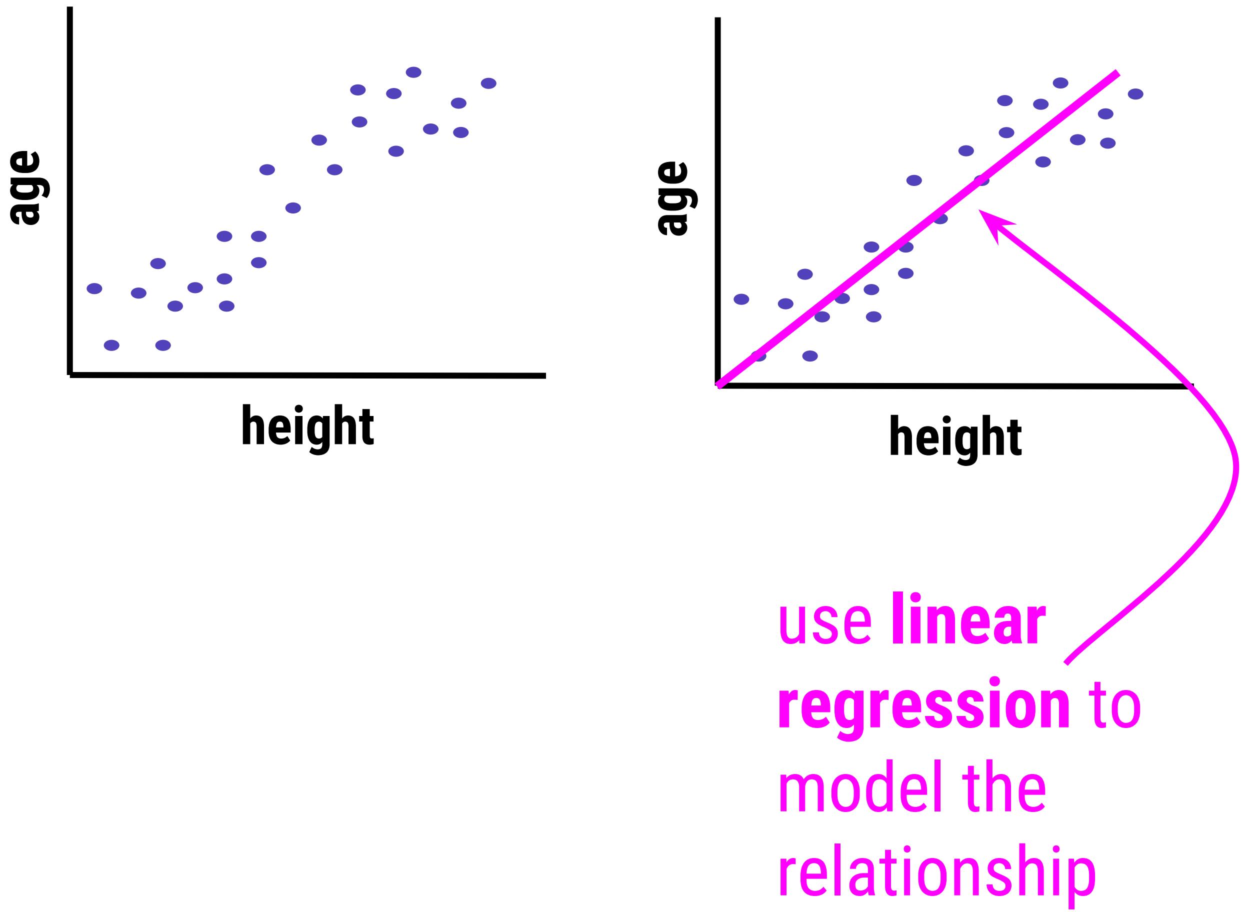
Classification:
predicting categorical variables
(i.e. education level)

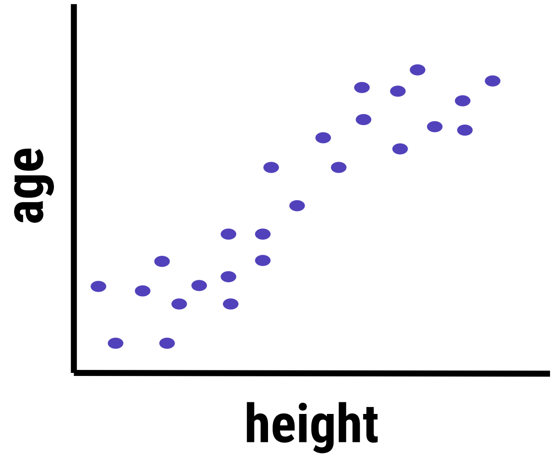


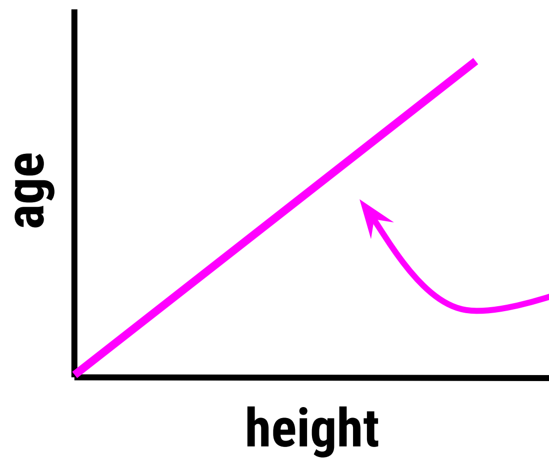
We'll use the linear relationship between variables to generate a **predictive model**!



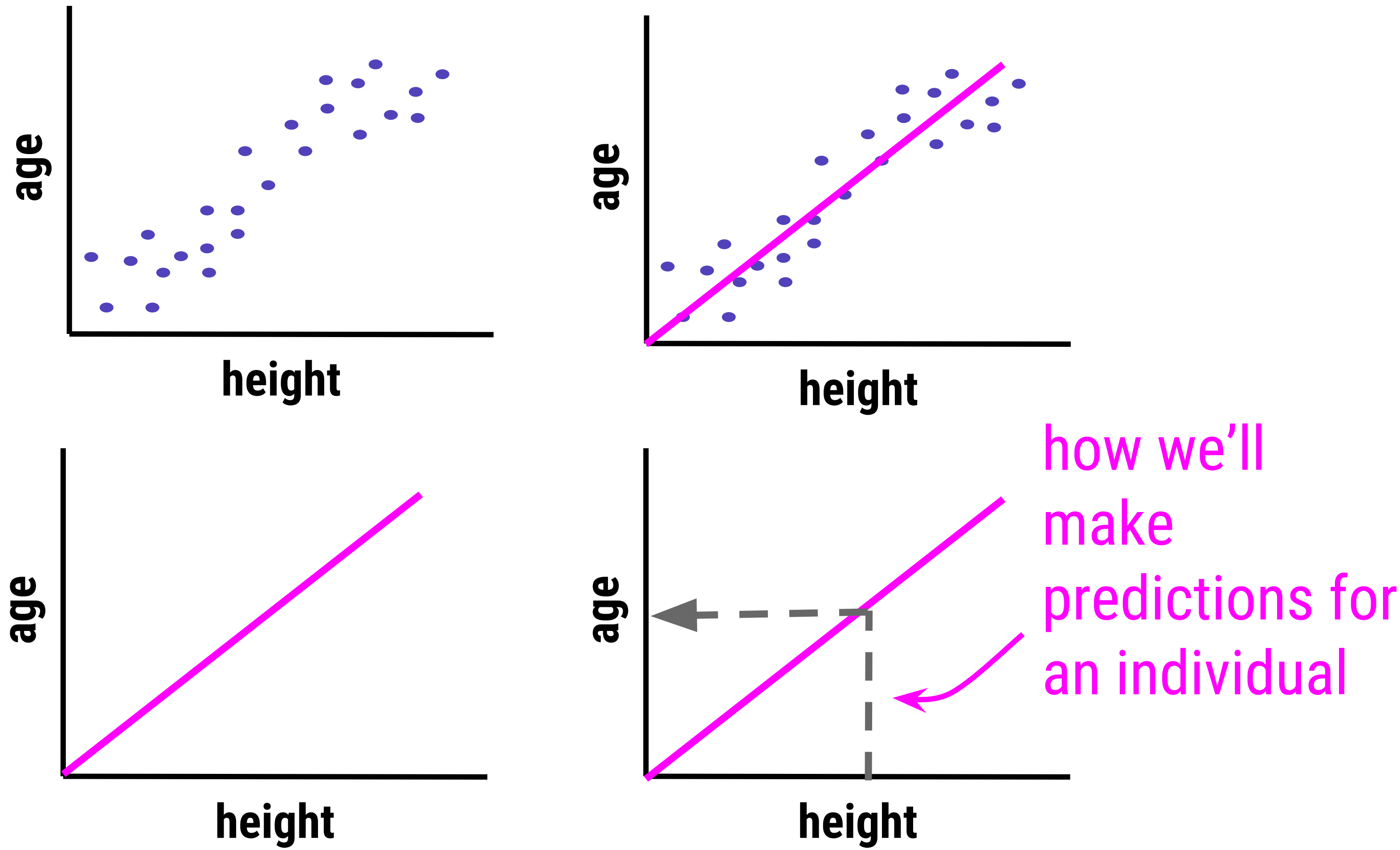
the training data
will be used to
build the
predictive model

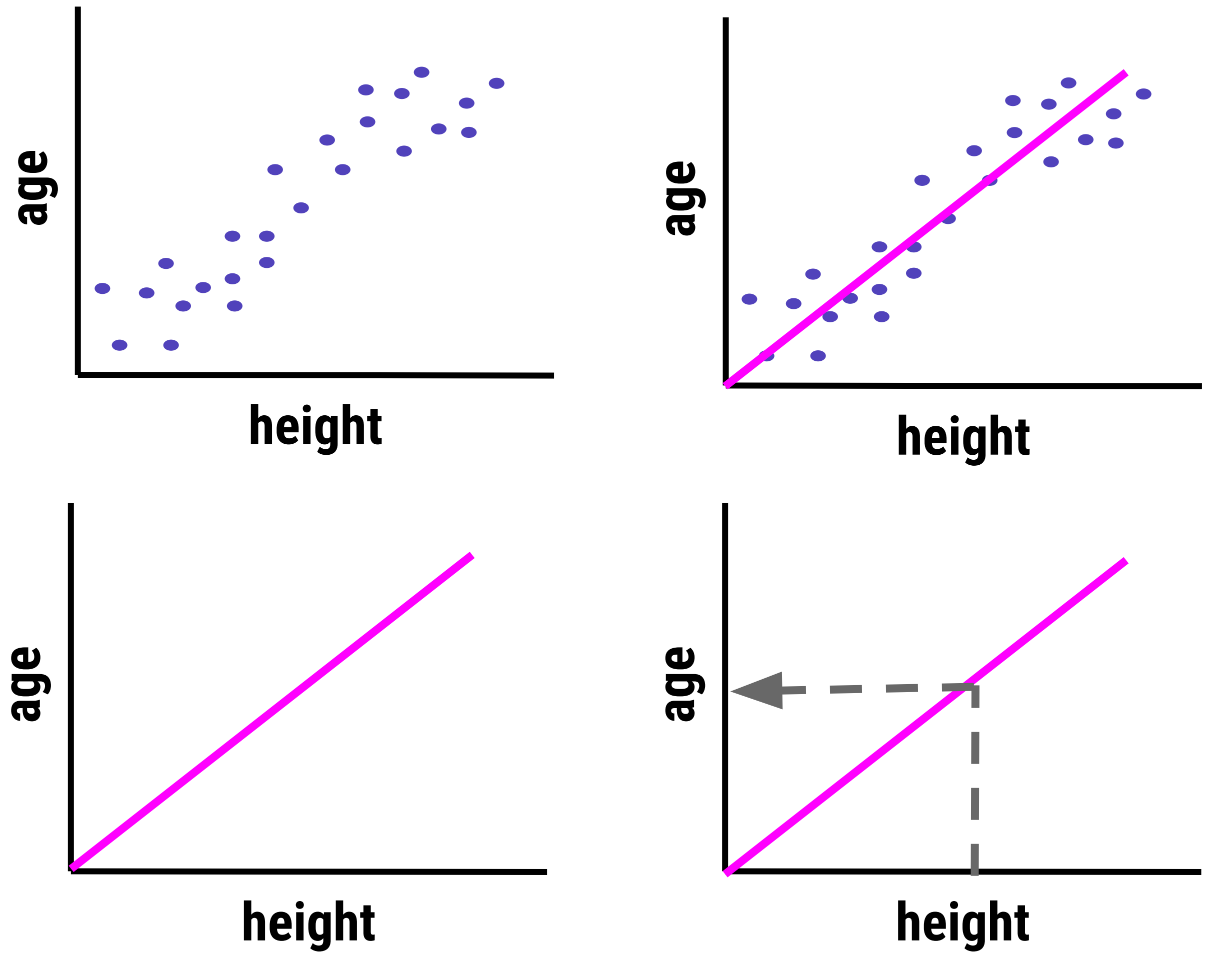

age
height
age
height
use **linear regression** to model the relationship

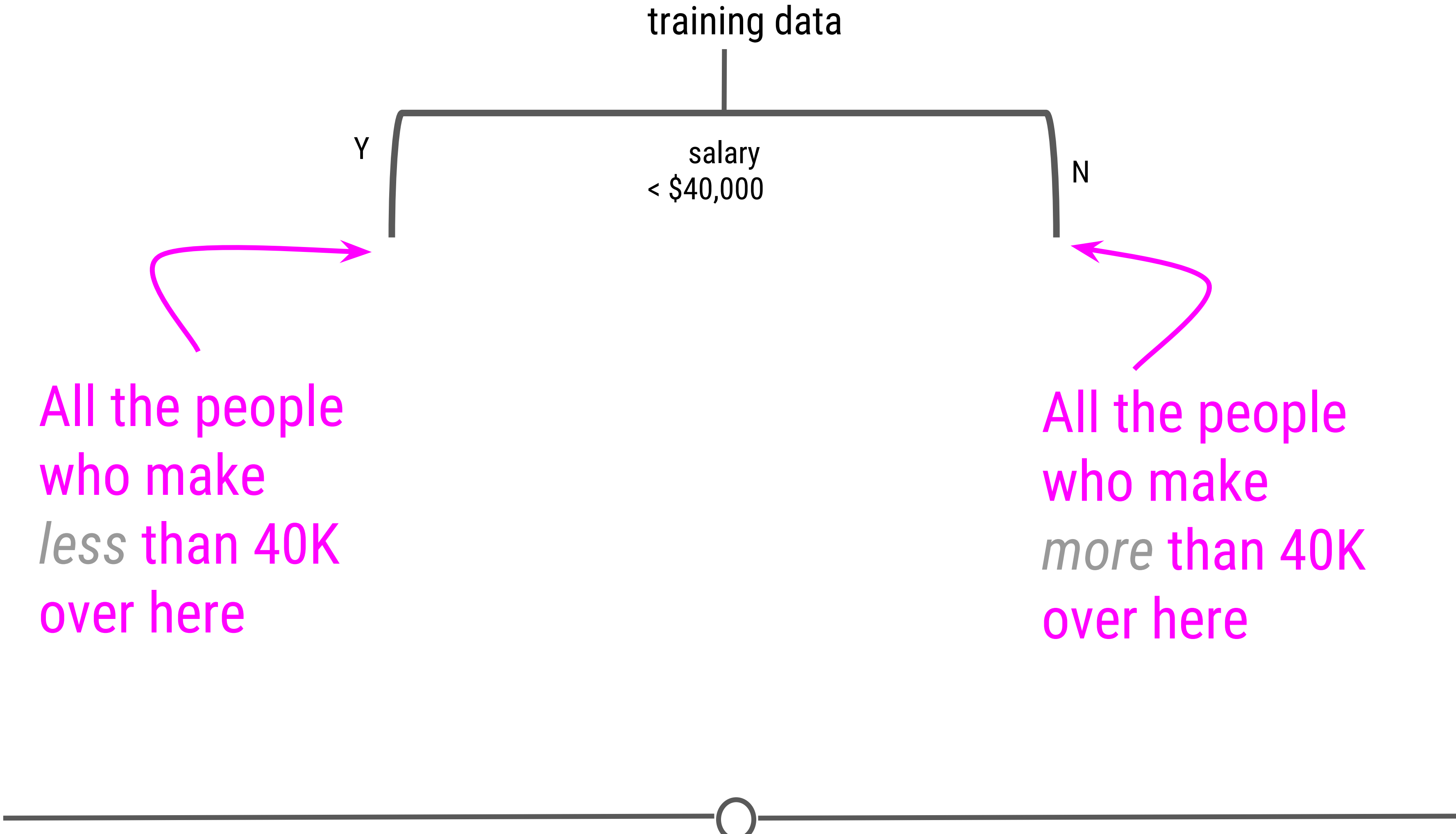


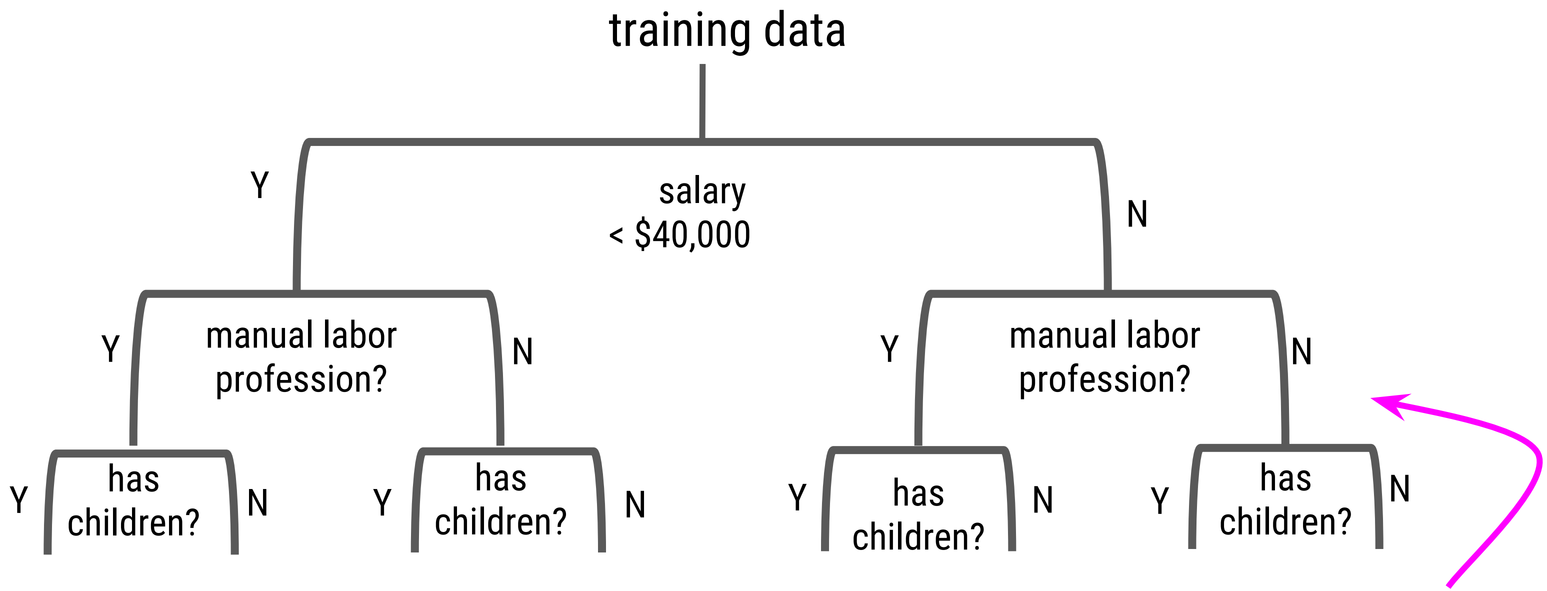


For prediction, the individual values in the training data are *not* important. We only need the model.

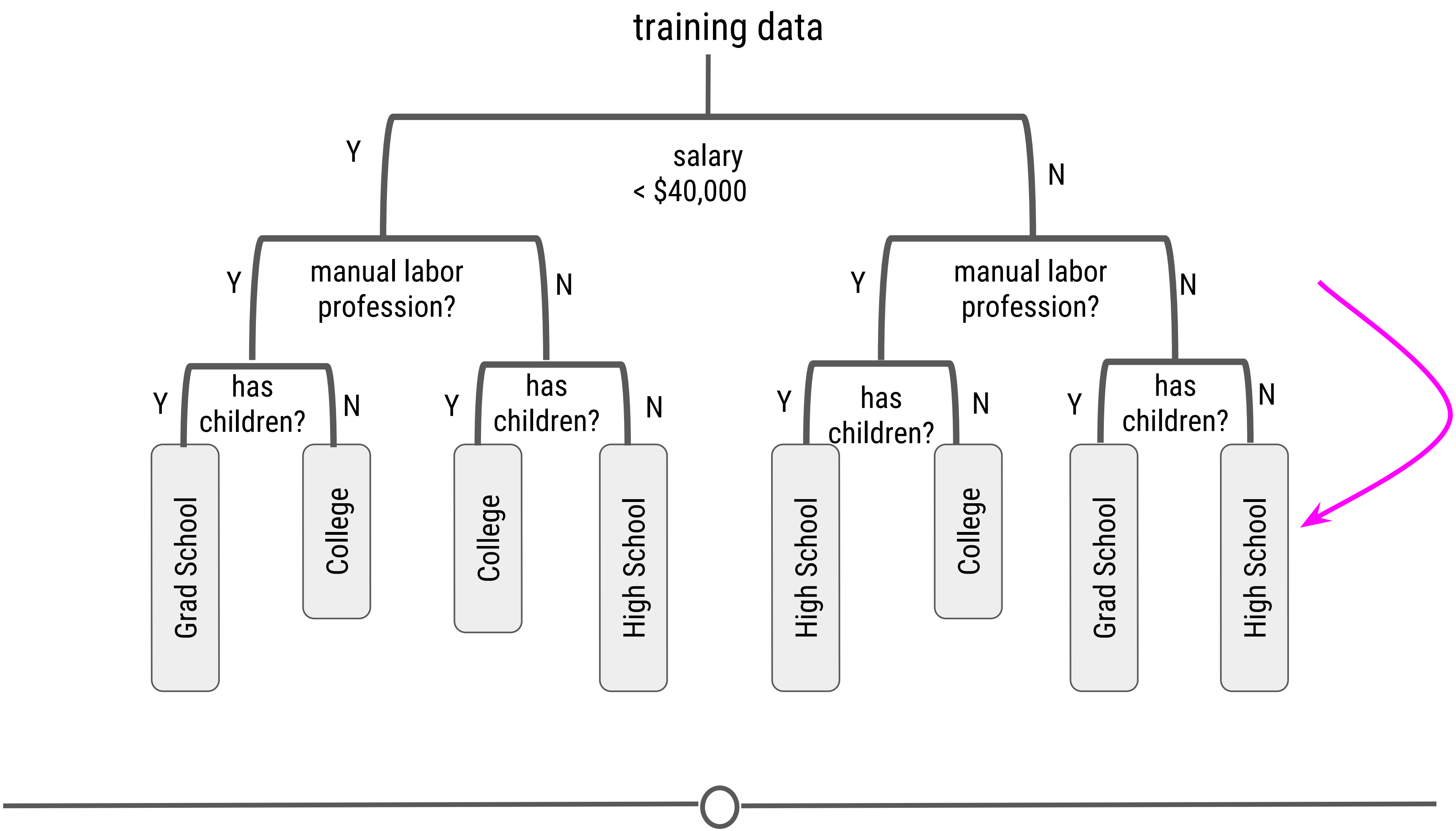

age
height
age
height
age
height
age
height
how we'll
make
predictions for
an individual

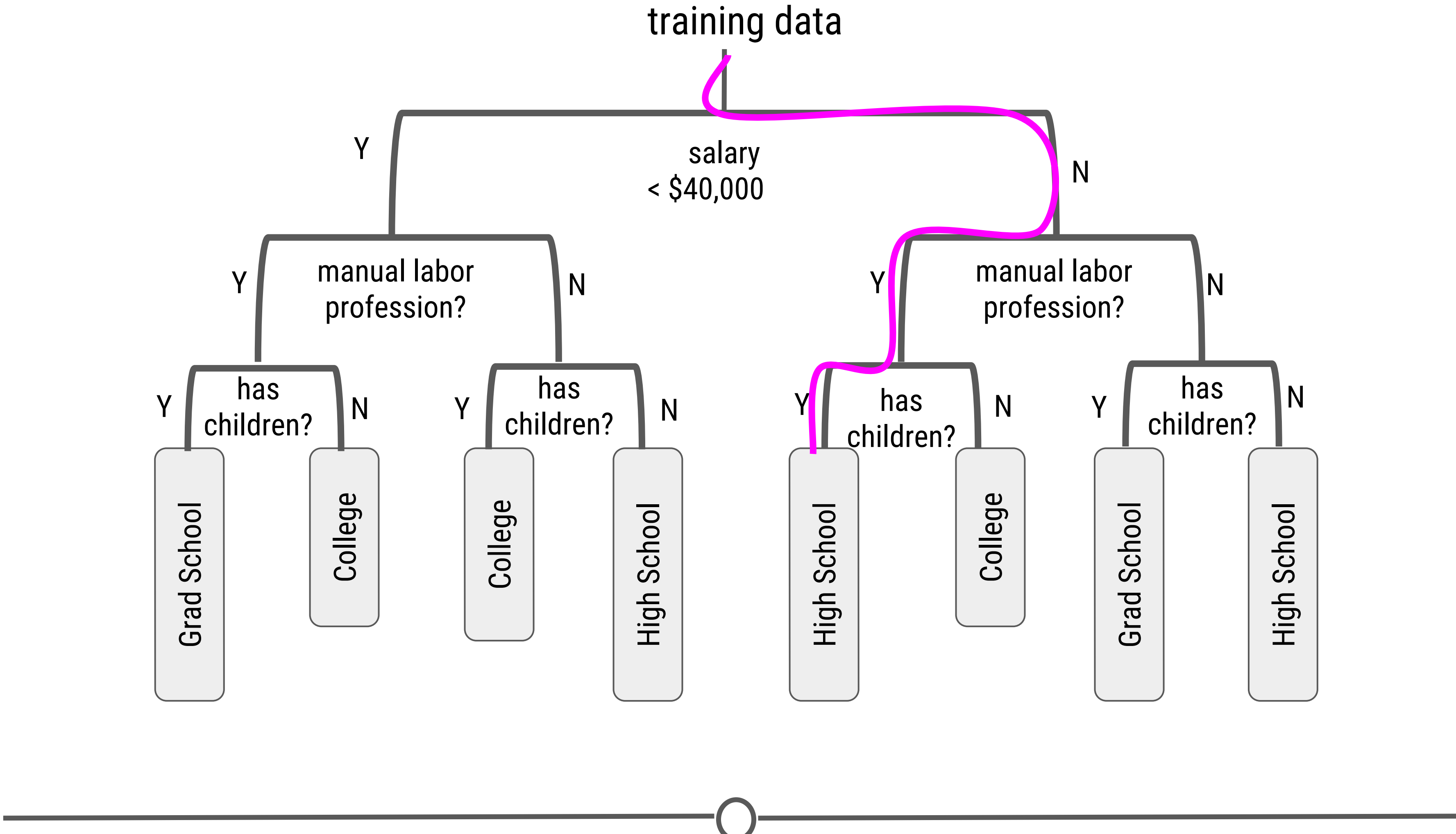

age
height
age
height
age
height
age
height

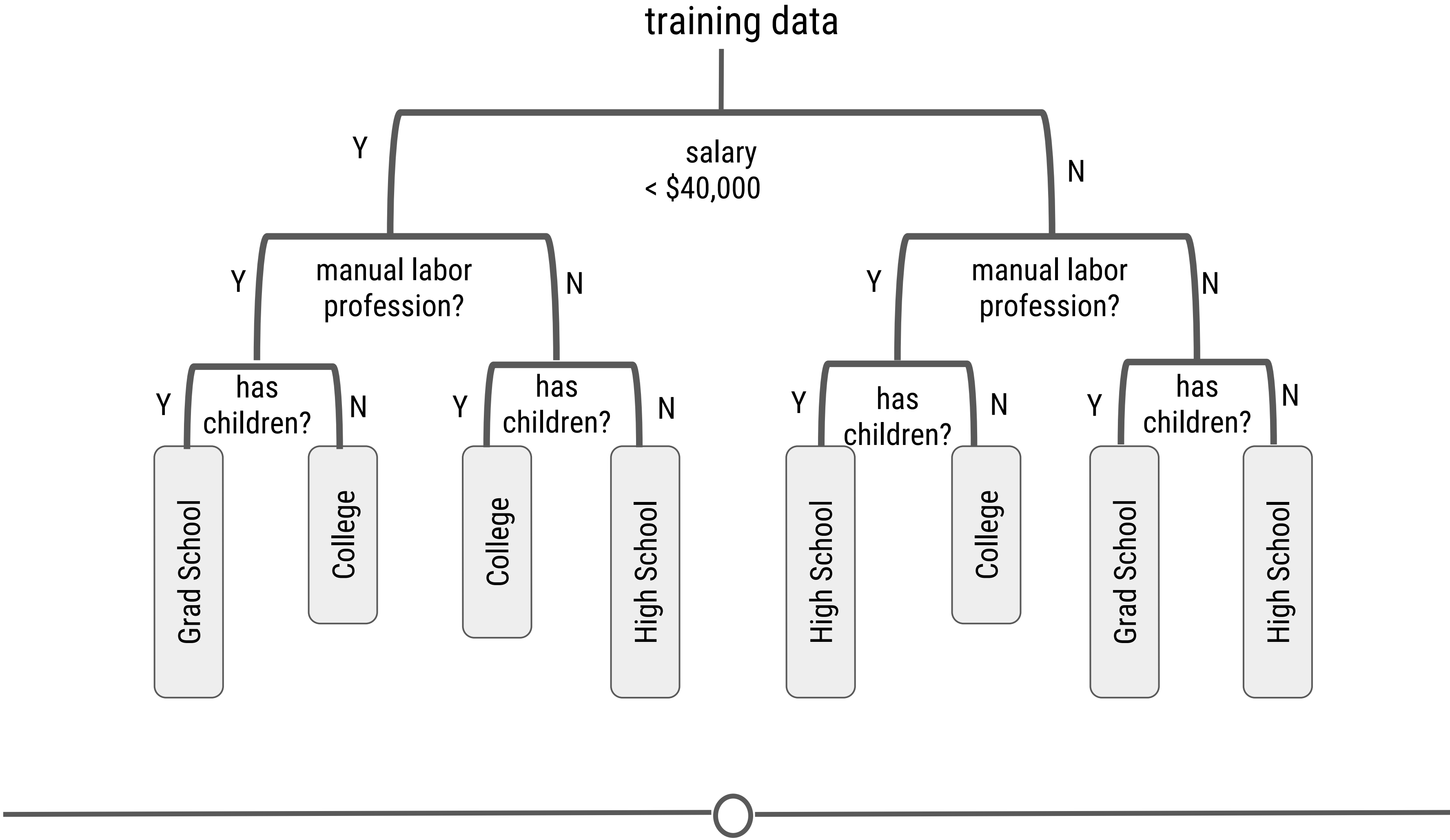

training data
salary
< $40,000
Y
N
All the people who make *less* than 40K over here
All the people who make *more* than 40K over here



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


training data
salary
< $40,000
Y
N
manual labor
profession?
Y
N
manual labor
profession?
Y
N
has
children?
Y
N
has
children?
Y
N
has
children?
Y
N
has
children?
Y
N
Grad School
College
College
High School
High School
College
Grad School
High School


training data
salary
< $40,000
Y
N
manual labor
profession?
Y
N
manual labor
profession?
Y
N
has
children?
Y
N
has
children?
Y
N
has
children?
Y
N
has
children?
Y
N
Grad School
College
College
High School
High School
College
Grad School
High School


training data
salary
< $40,000
Y
N
manual labor
profession?
Y
N
manual labor
profession?
Y
N
has
children?
Y
N
has
children?
Y
N
has
children?
Y
N
has
children?
Y
N
Grad School
College
College
High School
High School
College
Grad School
High School

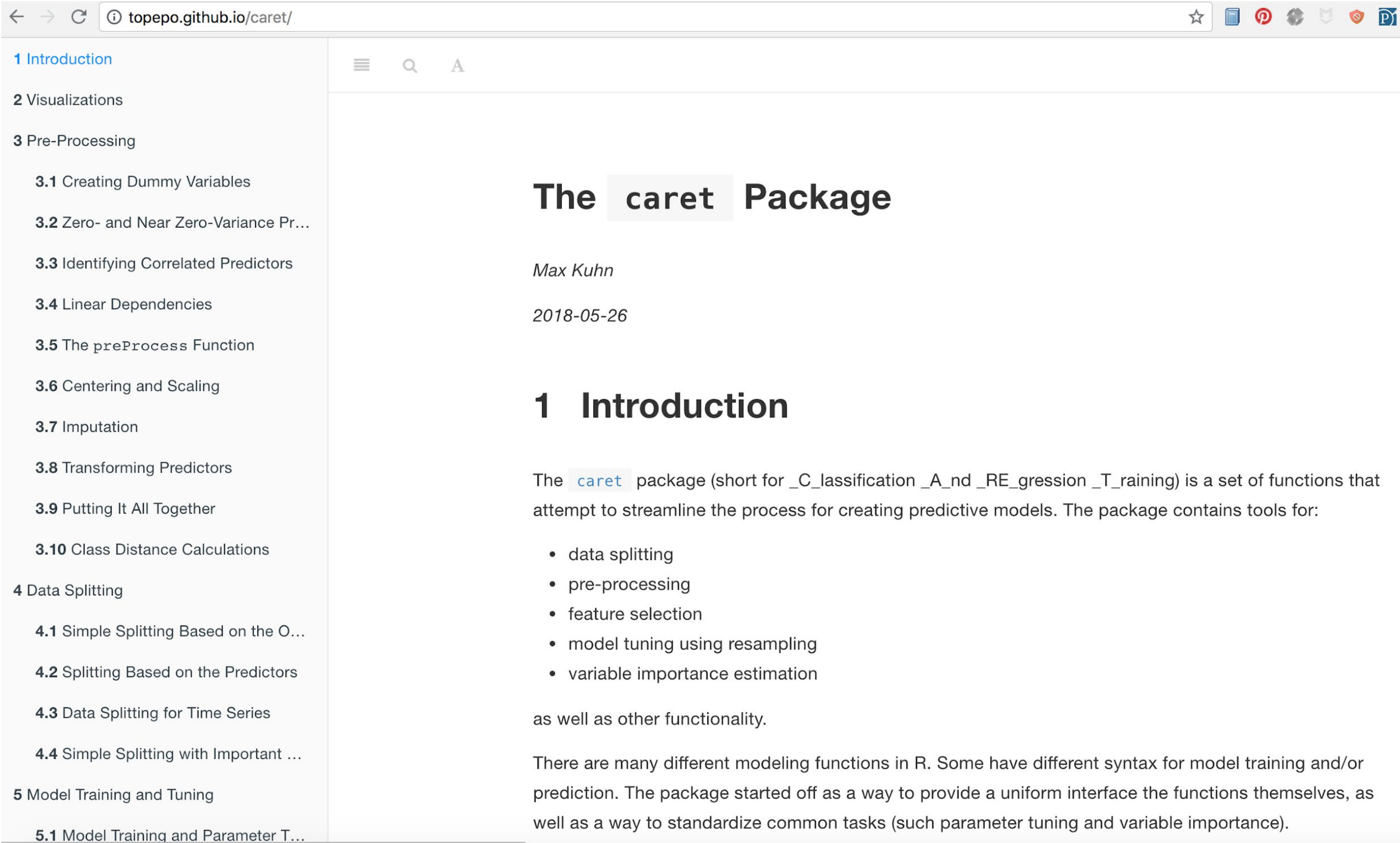
accuracy assessment

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} (Predicted_i - Actual_i)^2}{N}}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} (Predicted_i - Actual_i)^2}{N}}$$

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

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



topepo.github.io/caret/

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3.3 Identifying Correlated Predictors
3.4 Linear Dependencies
3.5 The `preProcess` Function
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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).

http://topepo.github.io/caret/

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`.)

```r
## install and load packages
install.packages("caret")
library(caret)
library(dplyr)

## 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)
```

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

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

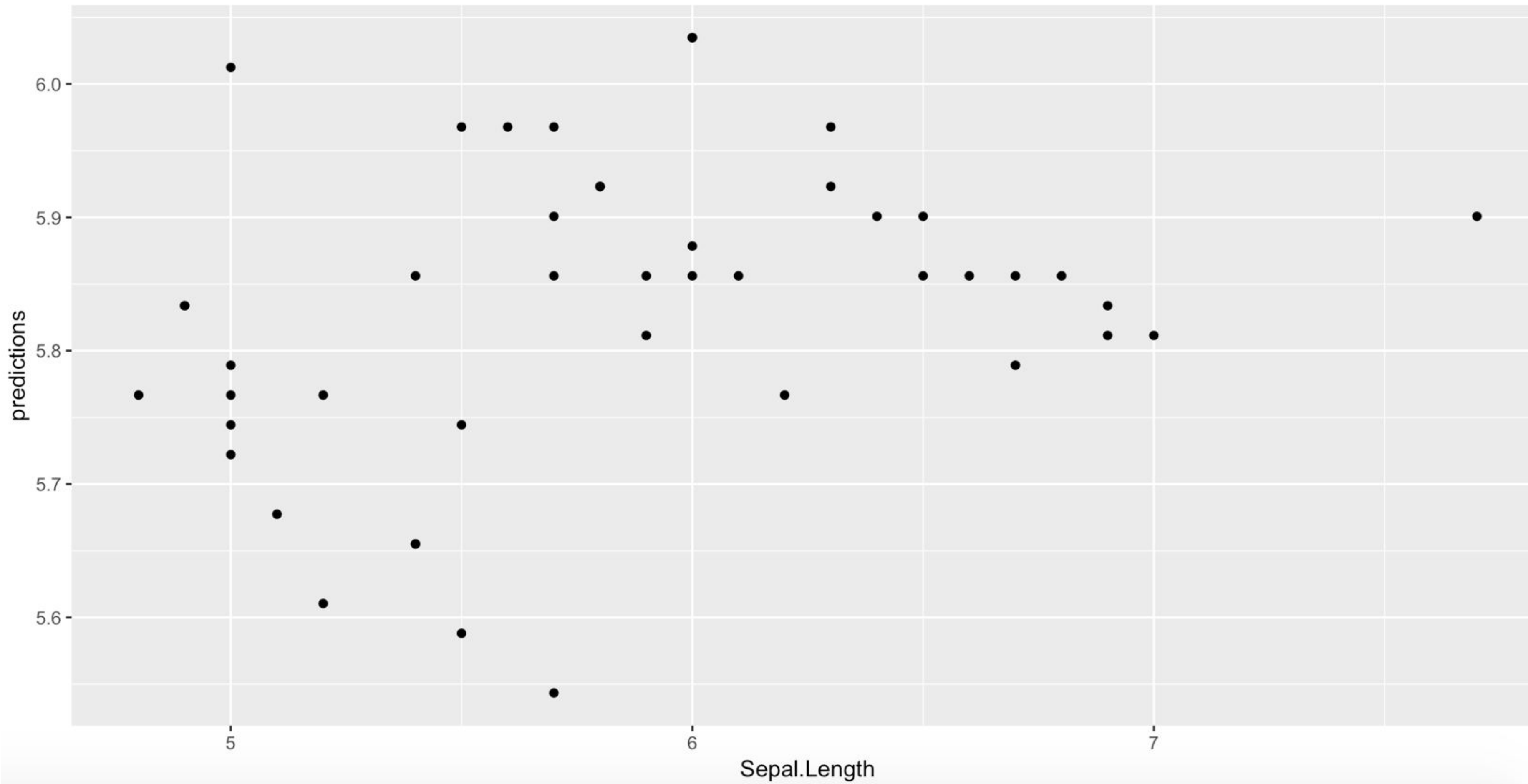
```
> str(iris_train)
'data.frame':	105 obs. of  5 variables:
 $ Sepal.Length: num  5.1 4.9 4.7 4.6 4.6 4.4 5.4 4.8 4.3 5.8 ...
 $ Sepal.Width : num  3.5 3 3.2 3.1 3.4 2.9 3.7 3 3 4 ...
 $ Petal.Length: num  1.4 1.4 1.3 1.5 1.4 1.4 1.5 1.4 1.1 1.2 ...
 $ Petal.Width : num  0.2 0.2 0.2 0.2 0.3 0.2 0.2 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

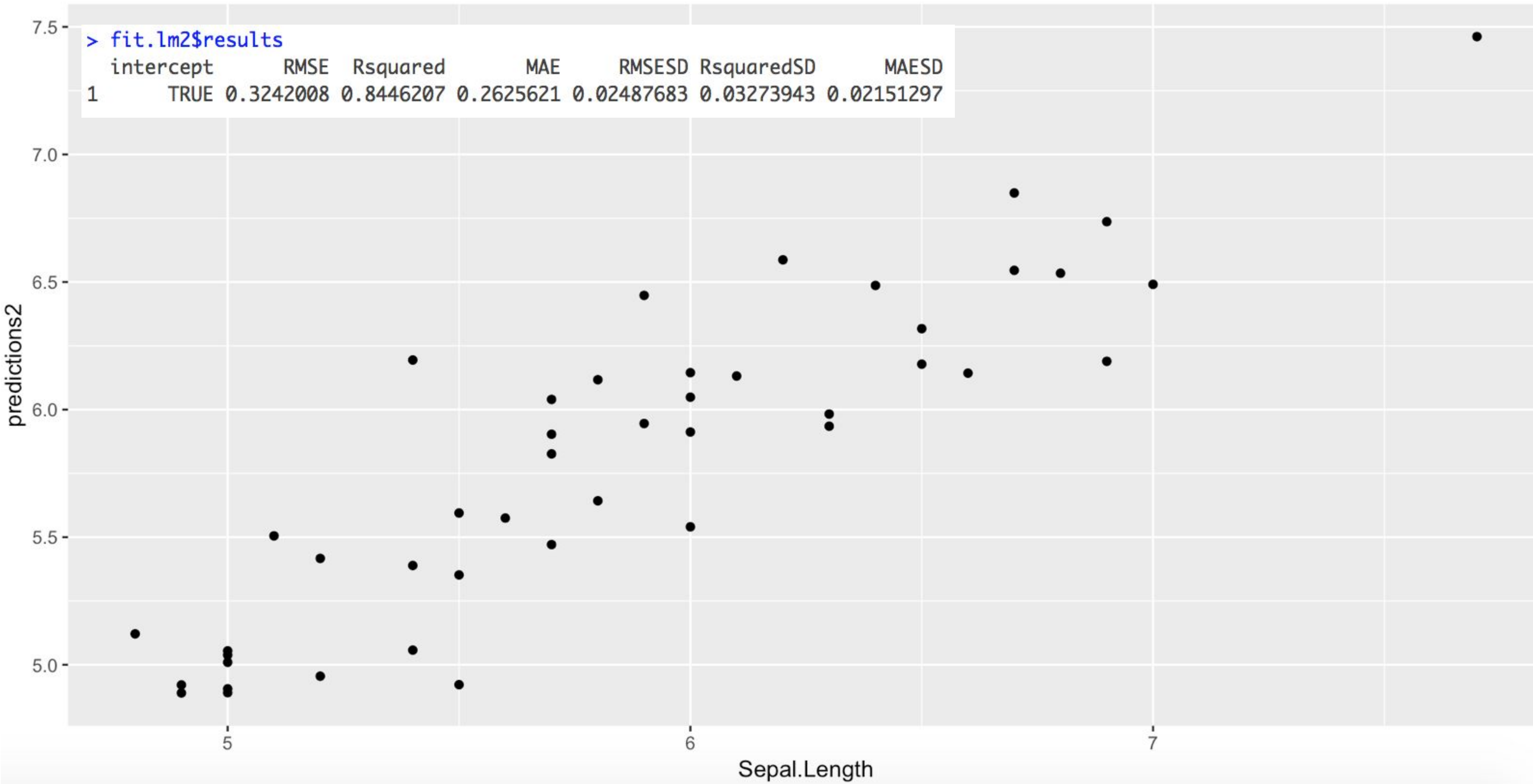
```
## train regression model
set.seed(123)
fit.lm <- train(Sepal.Length ~
Sepal.Width,
                data = iris,
                method = "lm",
                metric = "RMSE")
```

```
> ## 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
```

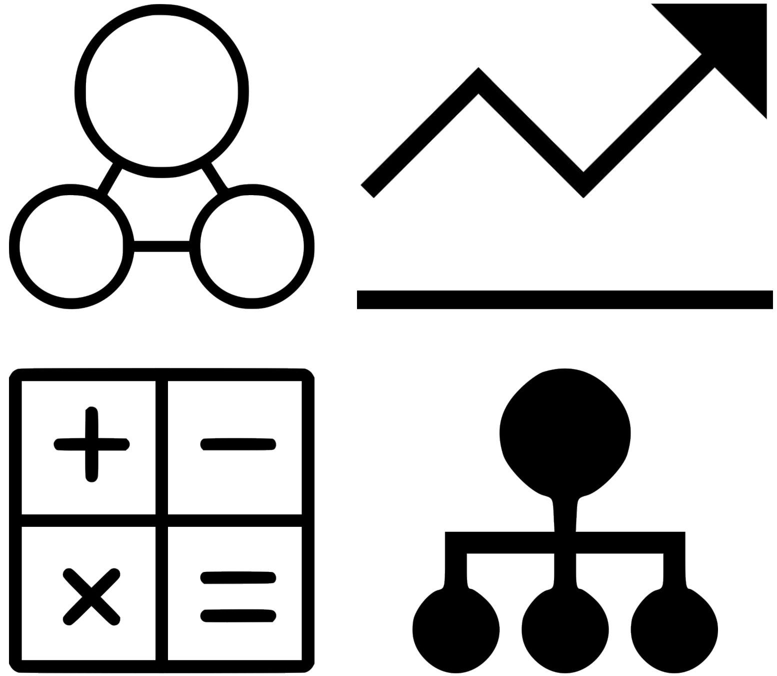
```r
## make predictions in tuning data set
predictions <- predict(fit.lm, iris_tune)


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


6.0
5.9
5.8
5.7
5.6
predictions
5
6
7
Sepal.Length

```r
## 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))
```



> fit.lm2$results
intercept RMSE Rsquared MAE RMSESD RsquaredSD MAESD
1 TRUE 0.3242008 0.8446207 0.2625621 0.02487683 0.03273943 0.02151297
predictions2
Sepal.Length
7.5
7.0
6.5
6.0
5.5
5.0
5
6
7



model selection

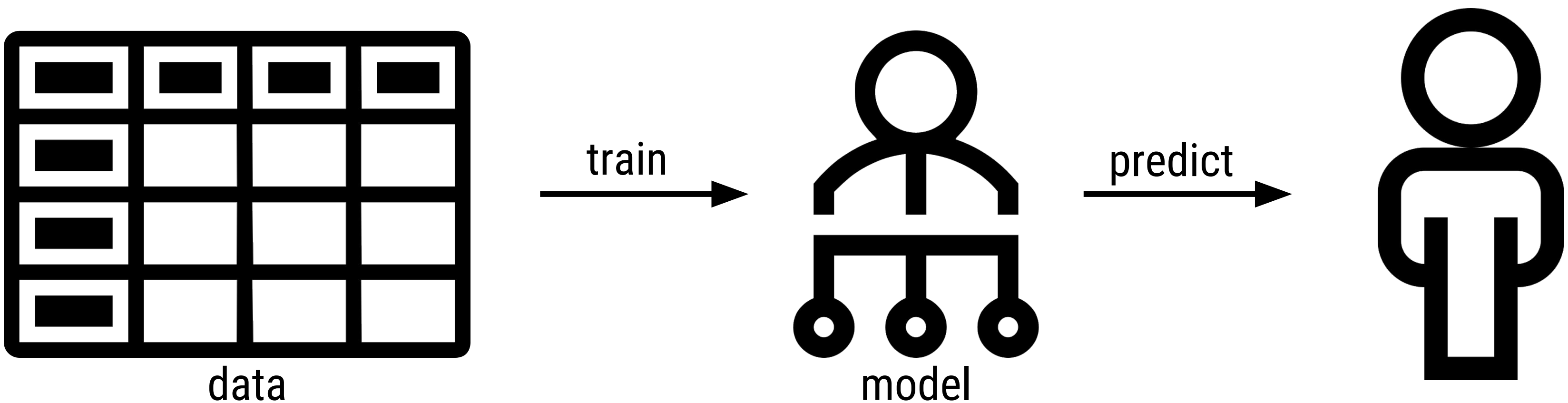
http://topepo.github.io/caret/model-training-and-tuning.html#fitting-models-without-parameter-tuning

```r
## CART
set.seed(7)
fit.cart <- train(Species~.,
                  data = iris,
                  method = "rpart",
                  metric = "Accuracy")

## look at Accuracy
fit.cart$results

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

rpart specifies to use a CART for classification 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


train
predict
data
model