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#Babraham Bioinformatics

Introduction to Machine Learning

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Agenda for the session

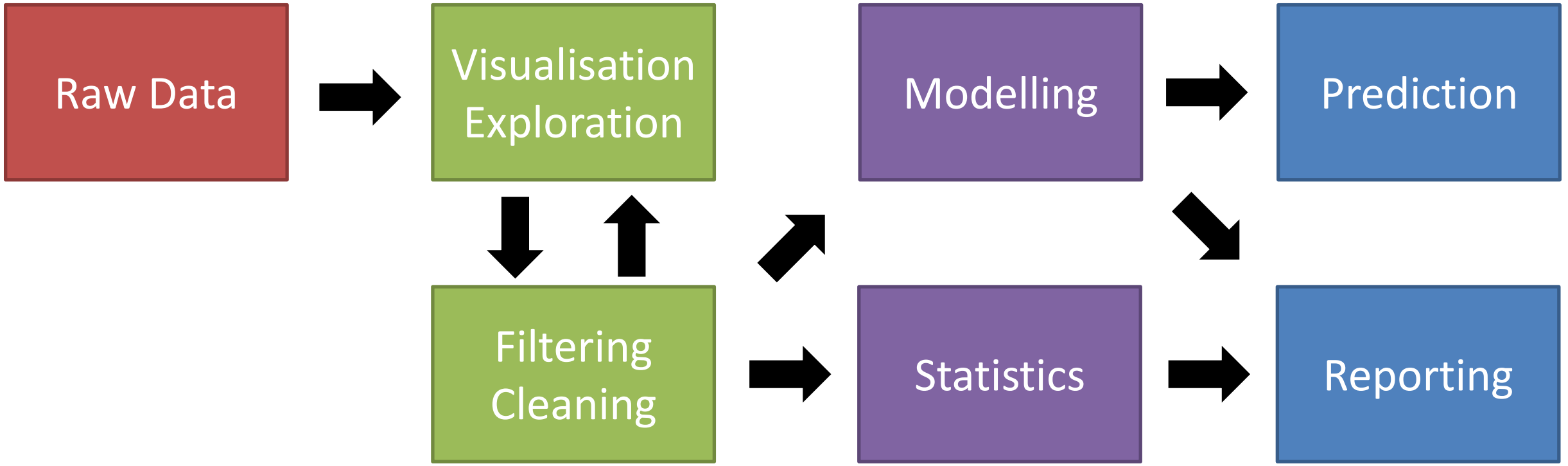
- What is machine learning
- Different types of machine learning model

- Running Models with tidymodels
- [Exercise] Building your first model

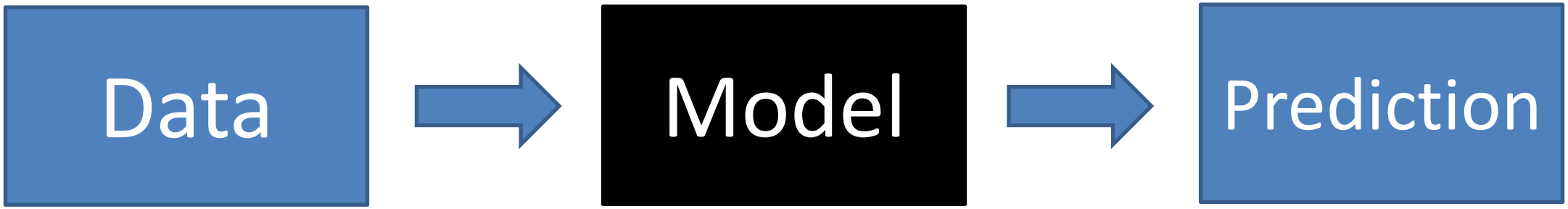
- How to evaluate models
- Preparing Input Data
- [Exercise] Evaluating Models

What is Machine Learning?

Data Analysis Workflow



Machine Learning Builds a **Model** to make **Predictions**



Sample	Weight	Age	Sex
A	27	4.5	Male
B	28	2	Female
C	19	6.7	Female

Classification

Sample	Healthy
A	No
B	Yes
C	No

Regression

Sample	Height
A	18
B	22
C	12

Biological Examples

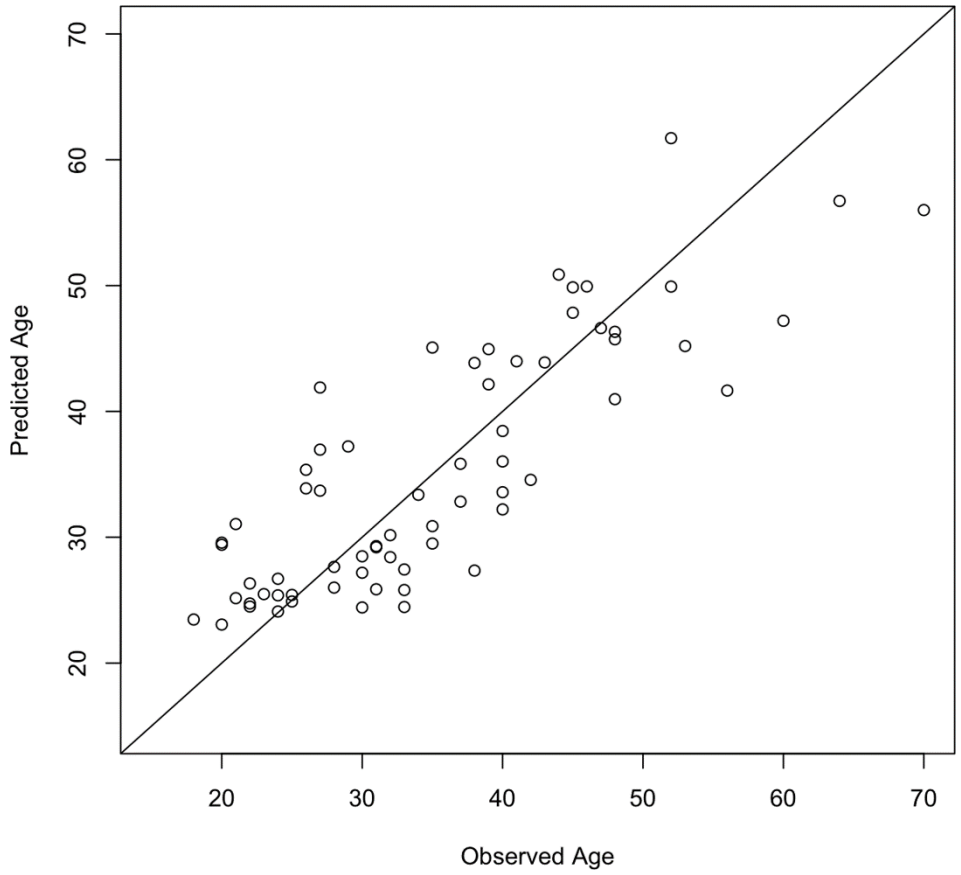
Input: DNA Methylation from genomic CpGs
Output: Estimated biological age

OPEN ACCESS Freely available online

PLoS one

Epigenetic Predictor of Age

Sven Bocklandt[1], Wen Lin[2], Mary E. Sehl[3], Francisco J. Sánchez[1,5], Janet S. Sinsheimer[1,2,4], Steve Horvath[1,2], Eric Vilain[1,5]*



Biological Examples

Input: DAPI stained cell images
Output: Predicted Cell Cycle Stage

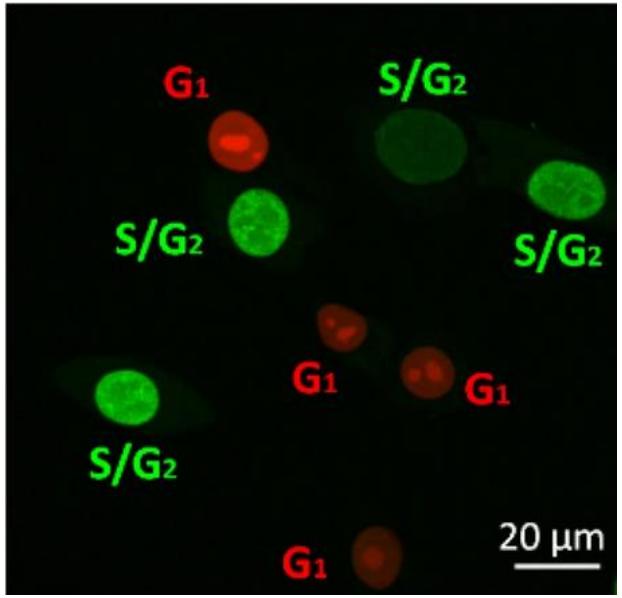
Visual Analysis	Automatic Labels: G1	S/G2	Total
G1	1371	16	1387
S/G2	5	1289	1294
Total	1376	1305	2681

scientific reports

OPEN

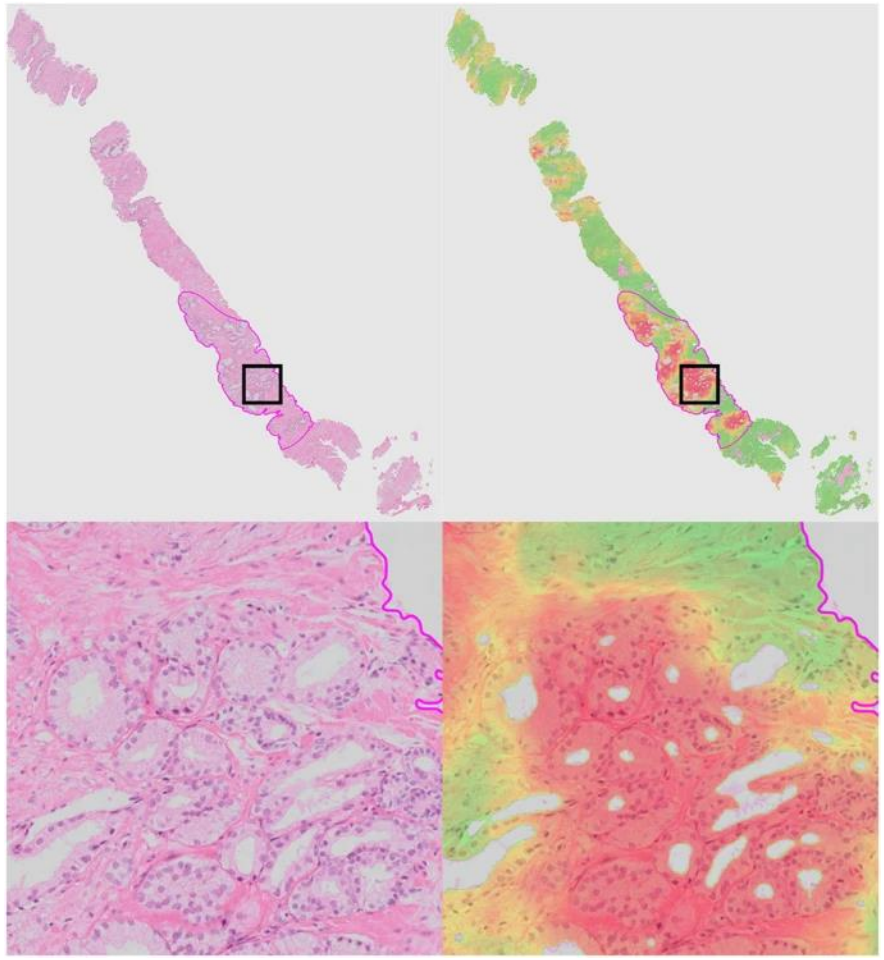
A machine learning approach for single cell interphase cell cycle staging

Hemaxi Narotamo[1,6], Maria Sofia Fernandes[2,3,6], Ana Margarida Moreira[2,3,4], Soraia Melo[2,3], Raquel Seruca[2,3,5✉], Margarida Silveira[1] & João Miguel Sanches[1]



Biological Examples

Input: Histopathology slide images
Output: Cancer likelihood score



SCIENTIFIC REPORTS

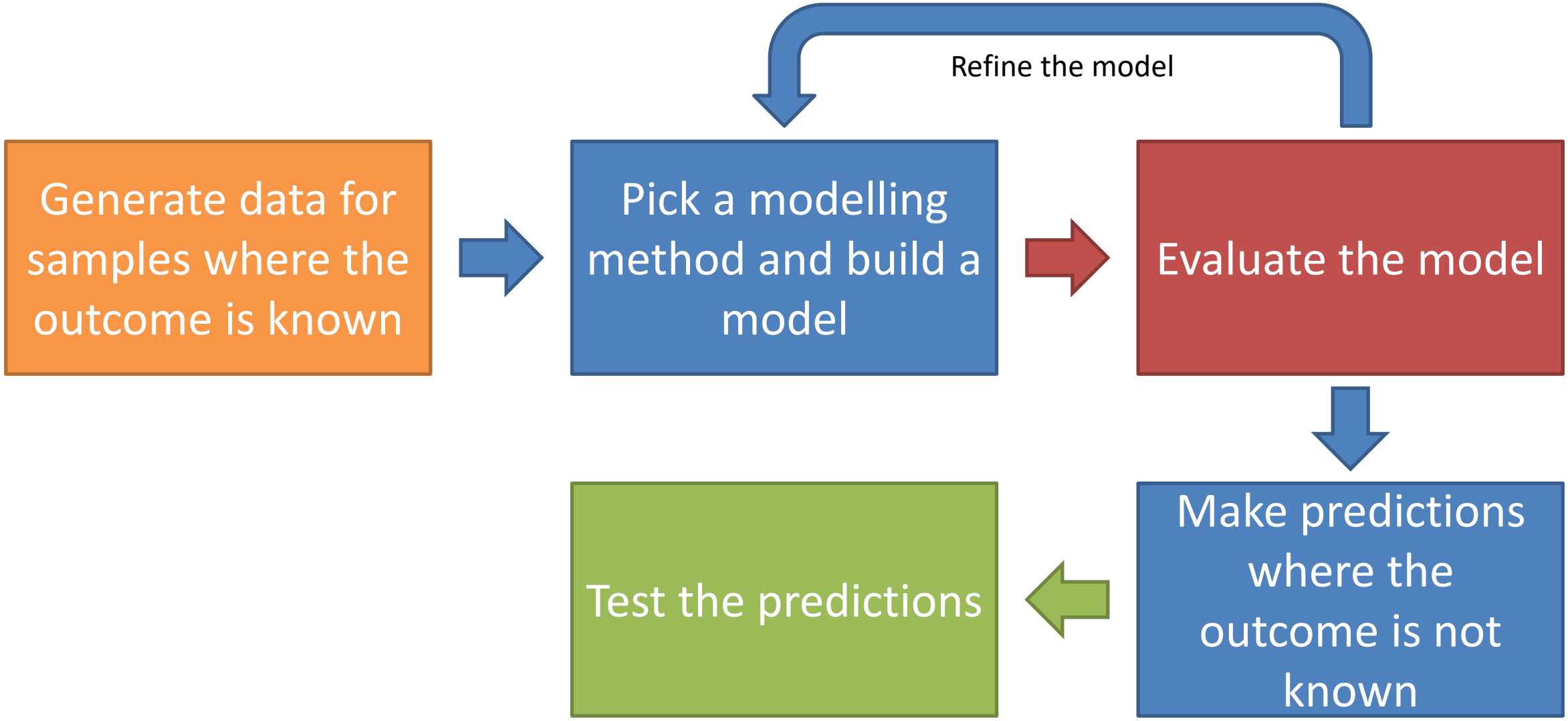
OPEN

Deep learning as a tool for increased accuracy and efficiency of histopathological diagnosis

Received: 28 January 2016
Accepted: 27 April 2016
Published: 23 May 2016

Geert Litjens[1], Clara I. Sánchez[2], Nadya Timofeeva[1], Meyke Hermsen[1], Iris Nagtegaal[1], Iringo Kovacs[3], Christina Hulsbergen - van de Kaa[1], Peter Bult[1], Bram van Ginneken[2] & Jeroen van der Laak[1]

Steps in Machine Learning



Different machine learning models

Model Name	Model Type
Linear Regression	Regression
Logistic Regression	Regression or Classification
K-nearest neigbours	Regression or Classification
Naïve Bayes	Classification
Decision Tree	Classification
Random Forest	Classification
Support Vector Machine	Regression or Classification
Neural Networks	Regression or Classification

Differences between models

- Outcome type
  - Regression models for quantitative predictions
  - Classification models for categorical predictions
  - Some model types can do both

Regression

Sample	Height
A	18
B	22
C	12

Classification

Sample	Healthy
A	No
B	Yes
C	No

- Input type
  - Some models require all of their variables to be numeric
  - May need to convert categorical values to numbers
  - Expected behaviour of input data
  - Variation in the number of viable measures

K-Nearest Neighbours (KNN) models

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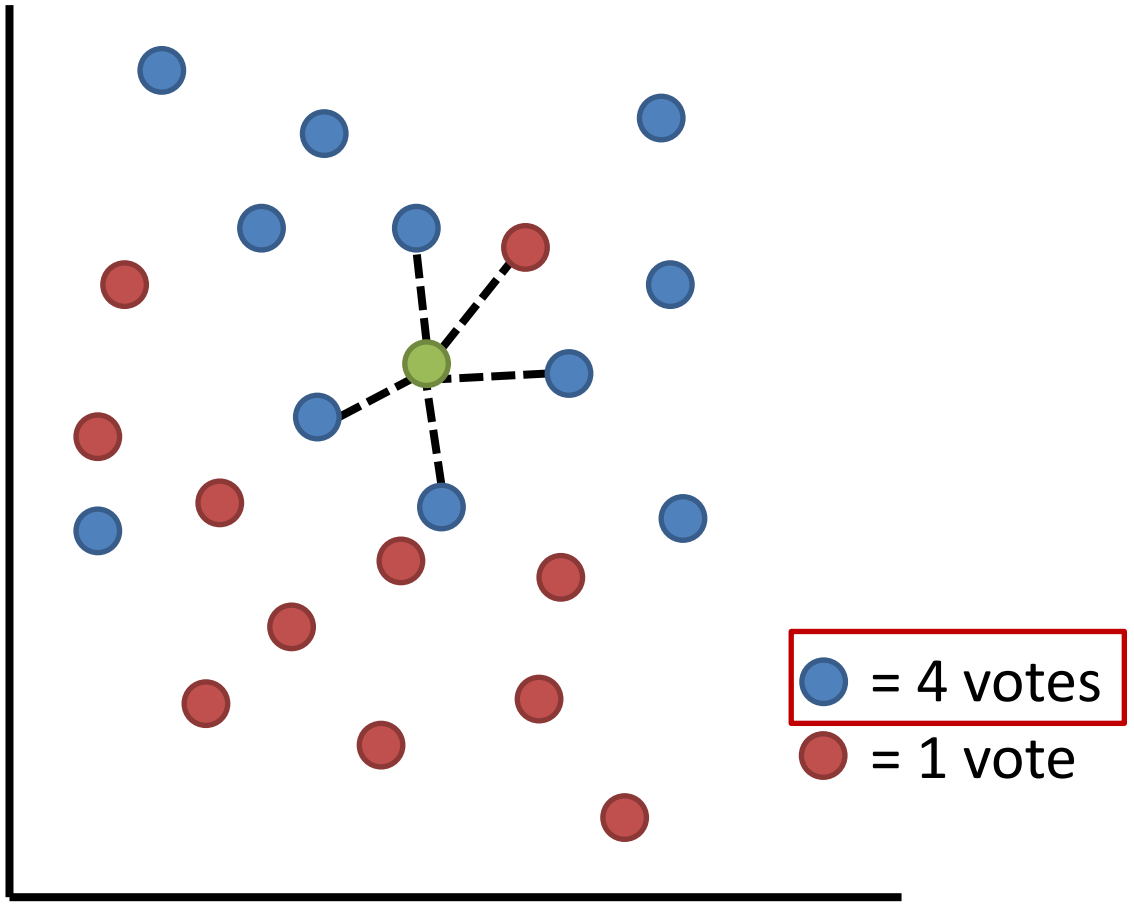
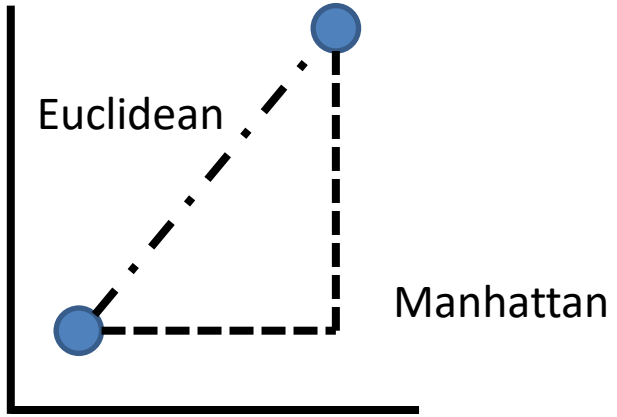
K-nearest neighbours

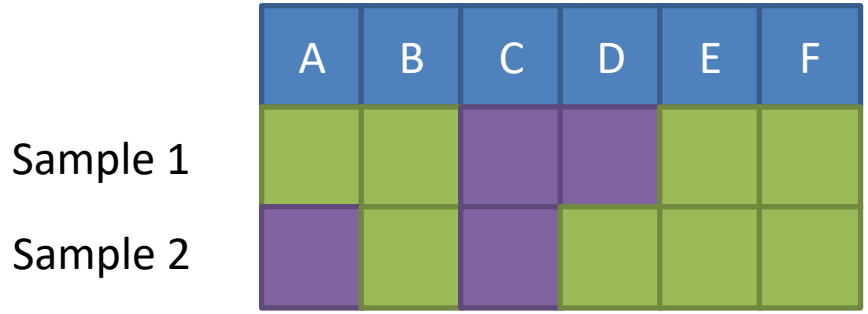


- Add a new point
- Find the K (5 in this case) closest points
- Count the categories in the closest points
- The highest vote wins

Distance Measures

- Quantitative:
  - Euclidean Distance (straight line)
  - Manhattan Distance (along each axis)
- Categorical:
  - Hamming Distance (how many categories need to switch to make match)
  - Jaccard Distance
- …





Hamming = 2 differences

Naïve Bayes Models

Naïve Bayesian

Bayes' Theorem states that the conditional probability of an event, based on the occurrence of another event, is equal to the likelihood of the second event given the first event multiplied by the probability of the first event.

Gene	Length	GC	Chromsome	Disease Linked
A	1kb	40	1	Yes
B	5kb	50	2	No
C	2kb	50	2	No
D	3kb	20	X	Yes
E	10kb	30	X	No

We calculate a set of probabilities for each variable, based on the "Disease Linked Classification"

Categorical Probabilities

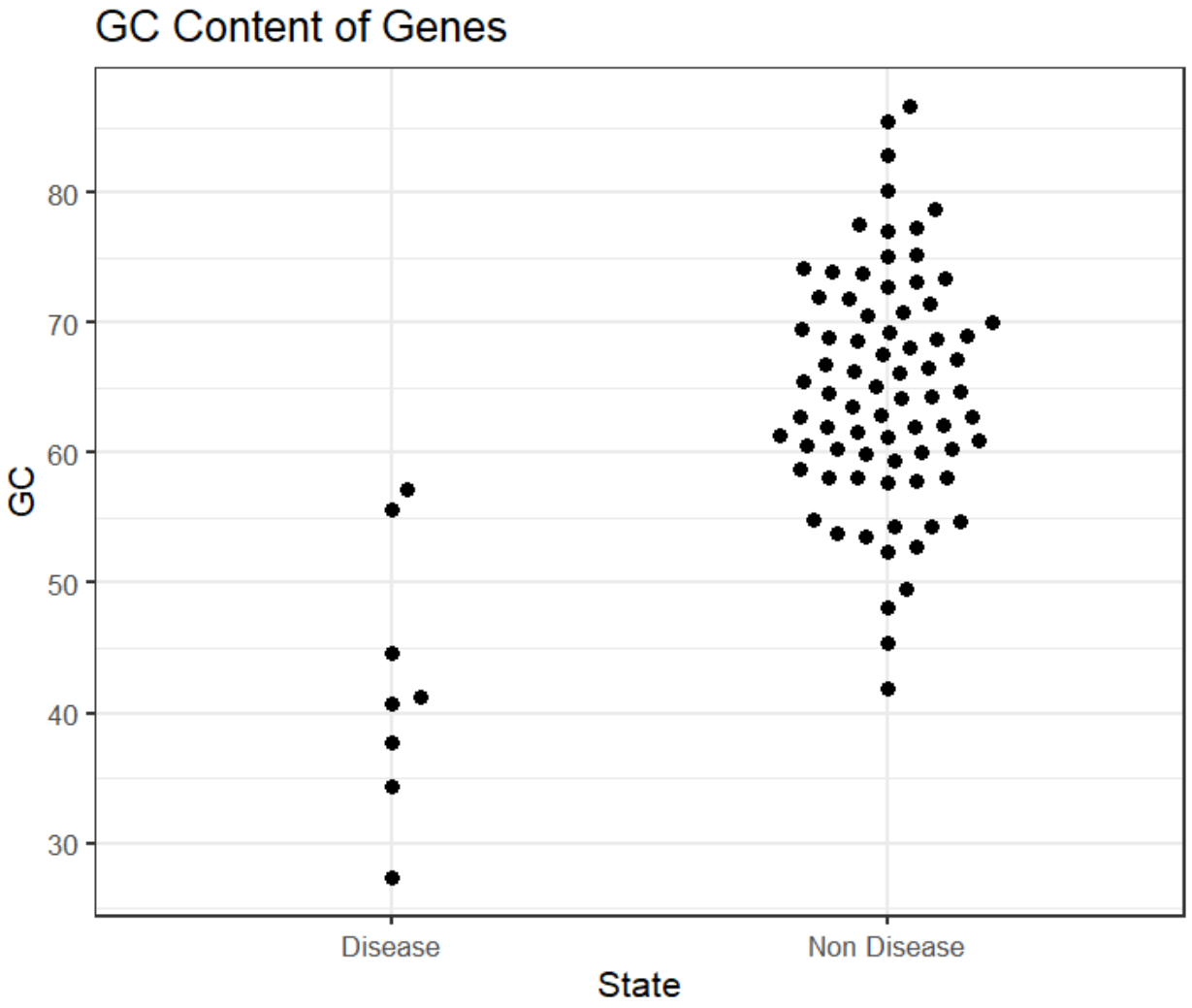
Chromosome	Disease Linked	Non Disease
1	5	6
2	2	20
X	1	50

p Chr1 | Disease = 5 / 8 = 0.625
p Chr2 | Disease = 2 / 8 = 0.250
p ChrX | Disease = 1 / 8 = 0.125

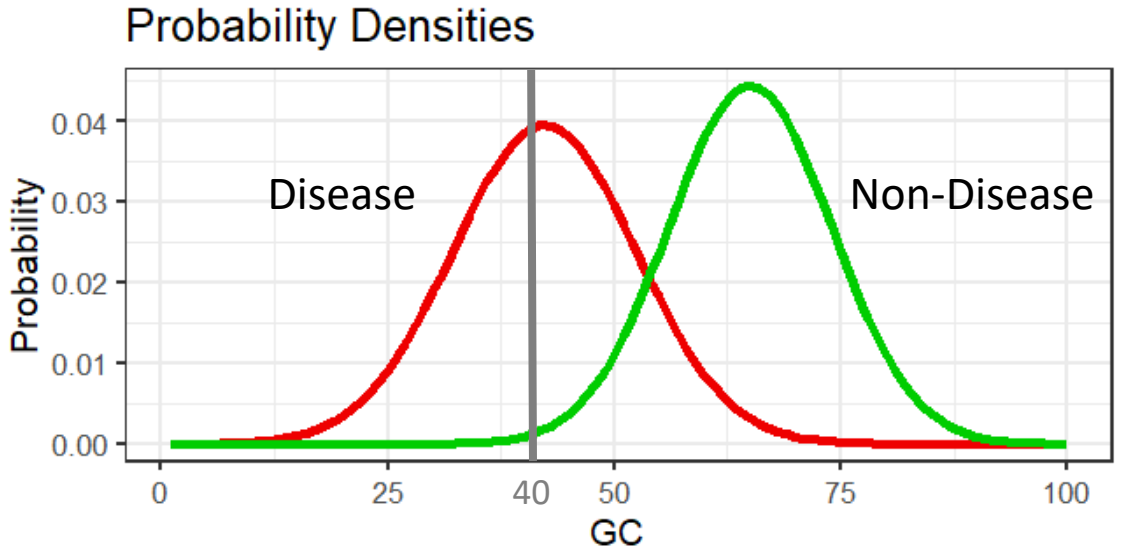
p Chr1 | Non Disease = 6 / 76 = 0.079
p Chr2 | Non Disease = 20 / 76 = 0.263
p ChrX | Non Disease = 50 / 76 = 0.658

Disease genes are more likely to be on Chr1 and Non Disease genes are more likely to be on ChrX

Quantitative Probabilities



State	mean	stdev
Disease	42.3	10.10
Non Disease	65.0	8.99



Assumption: quantitative values are normally distributed

Naïve Bayes Predictions

- Predict the state for a new datapoint
  - Chromosome is 1
  - GC content is 40%

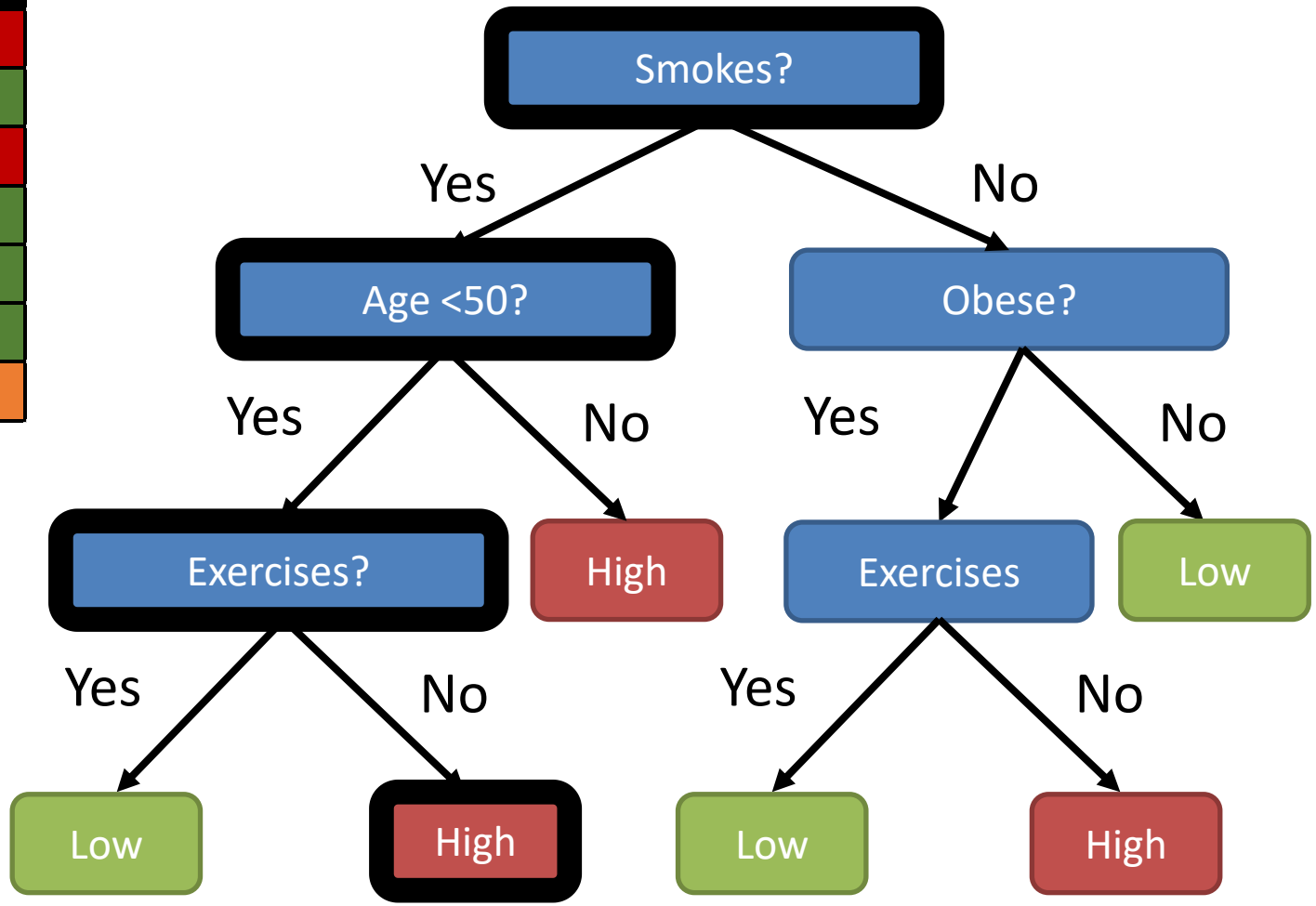
	Disease	Non-Disease
Prior (starting assumption)	(8/84) = 0.095	(76/84) = 0.905
Probability Chr1	0.625	0.079
Probability 40% GC	0.038	0.001
Total	**0.0022**	**0.00007**

New data is predicted to be **Disease**

Decision Trees

Predict Cancer Risk with a Decision Tree

Obese	Smoker	Exercises	Age	Cancer Risk
Yes	Yes	No	64	High
Yes	No	Yes	32	Low
Yes	No	No	58	High
No	Yes	Yes	25	Low
No	No	Yes	66	Low
No	No	Yes	34	Low
No	Yes	No	48	???



How do you build a tree?

- From a population of observations
  - Which variable do you use when?
  - [If quantitative] which cutoff do you use?

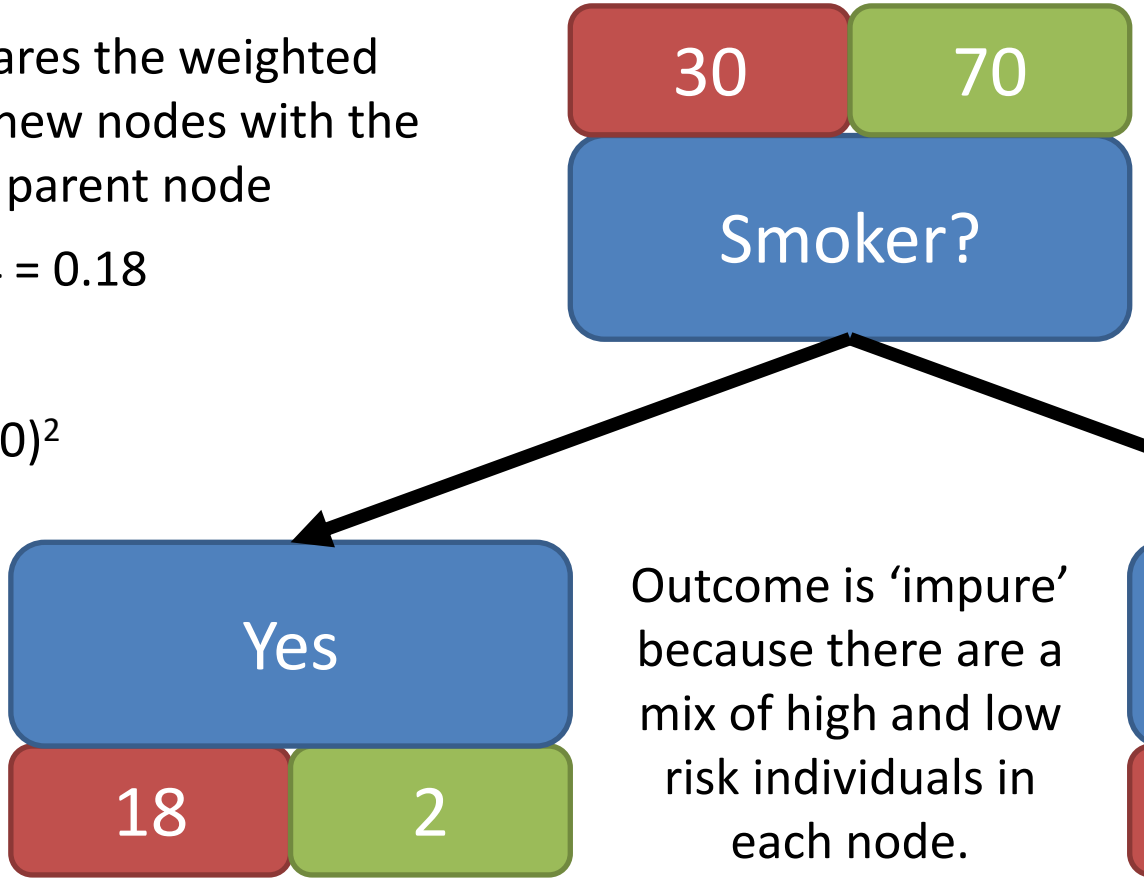
- Answer: you calculate an ‘impurity’ score and pick the least ‘impure’ variable to split the remaining data

- Want to use the most cleanly predictive question to improve the tree

Calculating Categorical Impurity

Gini gain compares the weighted average of the new nodes with the impurity of the parent node

0.42-0.24 = 0.18



Repeat for each question & select lowest impurity

$1 - (18/20)^2 - (2/20)^2$

0.180

$1 - (12/80)^2 - (68/80)^2$

0.255

Outcome is 'impure' because there are a mix of high and low risk individuals in each node.

Node impurity = $1 - (p\ \text{High})^2 - (p\ \text{Low})^2$ = Gini impurity

Weighted Average of Node Impurities = 0.18 * (20/100) + 0.255 * (80/100) = **0.24**

Calculating Quantitative Impurity

Age	Cancer Risk
25	Low
32	Low
34	Low
58	High
64	High
66	Low

Take mid-point between 34 and 58

Age <= 25 = 1 Low 0 High, Age >25 = 3 Low 2 High, Impurity = **0.40**

Age <= 32 = 2 Low 0 High, Age >32 = 2 Low 2 High, Impurity = **0.33**

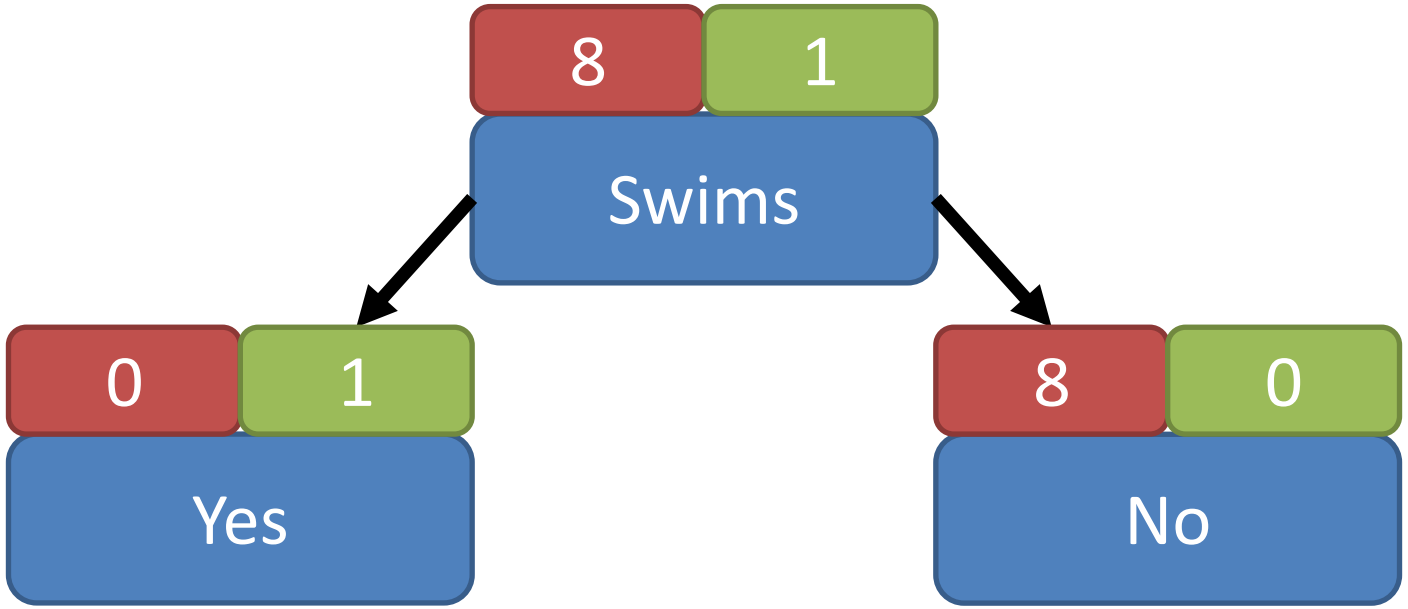
Age <= 34 = 3 Low 0 High, Age >34 = 1 Low 2 High, Impurity = **0.22**

Age <= 58 = 3 Low 1 High, Age >58 = 1 Low 1 High, Impurity = **0.42**

Age <= 64 = 3 Low 2 High, Age >64 = 1 Low 0 High, Impurity = **0.40**

Pruning Trees

- Lower branches may provide minimal additional information
- Leaves don’t need to be completely pure
- Can terminate the tree early and pick the majority answer
- When to stop can be determined by node size



Random Forests

Random Forest

- Decision trees can be fragile
  - Prone to overfitting – too specific to training data
  - Deterministic – same result every time
- Many trees are better than one!

Bagging

Bootstrapping
Selecting multiple random subsets of data

+

Aggregating
Making many predictions and voting

Bootstrapping

Two Levels of Randomisation

Original

	Obese	Smoker	Exercises	Age	Cancer Risk
x	Yes	Yes	No	64	High
	Yes	No	Yes	32	Low
	Yes	No	No	58	High
x	No	Yes	Yes	25	Low
	No	No	Yes	66	Low
x	No	No	Yes	34	Low

"Out of Bag"

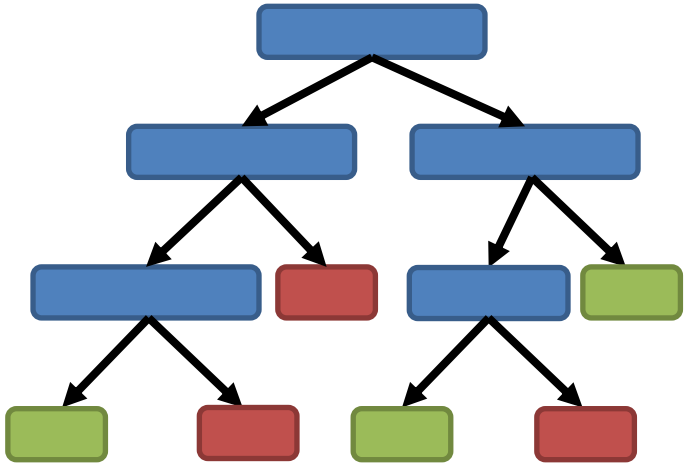
Random

Obese	Smoker	Exercises	Age	Cancer Risk
Yes	No	No	58	High
Yes	No	No	58	High
No	No	Yes	66	Low
Yes	No	Yes	32	Low
Yes	No	Yes	32	Low
Yes	No	No	58	High

Smoker | Exercises

Age | Exercises

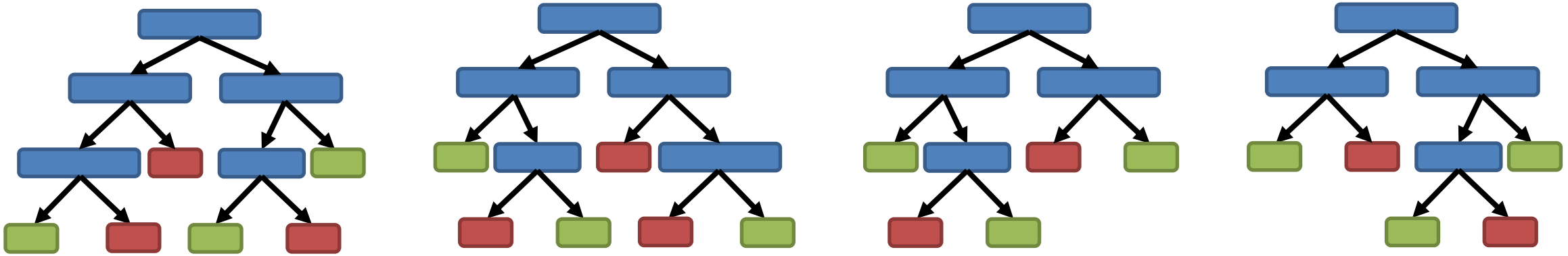
Age | Smoker



Build tree with random selection of variables at each branch point

Build a Forest

(hundreds of trees)



Evaluate

Run the “out of bag” data through the trees

See how often they predict correctly

Random variable number and
number of trees can be optimised

Predict

Run new data down all trees

Count the predicted outcomes

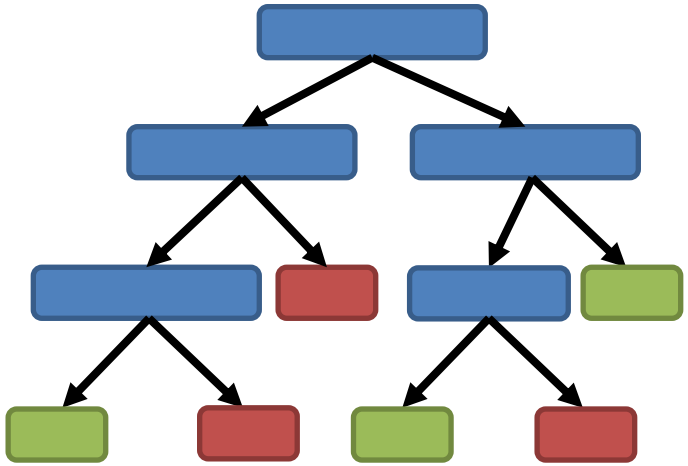
Most frequent outcome wins

Feature Selection

Smoker | Exercises

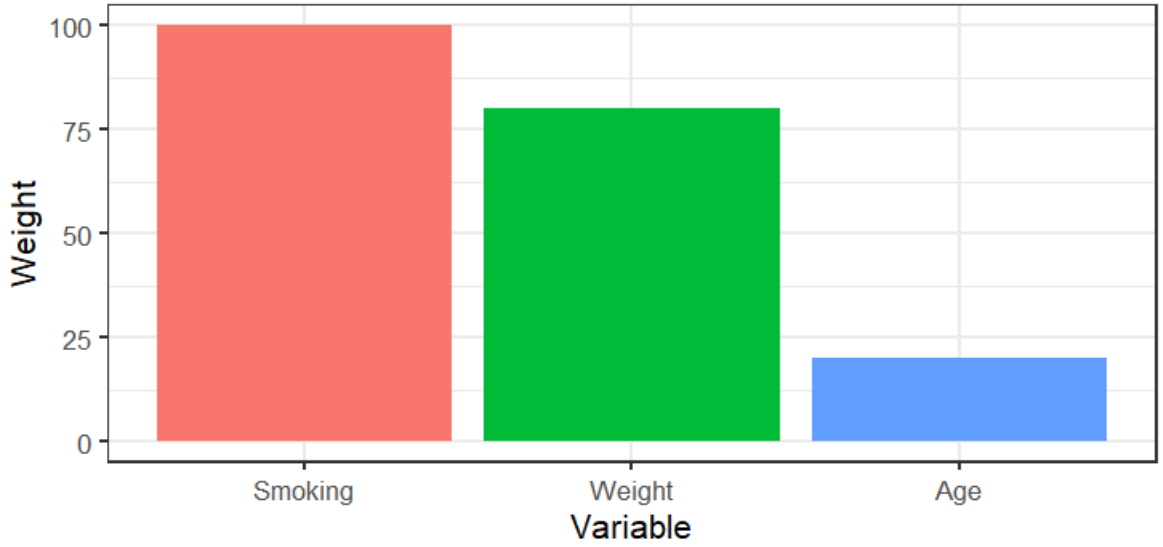
Age | Exercises

Age | Smoker



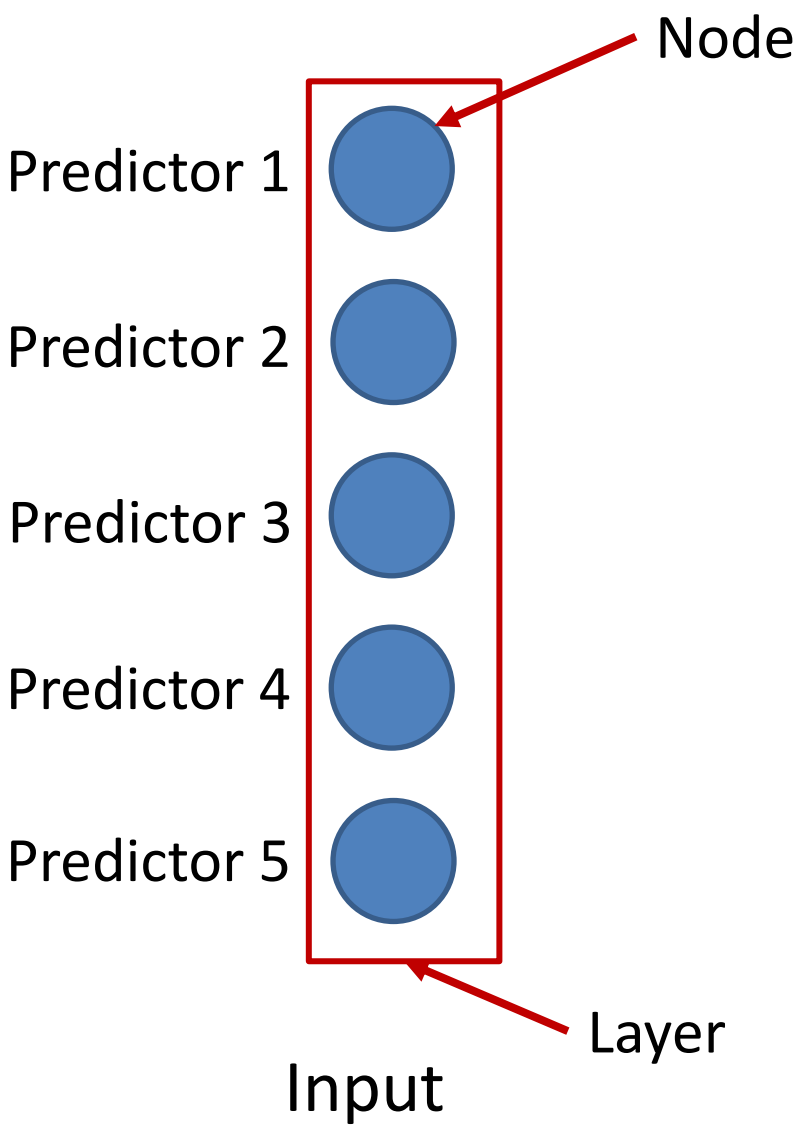
More informative features will appear higher up the tree.

Can aggregate this information across the forest

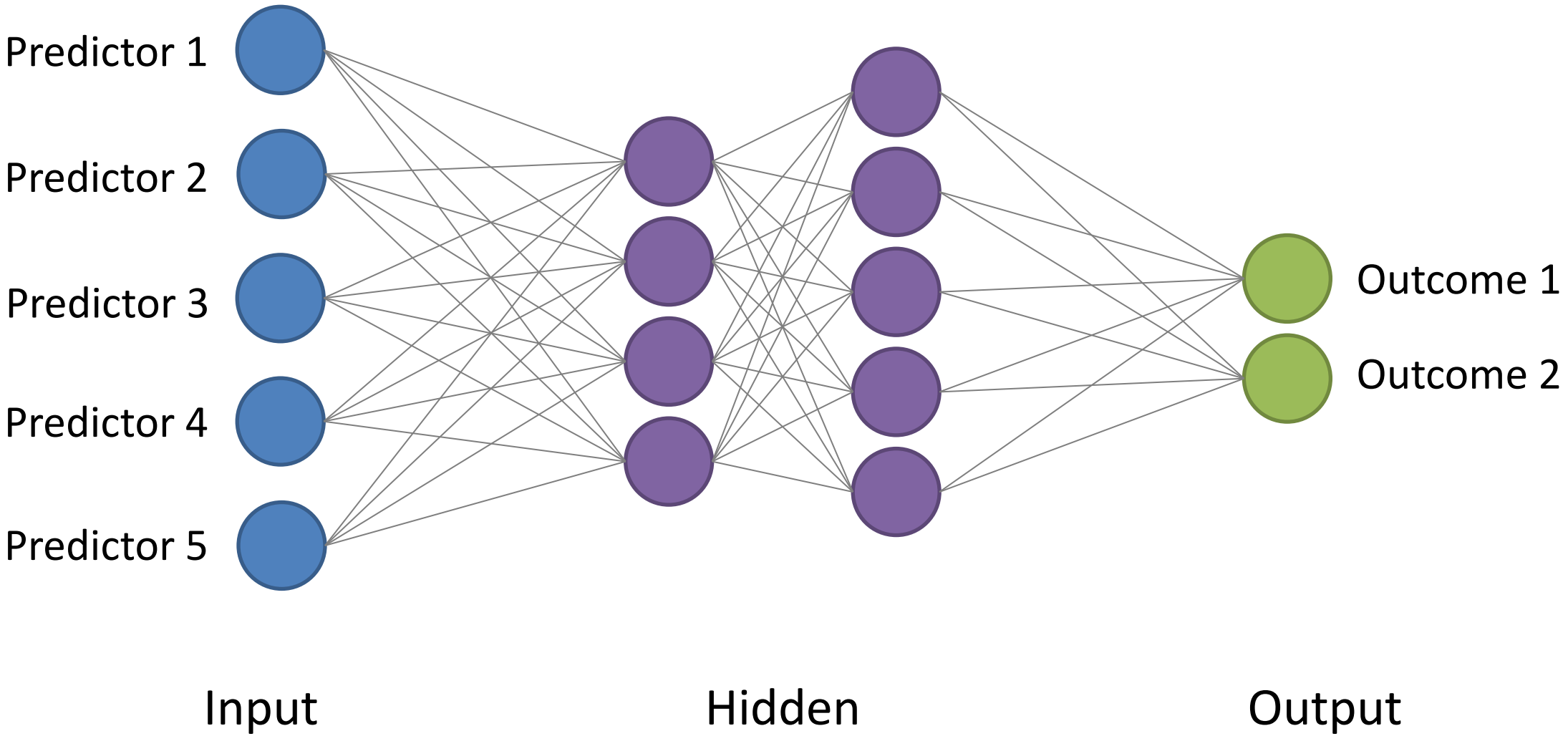


Neural Networks

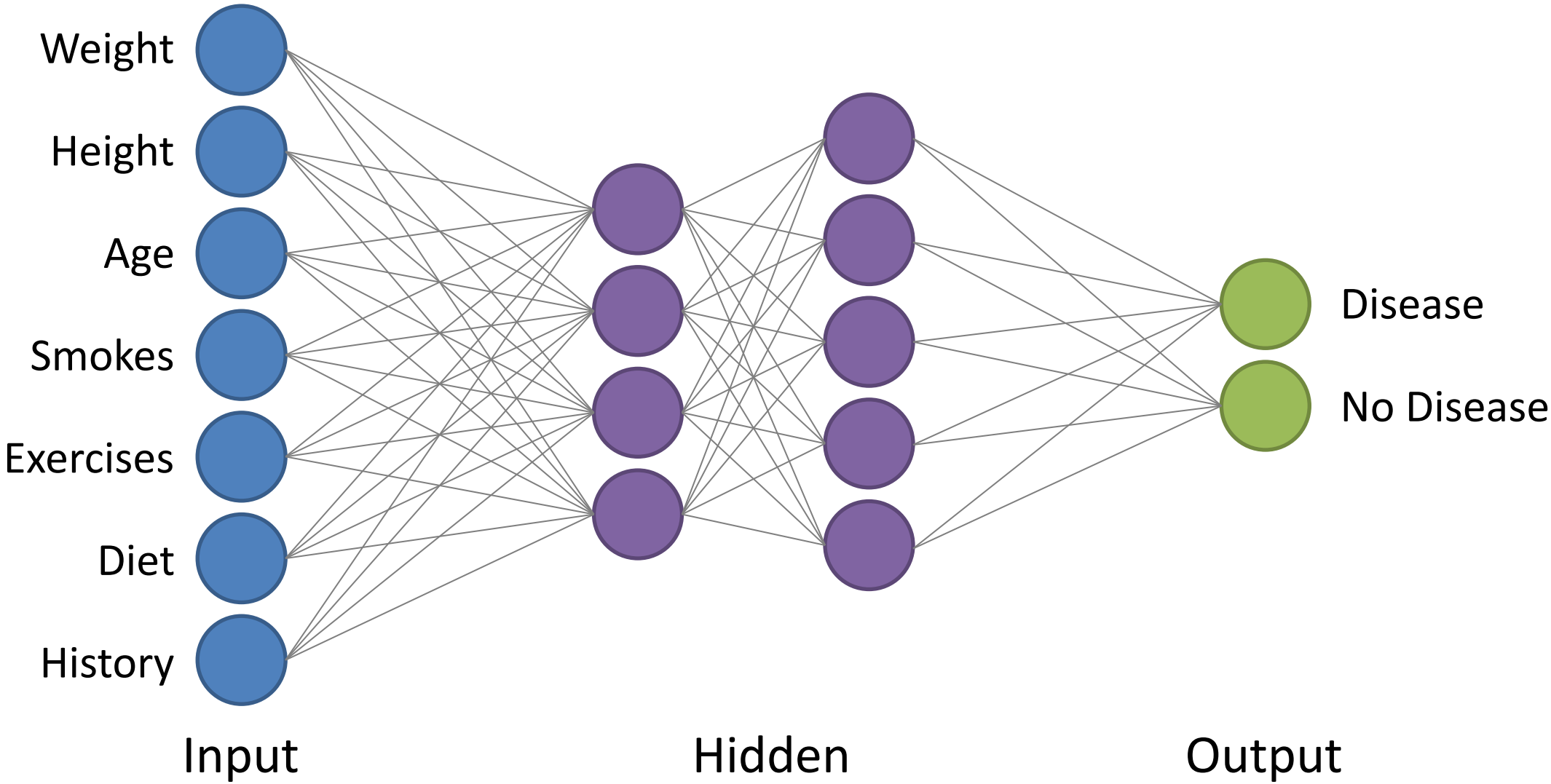
Neural Network Structure



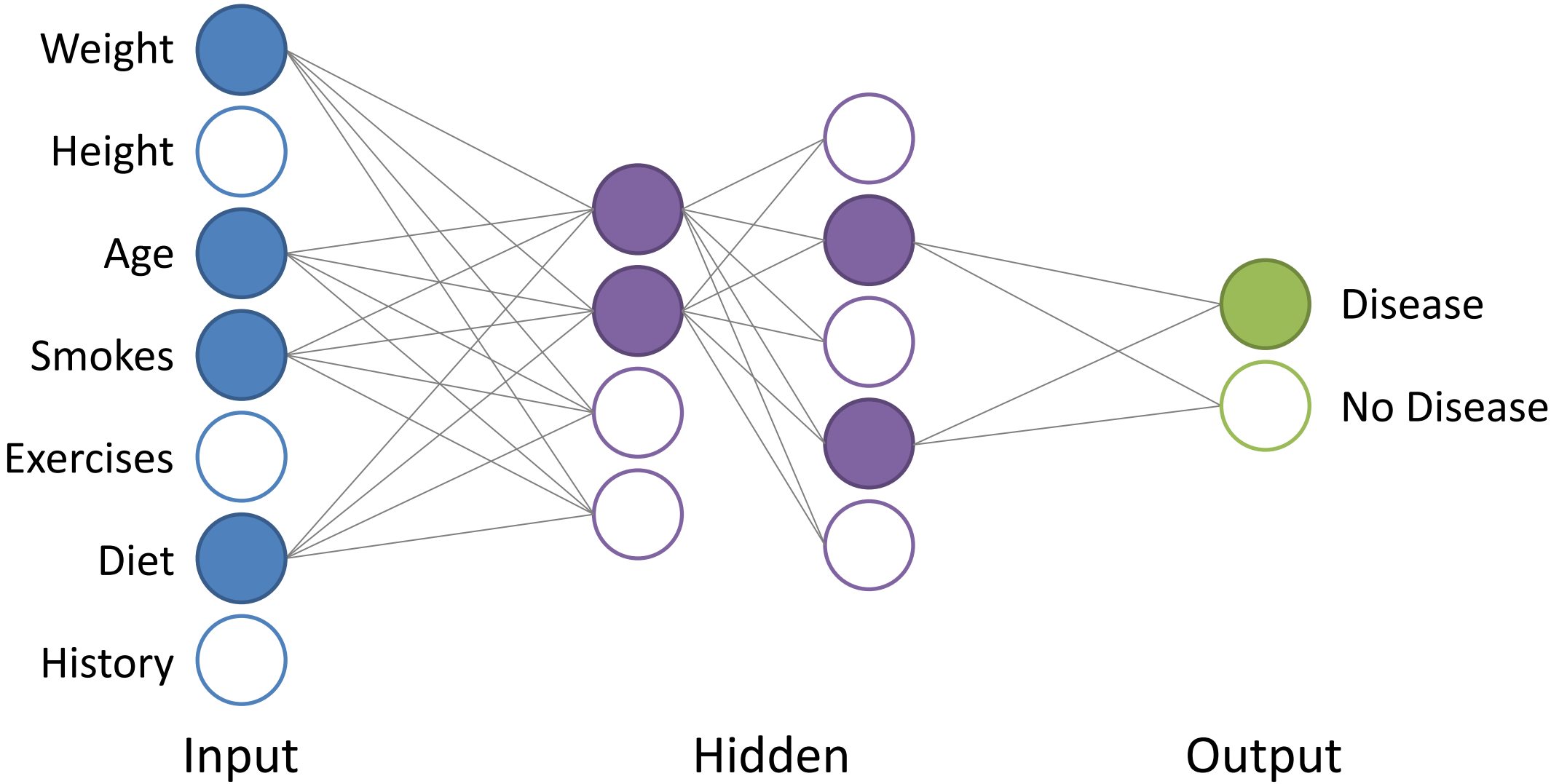
Neural Network Structure



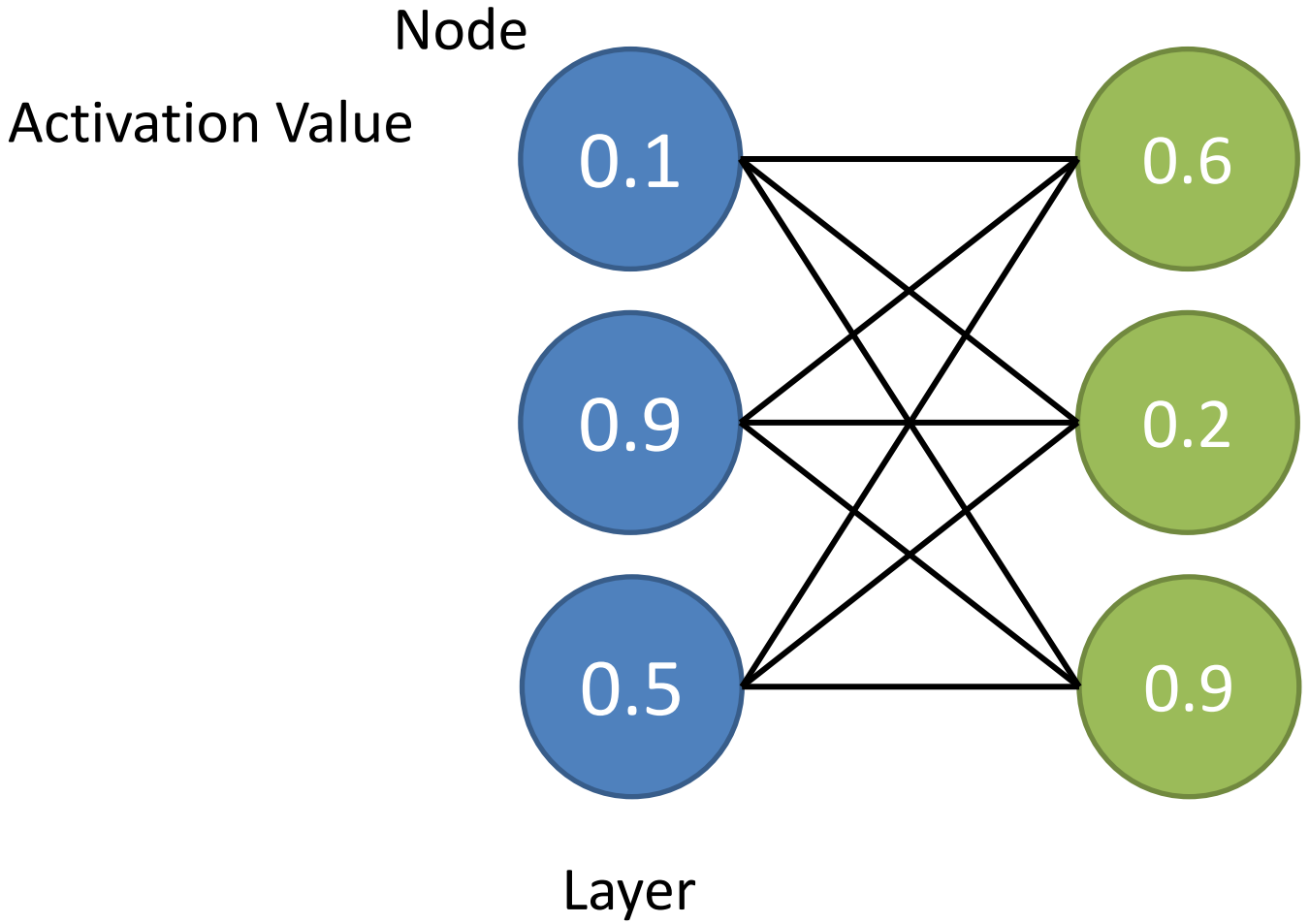
Neural Network Structure



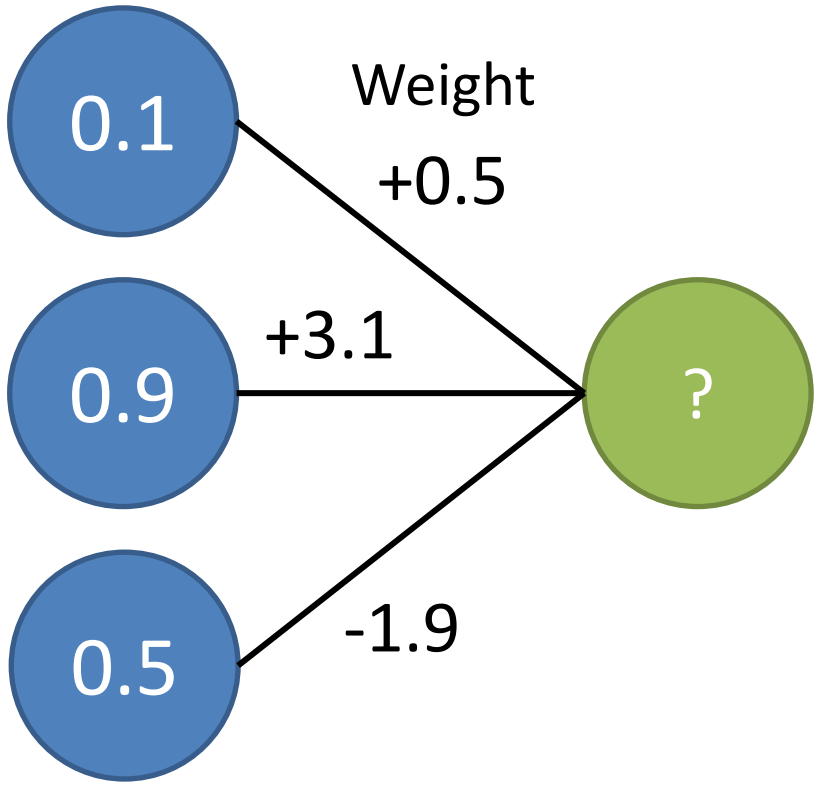
Using the network



Neural Networks



Calculating Node Values

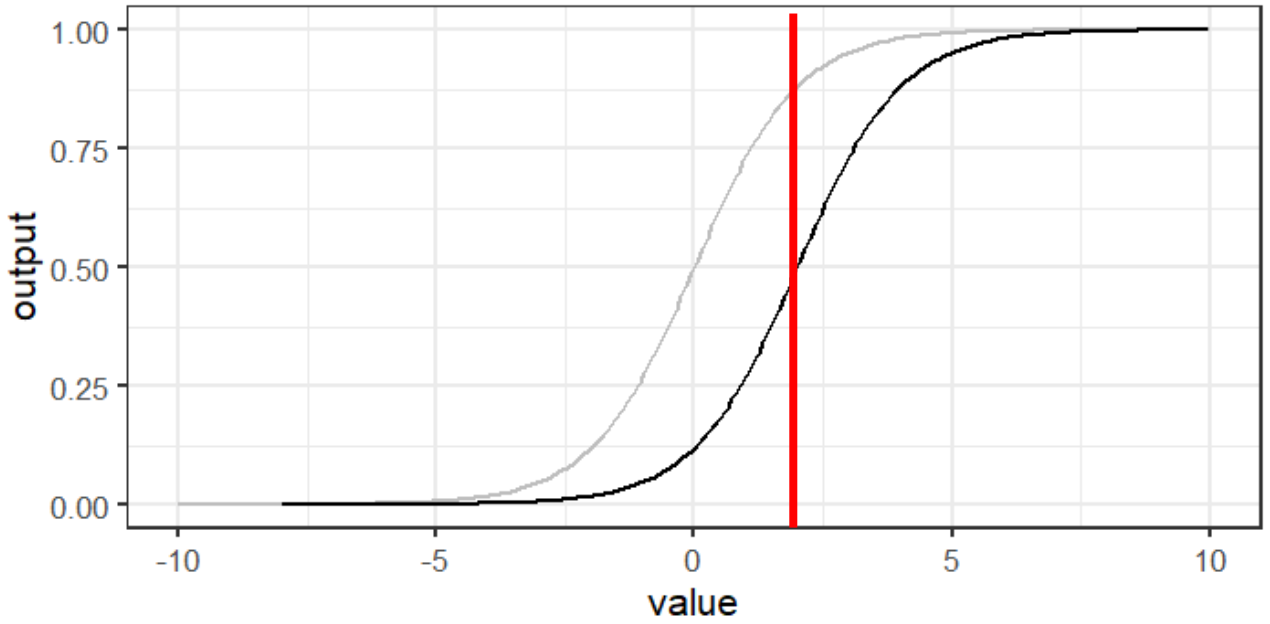


∑(activation x weight)

(0.1 x 0.5) + (0.9 x 3.1) + (0.5 x -1.9) = 1.89

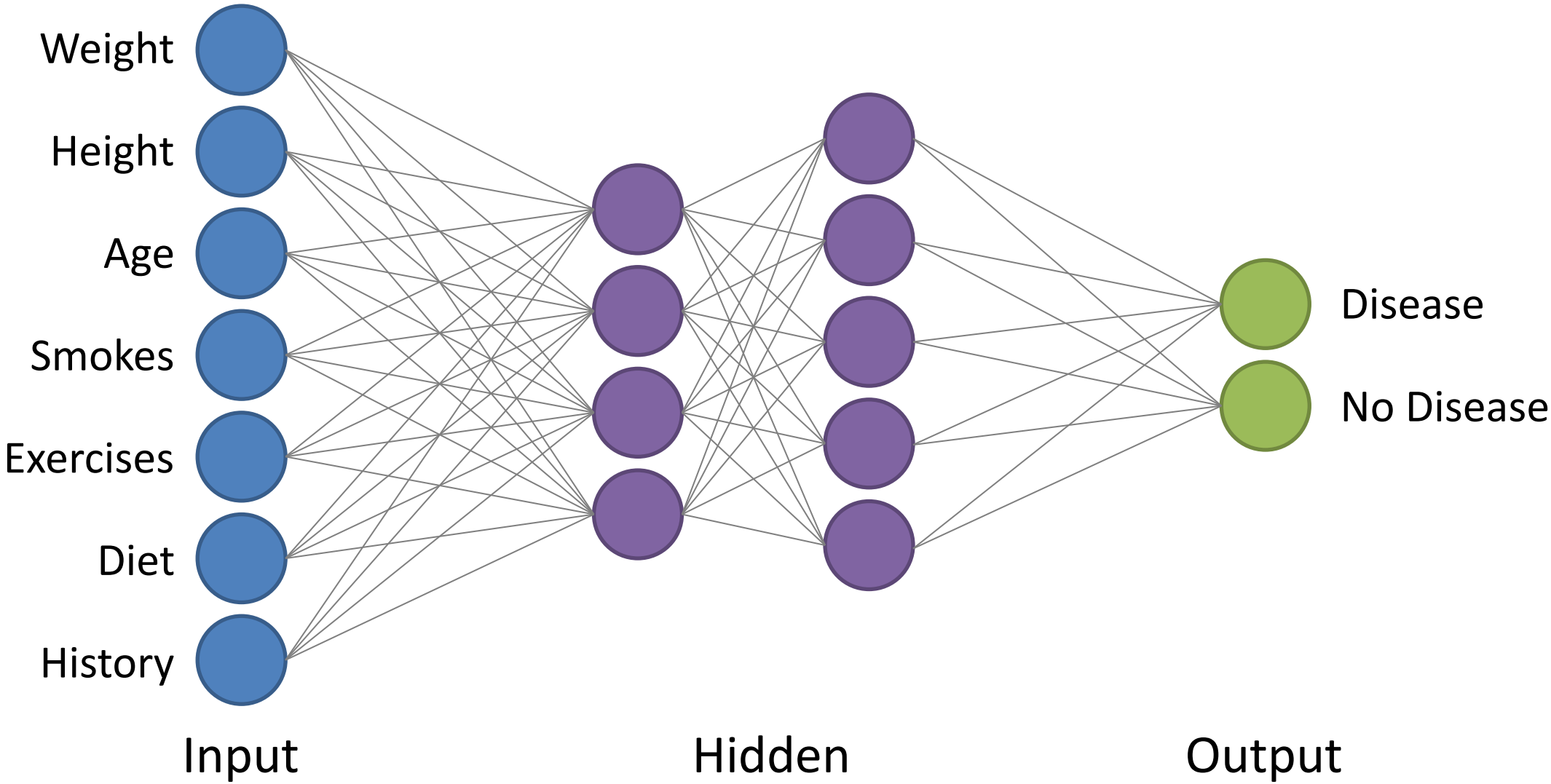
Sigmoid output = 0.87

Sigmoid output (bias 2) = 0.47



Training = Calculating Weights and Biases and optimising

Neural Network Structure



Training the network

Selecting the number of hidden layers

- Number of layers changes the type of relationships modelled

  0 hidden layers = linear relationship, similar to linear modelling

  1 hidden layer = nonlinear relationships

  2 hidden layers = nonlinear relationships with arbitrary boundaries

Most problems only require 1 hidden layer. More complex data can benefit from 2. Virtually nothing requires more than two.

Training the network

Selecting the number of nodes in hidden layers

Too few nodes will not allow enough complexity to model the system effectively

Too many nodes will overfit – essentially "memorising" the training data

Number of hidden layer nodes should be between the input number and the output number

Gives starting point, then can optimise

Simple

Try 2/3 input number plus output number

Complex

Nh = number of hidden nodes
Ni = number of input nodes
No = number of output nodes
Ns = size of training set
α = scaling factor (normally 2)

$$N_h = \frac{N_s}{(\alpha * (N_i + N_o))}$$

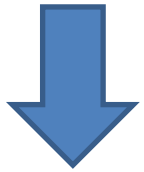
Training the network

Selecting weights and biases

Generate a "cost function" – a numerical value which says how well the model performed on the training data (high = bad, low = good)

Could just be how good the predictions are, but often good to include how complex the connections are

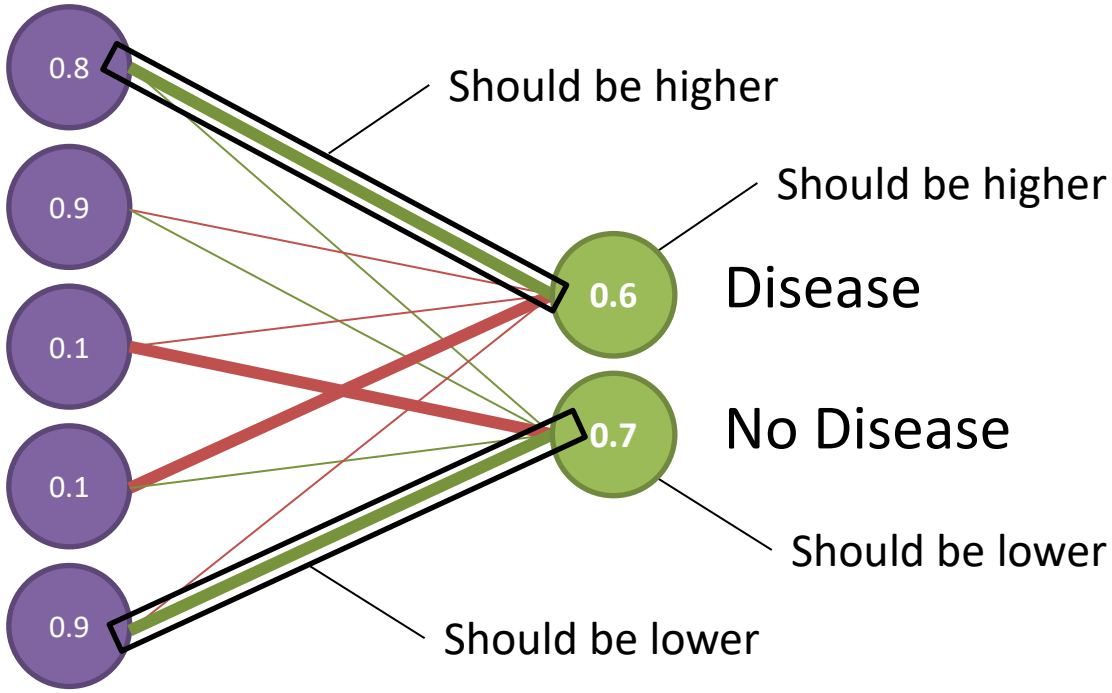
Start by initialising the weights / biases to random numbers



Shuffle the values to gradually minimise the cost function value

Training the network

Back Propagation



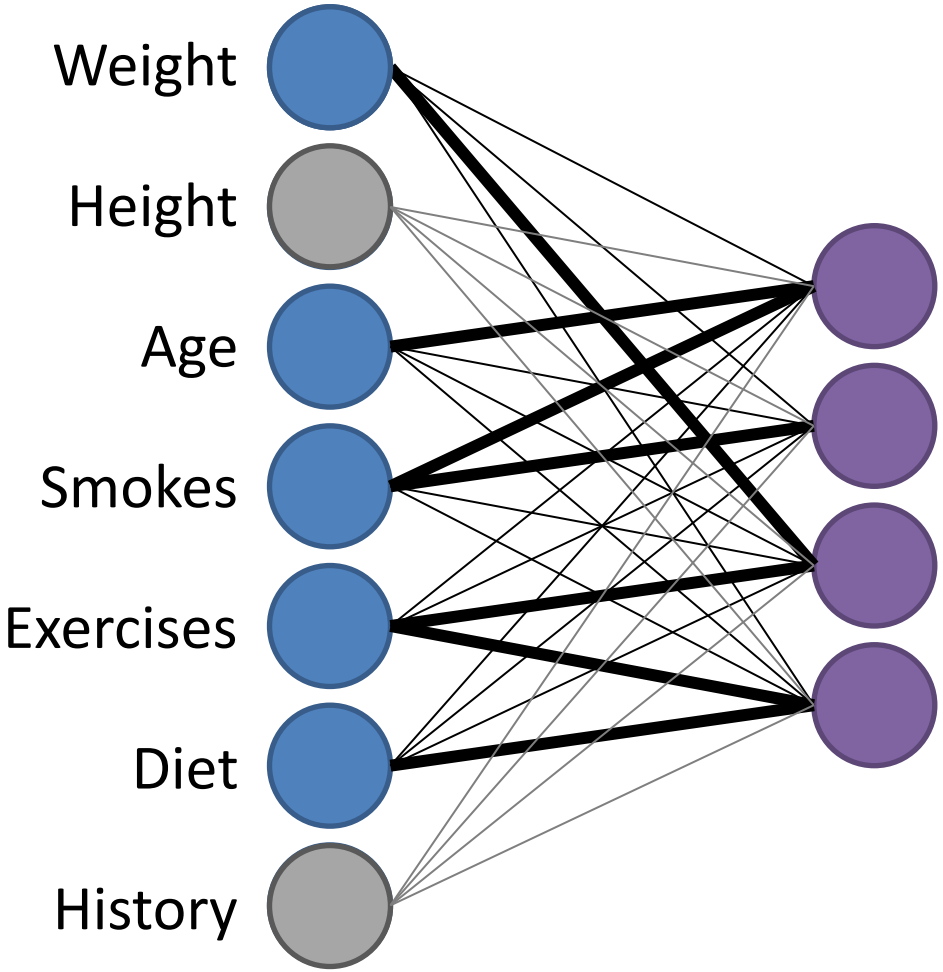
- How do you increase a value?
  - Increase positive weights
    - Tied to high activations upstream
  - Decrease negative weights
    - Tied to high activations upstream

- What doesn't matter?
  - Anything with a low weight
  - Anything with a low upstream activation

Prediction for a single **disease** sample

Average across all samples and then adjust

Cleaning the network



- Good idea to minimise the network
- Remove nodes where all output weights are low
- Having little effect on the rest of the network

Practical Machine Learning using R and tidymodels

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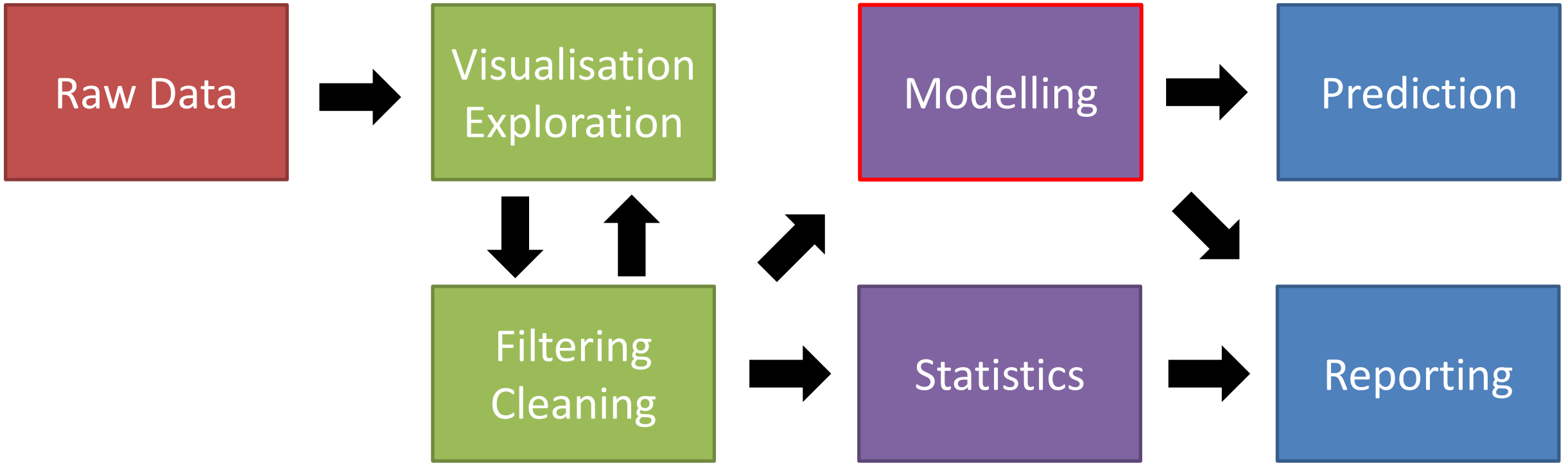
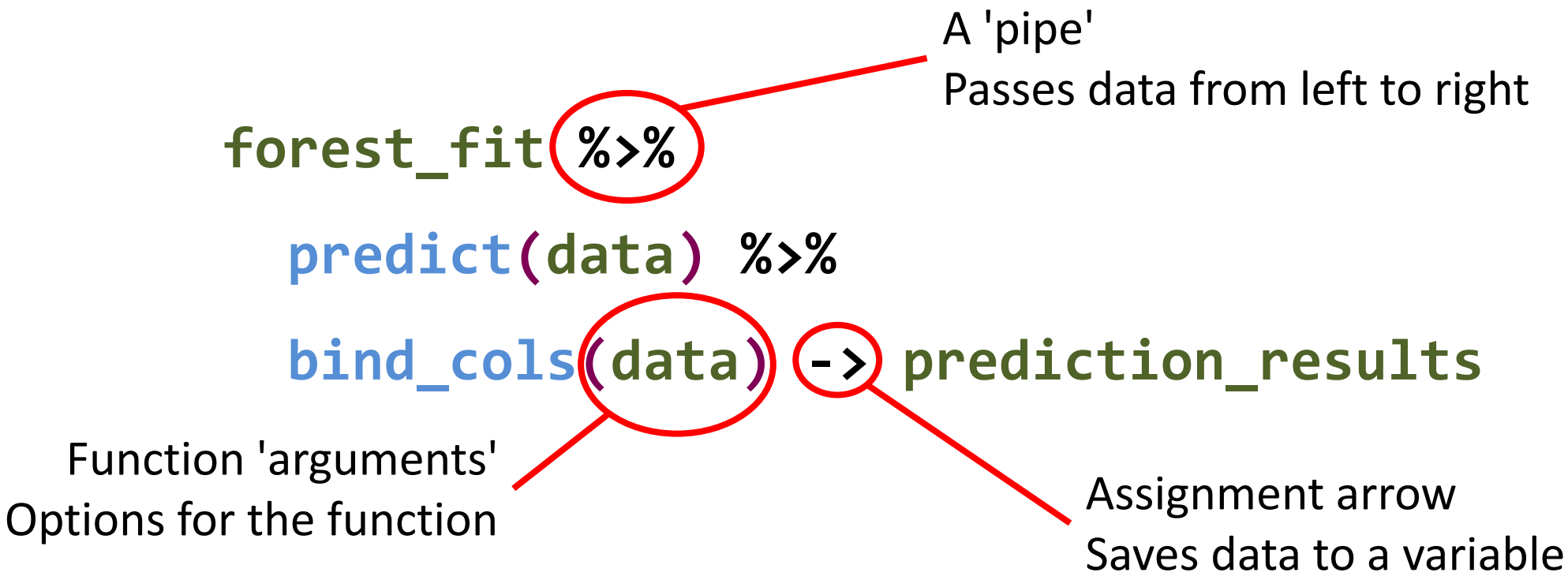
Data Analysis Workflow



R Syntax



Variables (data structures)

Functions (do stuff and give something back)

Packages for machine learning in R

- `lm`
- `nnet`
- `rpart`
- `brulee`
- `kknn`
- `ranger`
- `h2o`
- `mboost`
- `spark`
- `glmnet`
- `keras`
- `partykit`
- `aorsf`
- `stan`
- `kernlab`
- `thief`
- `tbats`
- `survival`
- `xrf`
- `hurdle`
- `aorsf`
- `gee`
- `lmer`
- `mgcv`

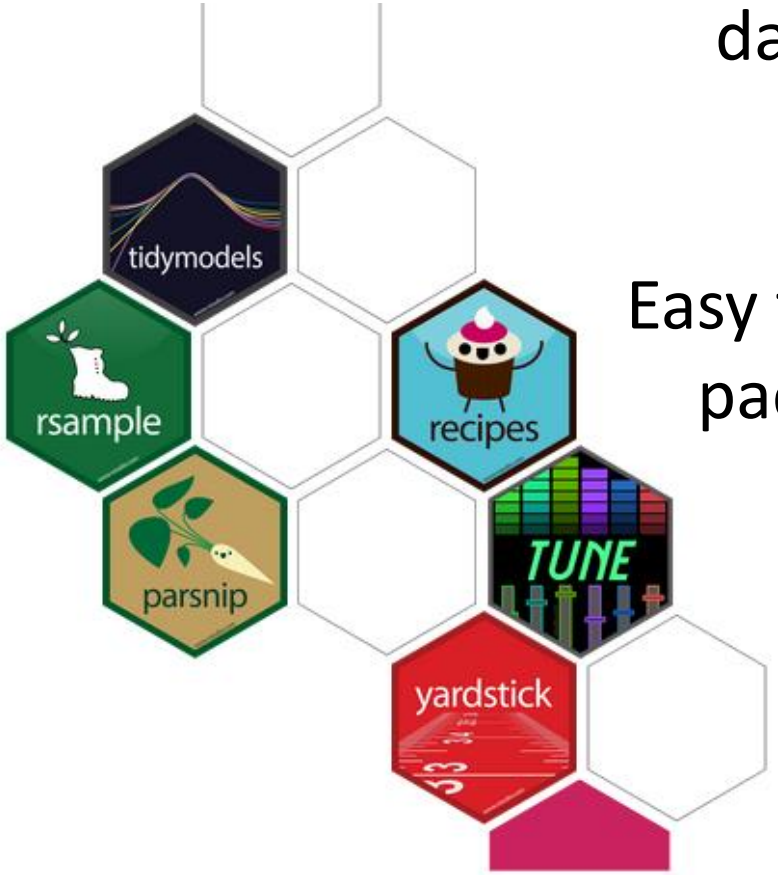
- Different model types
- Sometimes same model but with slight differences (tuneable factors, input data format, etc)
- Want to be able to easily try different model types

All have their own conventions for preparing data and building models

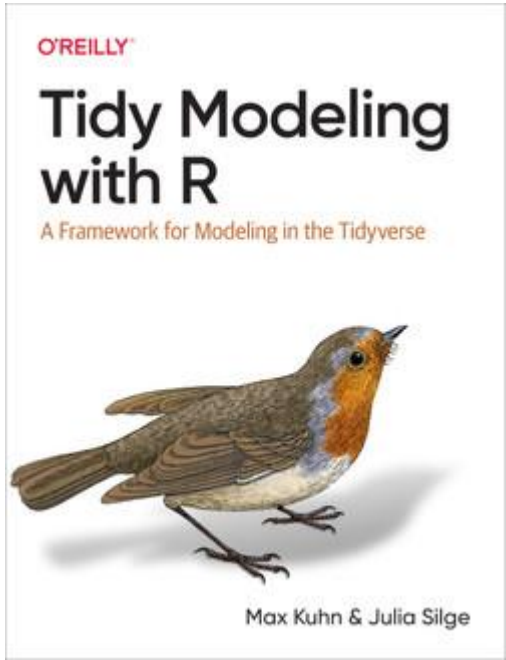
TidyModels

https://www.tidymodels.org/

Provides a consistent interface to prepare data, construct models and evaluate results.



Easy to move between different modelling packages with minimal code changes.



Input Data

- Tibble of data (2D Spreadsheet)
  - Read in as e.g. tsv, csv, excel spreadsheet
  - Rows are observations (cases) columns are variables
- Classification variables must be factors (not text)
- Standard exploration / plotting should happen before modelling *(not covered today)*

Code Structure

1. Create a model
   - No data yet, just the type of model and the settings to use
2. Create your data
   - Prepare and filter the input data (e.g. filtering/scaling/etc.)
   - Split off training / testing data
3. Train the model
   - Pass the data to the model and define the variable to predict
4. Test / Use the model
   - Use the trained model to predict new values

Create a Model

- parsnip = translation layer
- You need
  1. A model type
  2. An engine
  3. A mode
  4. Options

https://www.tidymodels.org/find/parsnip/

Search parsnip models

Find model types, engines, and arguments to fit and predict in the tidymodels framework.

To learn about the parsnip package, see *Get Started: Build a Model*. Use the tables below to find model types and engines.

Show 25 entries Search:

title	model	engine	topic	modes	package
All	and_forest	All	All	All	All
Oblique random survival forests via aorsf	rand_forest	aorsf	rand_forest_aorsf	censored regression	parsnip
Random forests via h2o	rand_forest	h2o	rand_forest_h2o	classification, regression	parsnip
Random forests via partykit	rand_forest	partykit	rand_forest_partykit	classification, regression, censored regression	parsnip
Random forests via randomForest	rand_forest	randomForest	rand_forest_randomForest	classification, regression	parsnip
Random forests via ranger	rand_forest	ranger	rand_forest_ranger	classification, regression	parsnip
Random forests via spark	rand_forest	spark	rand_forest_spark	classification, regression	parsnip

Create a Model

```
library(tidymodels)
tidymodels_prefer()

rand_forest(trees=100, min_n=5) %>%
    set_mode("classification") %>%
    set_engine("ranger") -> model
```

Model Options

The model function

Model Type

The back end engine

Creating Data

```
read_delim("development_gene_expression.txt") -> data

data %>%
    mutate(Development=factor(Development)) -> data

set.seed(123)
data %>%
    sample_frac() -> data
```

Basic R data manipulation – convert text column to factor

Control random element to make reproducible by setting the random seed

Shuffle data – random reordering to remove any structure

Splitting Data

```
data %>%
    initial_split(prop=0.8) -> split_data
```

```
training(split_data)
# A tibble: 992 × 93
```

```
testing(split_data)
# A tibble: 249 × 93
```

Convention = 80-90%
Consider how much data you have and frequency of cases

Training the Model

Create a formula

```
Variable to predict ~ Variables to use
```

```
Variable to predict ~ VarA + VarB + VarC
```

```
Variable to predict ~ .
```
(dot = everything else)

Training the Model

Performing a single fit

```
model %>%
    fit(Development ~ ., data=training(split_data)) -> model_fit

model_fit
```

```
parsnip model object

Ranger result

Call:
 ranger::ranger(x = maybe_data_frame(x), y = y, num.trees = ~100, min.node.size = min_rows(~5, x), num.threads = 1,
verbose = FALSE,seed = sample.int(10^5, 1), probability = TRUE)

Type:                             Probability estimation
Number of trees:                  100
Sample size:                      992
Number of independent variables:  92
Mtry:                             9
Target node size:                 5
Variable importance mode:         none
Splitrule:                        gini
OOB prediction error (Brier s.):  0.2412714
```

24% of out of bag predictions wrong

Evaluating / Using the Model

```
model_fit %>%
    predict(new_data=testing(split_data)) %>%
    bind_cols(testing(split_data))
```

.pred_class <fctr>	Development <fctr>	AdrenalCortex <dbl>	Appendix <dbl>
Development	Not_Development	6.787032	6.557910
Development	Not_Development	7.599913	7.794741
Development	Not_Development	9.914123	8.784308
Development	Development	5.608809	6.809286
Not_Development	Development	8.634448	8.676486
Development	Not_Development	6.692790	7.963474
Not_Development	Development	8.275368	7.859379
Development	Not_Development	8.375908	9.510962
Not_Development	Not_Development	2.867896	4.776104
Not_Development	Not_Development	9.104730	7.590587

1-10 of 249 rows | 1-8 of 94 columns

Evaluating / Using the Model

```
model_fit %>%
      predict(new_data=testing(split_data)) %>%
      bind_cols(testing(split_data)) %>%
      group_by(.pred_class, Development) %>%
      count()
```

.pred_class <fctr>	Development <fctr>	n <int>
Development	Development	23
Development	Not_Development	44
Not_Development	Development	71
Not_Development	Not_Development	111

Exercise: Building a model in tidymodels

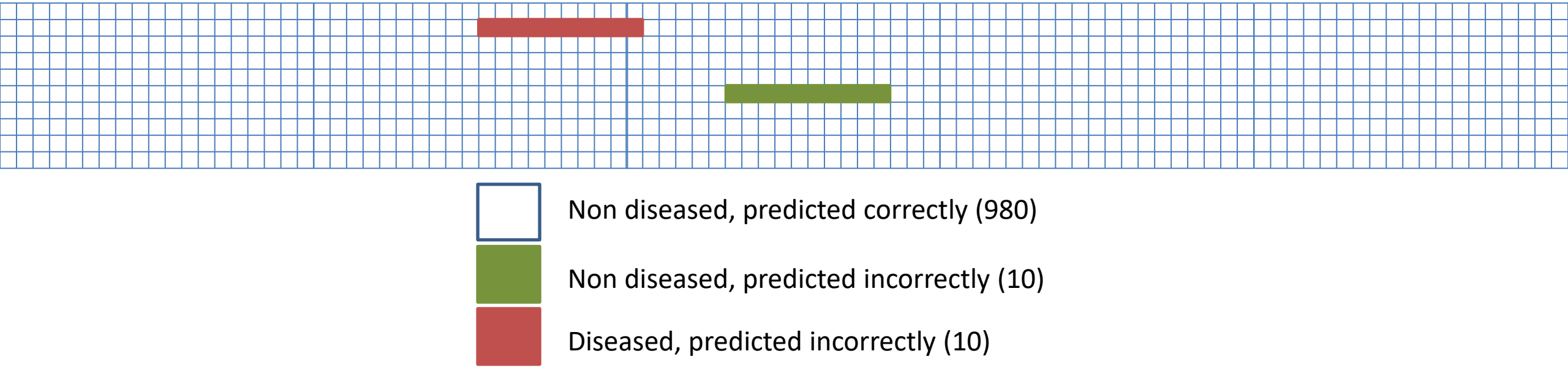
Evaluating Models

A good model?

DC

Disease Corp

In a recent study our new AI model correctly predicted the disease status of 980 out of 1000 patients – that's a 98% success rate!

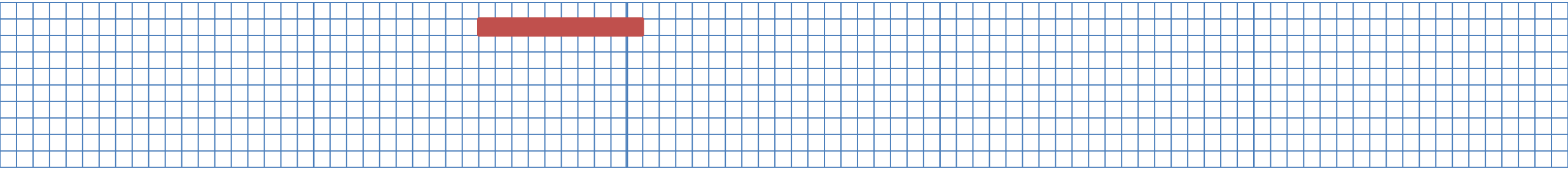


Non diseased, predicted correctly (980)

Non diseased, predicted incorrectly (10)

Diseased, predicted incorrectly (10)

Baseline for comparison



- 1000 patients, 10 have disease
- Assign most common category (healthy) to everyone

- 990 correct = 99% success!
- A good model must do better than this.

Evaluating Qualitative Models

Sample	Prediction	Truth	Correct
D	Healthy	Healthy	✓
E	Diseased	Diseased	✓
F	Diseased	Healthy	x
G	Healthy	Healthy	✓
H	Healthy	Diseased	x

Rather than overall success rate, break down by category

Confusion matrix

	True Healthy	True Diseased
Predicted Healthy	88	4
Predicted Diseased	6	24

False Negative

False Positive

Evaluating Qualitative Models

	True Healthy	True Diseased
Predicted Healthy	88	4
Predicted Diseased	6	24

(88+24) = 112 correct
(4+6) = 10 incorrect
Overall = 92% correct

	True Healthy	True Diseased
Predicted Healthy	88	4
Predicted Diseased	1	4

(88+4) = 92 correct
(4+1) = 5 incorrect
Overall = 95% correct

	True Healthy	True Diseased
Predicted Healthy	78	0
Predicted Diseased	16	28

(78+28) = 106 correct
(0+16) = 16 incorrect
Overall = 91% correct

Sensitivity vs Specificity

Sensitivity: How likely is the model to identify diseased patients correctly
Specificity: How likely is the model to identify healthy patients correctly

	True Healthy	True Diseased
Predicted Healthy	88	4
Predicted Diseased	6	24

Overall = 92% correct
Sensitivity = 24/28 = **86%**
Specificity = 88/94 = **94%**

	True Healthy	True Diseased
Predicted Healthy	88	4
Predicted Diseased	1	4

Overall = 95% correct
Sensitivity = 4/8 = **50%**
Specificity = 88/89 = **99%**

	True Healthy	True Diseased
Predicted Healthy	78	0
Predicted Diseased	16	28

Overall = 91% correct
Sensitivity = 28/28 = **100%**
Specificity = 78/94 = **83%**

Sensitivity vs Specificity

What matters more?

Overall = 92% correct
Sensitivity = 24/28 = **86%**
Specificity = 88/94 = **94%**

Overall = 95% correct
Sensitivity = 4/8 = **50%**
Specificity = 88/89 = **99%**

Overall = 91% correct
Sensitivity = 28/28 = **100%**
Specificity = 78/94 = **83%**

Getting both is ideal – obviously!

If **never missing disease** is the main concern favour **sensitivity**

If **not incorrectly false predictions** is important favour **specificity**

Need to consider the frequency of true positives

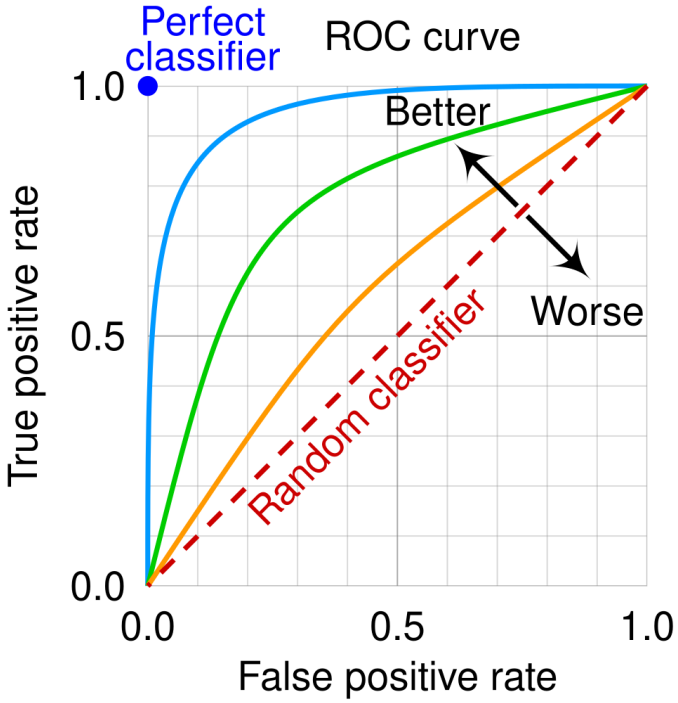
Cohen's Kappa Score

- Measures whether the predictions are correct more often that you'd expect if the model was just guessing
- Takes into account the proportion of predictions and observations in each class

Kappa	Agreement
<0	Less than chance agreement
0.01-0.20	Slight agreement
0.21-0.40	Fair agreement
0.41-0.60	Moderate agreement
0.61-0.80	Substantial agreement
0.81-0.99	Almost perfect agreement

Area Under the ROC Curve (AUC)

- ROC curves plot the model's True Positive Rate (TPR) as a function of its False Positive Rate (FPR)
- AUROC values of:
  - 1.0 = a perfect classifier
  - 0.5 = a classifier with random guessing performance
  - 0 = the worst possible classifier
- If not a binary classifier then it can be calculated for each class in turn and take a weighted average (e.g. by number of instances in each class)



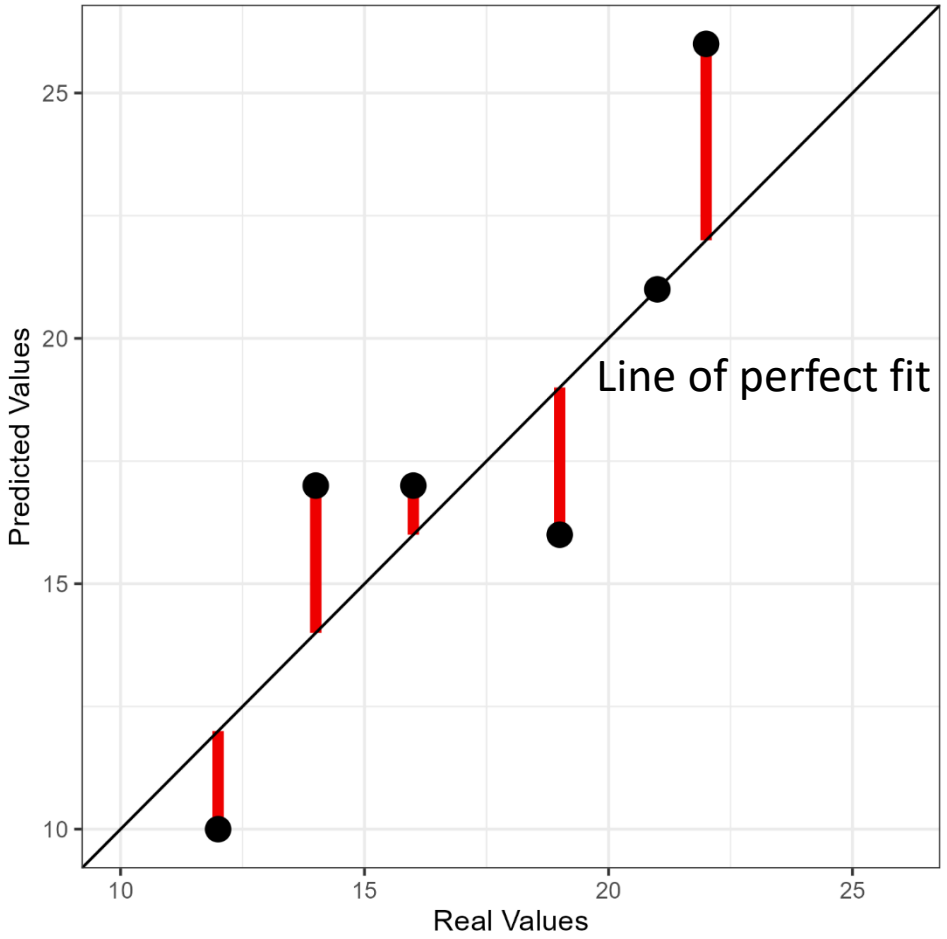
Evaluating Quantitative Models

- Correlation/association between predictions and true values (R or R^2)

- How close are the predictions to the true values?
- Doesn’t matter if the mistake is high or low

- Need a single value to summarise the total error

Evaluating Quantitative Models



Differences (+ and -)

Square differences (all positive)

Sum differences = single value

Sum of Squared Differences

SSD

Evaluating / Using the Model

```
model_fit %>%
predict(new_data=testing(split_data)) %>%
bind_cols(testing(split_data)) %>%
sens(Development,.pred_class)
spec(Development,.pred_class)
metrics(Development,.pred_class)
```

.metric <chr>	.estimator <chr>	.estimate <dbl>
sens	binary	0.2446809

.metric <chr>	.estimator <chr>	.estimate <dbl>
spec	binary	0.716129

.metric <chr>	.estimator <chr>	.estimate <dbl>
accuracy	binary	0.53815261
kap	binary	-0.04153785

Evaluating / Using the Model

Alternative is to use augment:

```
model_fit %>%
    augment(new_data=testing(split_data))
```

.pred_class <fctr>	.pred_Development <dbl>	.pred_Not_Development <dbl>	Development <fctr>
Development	0.5491667	0.4508333	Not_Development
Development	0.5236667	0.4763333	Not_Development
Development	0.5028333	0.4971667	Not_Development
Development	0.5778333	0.4221667	Development
Not_Development	0.4391667	0.5608333	Development
Development	0.5325000	0.4675000	Not_Development
Not_Development	0.4848333	0.5151667	Development
Development	0.5701667	0.4298333	Not_Development
Not_Development	0.4478333	0.5521667	Not_Development
Not_Development	0.4748333	0.5251667	Not_Development

Input Data

Garbage in = Garbage out

- Noisy Variables
- Outliers
- Poorly Scaled Variables
- Duplicates
- Conflated Signals
- Poorly Constructed Features
- Missing Data
- Data Leakage

Data Cleaning, Filtering, Scaling and Feature Construction

Common Data Problems

Data Leakage

Accidentally including something unintentional which reveals the true prediction for the case

- Audio clips from right whales were shorter than those from other species.
- The right whale clips were next to each other in the dataset

- Healthy scans came from children
- COVID scans came from people lying down
- Models recognised the font on the scan pictures

Common Data Problems

- Outliers
  - Extreme values, or just mistakes, will skew summary metrics
- Missing values
  - Handled poorly by many models, either remove, or impute (with care)
- Noisy variables
  - Variables with no connection to the question. Slow modelling and make results worse
- Different scales
  - Quantitative models benefit from having variables with similar ranges of values

Preprocessing

Converting to Numbers

- Some models require all data to be numeric
  - Linear Models, SVM, Neural Nets
  - Create ‘dummy variables’
- Some don’t care
  - Decision trees, Random Forest

Blue	Red	Purple	Orange	Green
0	1	2	3	4

Blue	Red	Purple	Orange	Green
1	0	0	0	0
0	0	1	0	0
0	1	0	0	0
0	0	0	0	1

Preprocessing

Scaling and Normalising

- Some models expect numerical data which behaves in a roughly normal manner
  - Naïve Bayes, Linear Modelling, Neural Nets
- Transformations make data more usable
  - Log transformation
  - Mean centering
  - Z-score normalisation
  - Converting to ranks
- Often dealing with high-dimensional data → More advanced transformations
  - PCA to remove noise (e.g. single cell data)

Preprocessing

Data Filtering

- Good idea to reduce the data complexity
  - Remove noise
  - Reduce size (runs quicker)
- Remove variables or cases which aren't helpful
  - Outlier values
  - Poorly measured features
  - Redundant features, e.g. highly correlated variables
  - Features with no variability

Exercise: Evaluating Models

BioTrain.TV

#Babraham Bioinformatics

That's it! - What Next?

Scan or Click to tell us what you thought

- Other relevant courses?
  - Introduction to R (with tidyverse): TBC
  - Advanced R (with tidyverse): TBC
  - Creating Complex Figures with GGPlot: TBC
- Stay in touch: contact@biotrain.tv

Automation with Recipes and Workflows

- Preprocessing often has multiple steps
- Need to apply these to training, testing and future data
- Manually preprocessing is tedious and potentially inconsistent

- Recipes let you automate this
  - More work initially but more reproducible
- Workflows bring everything together

Automation with Recipes and Workflows

- Create a recipe
  - Specify formula and optionally data (shows what looks like)
- Add processing steps
  - Filtering, Transformation etc.
- Create a model
  - Same as we did before
- Create a workflow
  - Combine the recipe and model together

Creating a Recipe

```
recipe(
    var_to_predict ~ .,
    data=training(split_data)
) -> my_recipe
```

You add data here but it's only used to list and type the variables.
You still need to provide it when you train or use the model

Recipe Preprocessing Steps

- `step_rm` : Remove one or more variables
- `step_log`: Log transform variables
- `step_normalize`: Convert values to z-scores
- `step_dummy`: Create numerical dummy variables from text
- `step_other`: Combine infrequent categories into an 'other'
- `step_corr`: Remove variables which are highly correlated
- `step_naomit`: Remove rows/columns with missing values

Full list of steps at https://recipes.tidymodels.org/reference/index.html

Applying Steps to Variables

Individually named variables

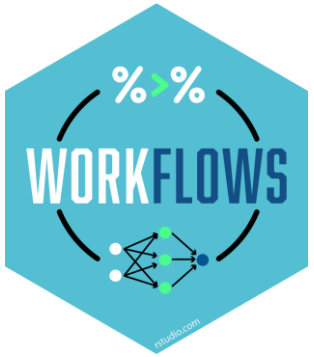
```
step_rm(Unsued1, Unused2)
```

Role selectors

```
step_normalize(all_numeric_predictors())
step_dummy(all_nominal_predictors())
```

Adding Preprocessing Steps

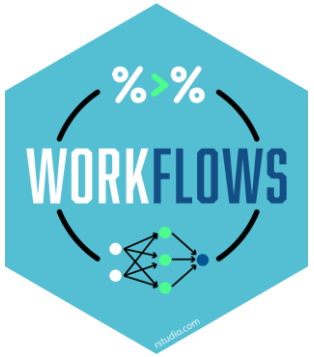
```
my_recipe %>%
    step_rm(Unsued1, Unused2) %>%
    step_log(expression, gene_length) %>%
    step_normalize(all_numeric_predictors()) %>%
    step_dummy(all_nominal_predictors()) -> my_recipe
```



Creating a workflow

- Workflows bring together
  - Recipe (training data, preprocessing, formula)
  - Model

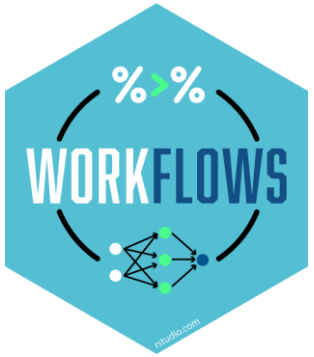
```
workflow() %>%
    add_recipe(my_recipe) %>%
    add_model(my_model) -> my_workflow
```



Training via a workflow

```
my_workflow %>%
    fit(training(my_data)) -> my_workflow
```

Fits the model, but also finalises choices in the recipe inside the workflow



Testing via a workflow

```
my_workflow %>%
    predict(new_data=testing(my_data)) %>%
    bind_cols(testing(my_data)) %>%
    select(.pred_class, var_to_predict)
```

Predict will automatically pull the trained model out of the workflow and will run the recipe on the new data

Exercise: Automating models with workflows