

# Putting the CART before the horse

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# Classic modelling

## Multiple Regression approach

Simple linear regression:

$$\text{Age} = X(\text{marker1}) + c$$

We try to find values for  $x$  &  $c$  that come as close as possible to solving the equation for each set of values for *Age* and *marker1* we have.

Two predictors:

$$\text{Age} = X(\text{marker1}) + Y(\text{marker2}) + c$$

Many predictors

$$\text{Age} = X(\text{marker1}) + Y(\text{marker2}) + Z(\text{marker3}) + W(\text{marker4}) + \dots + c$$

Where we have many different markers, we can find values of  $x$   $y$   $z$   $w$  etc that solve this equation very well but don't provide

# How do we avoid overfitting?

We want:

Modelling approach that can capture the signal without simply reproducing all the noise present in our dataset

To maximise predictive power

Approaches:

Data partitioning:

train-test split  
cross-validation)

Model type

Ensemble methods!

Model parameters

Exploring parameter space

# Machine Learning terminology

## Supervised vs unsupervised learning

Unsupervised learning: find the shape of the data (  
(eg: PCA, kmeans clustering)

Supervised learning: train an algorithm to recapitulate the examples  
it sees in a dataset  
(eg: linear regression)

## Classification vs Regression

Classification: categorise examples into one of a number of discrete  
categories

Regression: determine value along range

# Tree ensemble approaches

## Decision tree

Classify or perform regression by asking binary questions of data: whether value of marker X is above or below key value Y, whether marker Z is above or below. . . .

## Random Forest

Ensemble of decision trees, each using a random subset of the predictors to classify/perform regression on a random subset of the data

Resists overfitting

## Gradient Boosting Machine

Start with simple model (eg: mean of values in training dataset)

# Random Forest parameters

`ntree`: number of trees

`mtry`: Number of variables randomly sampled as candidates at each split

`min.node.size`: sets depth of trees

`cross-validation folds`: number of repartitions of data for testing

`splitting model`: variance or “extratrees”

# My project as example

## Project

Examine the effect of regeneration on the molecular age profile of *Parhyale* limbs

## Designing codeset

- \*Nanostring as method to quantify gene expression
- \*200 genes in codeset
- 195 genes chosen on the basis of differential expression analysis
- 5 control genes: do not vary in expression between conditions