Tree-based methods

Oxford Spring School in Advanced Research Methods 2025

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Day 3/5

Recap

Over past two sessions:

- Got to grips with important concepts re. machine learning
  - Gradient descent
  - Regularisation
- Explored extensions to **linear** prediction strategies
  - LASSO as a regularised version of OLS
  - Other extensions like ridge regression

But what if we want to model unknown and potentially *complex* relationships?

- Multi-way interactions
- Unknown polynomial terms
- Non-parametric relationships

Today's session

Explore a form of ML that helps find the optimal model:

- Uses "trees" to subset training data
- Making predictions on the basis of subsets
- Same foundational ML concepts recur...
    - Regularisation
- ...And we introduce some new ones:
    - Hyperparameter tuning

Remainder of the session:

1. Introduction to decision trees
2. Random forest
3. Hyperparameter tuning
4. Bayesian Additive Regression Trees

Decision trees

Motivation I

Consider the following data:

y_i	X_{1i}	X_{2i}
1	a	q
0	b	q
1	a	q
0	b	q

Suppose we observed the following new observation:

y_j	X_{1j}	X_{2j}
?	a	q

- What is $\hat{y}_j$?

Motivation II

Now consider this modified data:

y_i	X_{1i}	X_{2i}
1	a	q
1	a	q
1	a	r
0	b	q
0	b	q
1	b	r

Suppose we observed the following new observations:

y_j	X_{1j}	X_{2j}
?	a	r
?	b	r

- What are the predicted values here?

Homogenous subsets of $\boldsymbol{X}$

Example 1

- $\mathbb{E}[Y|X_1 = a] = 1$
- $\mathbb{E}[Y|X_1 = b] = 0$

Y_i	X_{1i}	X_{2i}
1	a	q
0	b	q
1	a	q
0	b	q

Example 2

- $\mathbb{E}[Y|X_1 = a, X_2 = q] = 1$
- $\mathbb{E}[Y|X_1 = b, X_2 = q] = 0$
- $\mathbb{E}[Y|X_1 = a, X_2 = r] = 1$
- $\mathbb{E}[Y|X_1 = b, X_2 = r] = 1$

Y_i	X_{1i}	X_{2i}
1	a	q
1	a	q
1	a	r
0	b	q
0	b	q
1	b	r

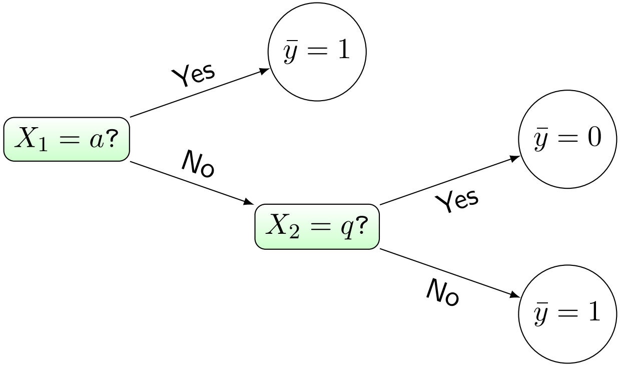
Prediction via subsetting

Tree-based ML methods make predictions on the basis of subsetting the data:

1. We start with training data $\boldsymbol{X}$
2. Choose a variable $\boldsymbol{X}_j$
3. Split $\boldsymbol{X}_j$ at some point c along that dimension
4. Either:
    a. Calculate the conditional mean for each of the two splits
    b. Repeat steps 2-3

Graphical depiction of a tree

Using the data from the second example yields a decision tree:



Tree terminology

Decision Node

- A junction in the network where we split the data in two
- Requires some splitting rule or decision

Branch

- A path along the tree

Terminal node or “leaf”

- The final node along a tree branch (i.e. no further splits)
- Returns a prediction or label for y

Depth

- The maximum number of nodes between the “root” node (i.e. original full data) and a leaf node

Alternative visualisation

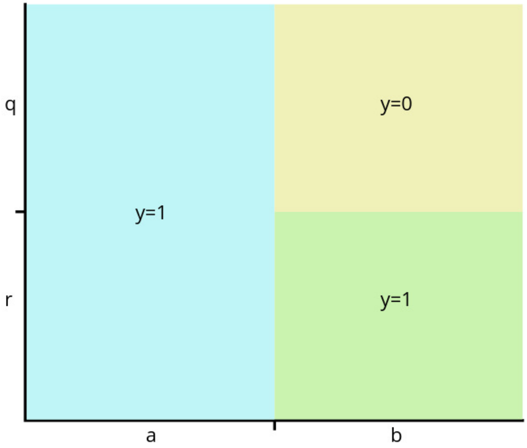


Figure 1: Partitioning the feature space

Classification and regression trees (CART)

A single-tree model trained on data $\boldsymbol{X}$ to make predictions about data $\boldsymbol{X}'$

- There are two types depending on the prediction problem:
  - **Classification trees**: predict which *class* an observation belongs to (i.e. $\boldsymbol{y}$ is a vector of labels)
  - **Regression trees**: predict the outcome of an observation (i.e. $\boldsymbol{y}$ is a continuous variable)

Across both types, model training determines:

- Structure of the tree
- The variable to split on at each decision node
- The splitting criteria c at each decision node

This is algorithmically more complicated than the ML extensions of OLS regression

Classification problems

Training objective: minimise the classification error for $\boldsymbol{y}$ corresponding to training data $\boldsymbol{X}$

Intuitively, we want to select features of $\boldsymbol{X}$ such that:

- Dividing on those features yields more *certain* predictions about $\boldsymbol{y}_k$ for each k

We call the increase in certainty as a result of splitting on a variable the **information gain**, denoted as

$$IG = I(\boldsymbol{y}^{\text{Parent}}) - \left(\frac{n_{\text{Left}}}{n_{\boldsymbol{y}^{\text{Parent}}}} I(\boldsymbol{y}^{\text{Left}}) + \frac{n_{\text{Right}}}{n_{\boldsymbol{y}^{\text{Parent}}}} I(\boldsymbol{y}^{\text{Right}}) \right)$$

In turn, this will depend on:

- The function $I()$
- The variable we split on
- The threshold that determines the split between Left and Right

$I()$ as the Gini Index

For classification trees, $I()$ is typically the **Gini Index**

- A (substantive) measure of inequality
- Countries with income equality have Gini Index values near 0
- Useful for our purposes because we want greater equality in the outcomes of each partition in $\mathcal{R}$

The Gini Index is calculated as:

$$I_{\text{Gini}}(\boldsymbol{y}) = \sum_a P(\boldsymbol{y} = a)(1 - P(\boldsymbol{y} = a))$$

- With two classes and $P(\boldsymbol{y} = 1) = 1, I_{\text{Gini}} = 0$
- With two classes and $P(\boldsymbol{y} = 1) = 0.5), I_{\text{Gini}} = 0.5$

Classification algorithm

We start with the full data $\boldsymbol{X}$:

1. For every possible variable, and splitting point in each variable, split the data and calculate the information gain
2. Choose the variable and splitting value which yields the greatest information gain
3. Repeat this process recursively for each partition of data

Clearly this results in a branching structure!

- But how do we know when to stop?

Stopping criteria

The algorithm will stop automatically when when $I(\boldsymbol{y}^{\text{Parent}}) = 0$

But with some small residual inequality we could get very deep networks, raising a familiar problem of **overfitting**

- I.e. we need to add some form of regularisation

Various alternative ways to do this:

- Stop splitting after λ decision nodes
- Stop splitting when there are fewer than λ observations in a subset

Alternatively we can "prune" a deep tree:

1. Hold out some validation data and train the model on the remaining training data
2. Successively remove splits from the trained model ("pruning") and calculate the classification error
3. Choose the pruned tree with the lowest classification error

Prediction (regression) problems

Training objective: minimise the *prediction* error for $\boldsymbol{y}$ corresponding to training data $\boldsymbol{X}$

One obvious candidate to focus on:

$$\text{Prediction error} = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2,$$

where

$$\hat{y}_i = \frac{1}{\sum_i \mathbb{I}(\boldsymbol{x}_i \in \mathcal{R}_k)} \times \sum_i \mathbb{I}(\boldsymbol{x}_i \in \mathcal{R}_k) y_i$$

- Similar idea as linear regression but not identical
- Recursively partition the data so that the split at node k only uses the data from its parent node

Regression algorithm

We start with the full data $\boldsymbol{X}$:

1. For every possible variable, and splitting point in each variable, split the data and calculate the conditional mean for the two branches: $\beta_{\text{Left}}, \beta_{\text{Right}}$
2. Calculate the total loss as,

$$\sum_{i \in \boldsymbol{X}^{Left}} (y_i - \beta_{\text{Left}})^2 + \sum_{i \in \boldsymbol{X}^{Right}} (y_i - \beta_{\text{Right}})^2$$

3. Choose the variable and splitting value which yields the smallest total squared loss
4. Repeat this process recursively for each new partition of data

Benefits and limitations of CART

Benefits

- Reasonably intuitive and interpretable
  - We can inspect the tree structure and make meaningful claims about the “role” of variables
- Easy to compute
  - Even with continuous predictors!
- Flexible – can model complex relationships reasonably well

Limitations

- It relies on a **greedy** algorithm
  - We fix the first split of the data
  - Then we find the best split conditional on that first split
  - Not necessarily optimal tree structure
- CART is a heuristic approach

Random forest

From one tree to a forest trees

CART is a simple ML procedure, but being "heuristic" in form means it is quite limited:

- Finding the optimal network structure is just computationally very difficult
  - Entails considering how any specific splitting rule affects the tree structure as a whole
  - Leads to an explosion of parameter combinations to consider

Random forests are an extension of CART models, and rests on two major alterations to the estimation strategy:

1. The number of trees estimated
   - Forest methods rely on fitting multiple trees to improve predictive performance
2. How individual trees grow
   - Randomising splitting decisions to regularise the estimation

Deterministic individual trees

Individual tree models are deterministic:

- Suppose we have training $\boldsymbol{X}^{\text{Train1}}$ and $\boldsymbol{X}^{\text{Train2}}$, and some constant test dataset $\boldsymbol{X'}$
- Let $\hat{f}_{\boldsymbol{X}^{\text{Train1}}}$ and $\hat{f}_{\boldsymbol{X}^{\text{Train2}}}$ be the trained CART models for the two training datasets

If $\boldsymbol{X}^{\text{Train1}} = \boldsymbol{X}^{\text{Train2}}$,

- $\hat{f}_{\boldsymbol{X}^{\text{Train1}}}(\boldsymbol{X'}) = \hat{f}_{\boldsymbol{X}^{\text{Train2}}}(\boldsymbol{X'})$

But if $\boldsymbol{X}^{\text{Train1}} \neq \boldsymbol{X}^{\text{Train2}}$,

- $\hat{f}_{\boldsymbol{X}^{\text{Train1}}}(\boldsymbol{X'})$ and $\hat{f}_{\boldsymbol{X}^{\text{Train2}}}(\boldsymbol{X'})$ likely differ

If we want to leverage multiple trees, we need multiple *different* training datasets

Bootstrapping

Collecting masses of new training data would be inefficient and expensive!

Instead, we can "pull ourselves up by our bootstraps" to generate multiple datasets from $\boldsymbol{X}$:

- Ramdomly *sample with replacement* data of the same size as $\boldsymbol{X}$
- Some $\boldsymbol{x_i} \in \boldsymbol{X}$ can appear more than once in a bootstrapped dataset
- In other words, we pretend $\boldsymbol{X}$ is a population, and take new random samples from it

Since $\{\boldsymbol{X^1}, \boldsymbol{X^2}, ..., \boldsymbol{X^B}\}$ will be (slightly) different:

- Training models on each will yield (slightly) different model predictions
- And hence we can get a "forest" of predictions

Averaging across the forest

Random forest estimators estimate T separate trees, by bootstrapping $\boldsymbol{X}$

- To get a final prediction, we pass our test data $\boldsymbol{X'}$ through each of the T trees,
- Recover the T corresponding estimates for each observation
- And take the average

$$\hat{\boldsymbol{y}} = \frac{1}{T} \sum_{t=1}^{T} \hat{f}_t(\boldsymbol{X'}),$$

where $\hat{f}_t$ is the tth trained tree model in the forest

Regularisation: Feature bagging

Unlike CART models, random forest does not employ pruning or maximum depth limits:

- We allow each individual tree to grow to its full length
- Individual trees may be overfit...
- ... but averaging across tree models helps smooth this overfitting

Likely not enough regularisation, so random forests also randomise access to variables:

- Involves setting a **hyperparameter** m:
  - The number of variables to be chosen at random for each decision node
- Forces different trees to learn different aspects of the relationship between $\boldsymbol{y}$ and $\boldsymbol{X}$
- Counteracts the “greedy” nature of CART estimation

Recap of random forest estimation

Procedure:

1. Take T bootstrapped samples of training data $\boldsymbol{X}$
2. For each sample b, estimate a single decision tree
   - At each splitting decision, randomly sample m variables and choose best variable and splitting value from this subset
3. Allow each tree to grow to full-length
4. Pass $\boldsymbol{X'}$ through *each* tree in the forest
5. Average the resultant predictions across each tree

Benefits of random forest

Averaging helps smooth overfitting, so trees can be deeper than in a CART model

- I.e. allow each individual tree to be more complex
- Out-of-sample accuracy should increase because we rely on not one, but many, trees to make the prediction!

Since we recover multiple estimates of $\hat{y}_i$, we can characterize the uncertainty of this prediction:

- For example, $\mathbb{V}(\hat{y}_i) = \frac{\sum_{t=1}^{T} \left(\hat{f}_t(\boldsymbol{x_i'}) - \hat{y}_i\right)^2}{t-1}$
- Or take 2.5th and 97.5th percentiles of distribution to construct a 95% interval

Limitations

Some additional computational cost:

- We are now training 1000 trees (by default)!
- Slightly offset by restricting choice of variables at each decision node
- Algorithmic implementations of random forest are pretty fast

Interpretability:

- Cognitively, unlike CART, intepreting all the trees is near impossible
- Conceptually, too, individual tree structures are meaningless
    - We care about the average performance of the trees

Optimisation

- Averaging improves performance by lowering variance
    - But each tree is grown independently
    - What if we could optimise trees with respect to each other?

Hyperparameter tuning

(Hyper)parameters

Models attempt to learn relationships in data by setting/adjusting *parameters*:

- Beta coefficients (in linear and LASSO regression)
- The splitting point and variable at a non-terminal node

Hyperparameters determine *how* the model learns these relationships:

- The λ value in LASSO
- The maximum depth of a tree in CART
- The number of bootstrapped variables
- The splitting criteria
- The number of trees
- ...

Hyperparameter values are set *prior* to estimating the model!

Choosing λ

Recall in a LASSO model that:

$$\mathcal{L} = \sum_{i=1}^{N} \big(y_i - f(x_i)\big)^2 + \lambda ||\hat{\boldsymbol{\beta}}||_1$$

λ regulates how much bias we add to the model:

- Too large a value = overly constricted model, large MSE
- Too small a value = overly complex model, large MSE

We need to find a value that helps us get near the bottom of the total-error curve!

- This process is called hyperparameter tuning
- It is a recurrent feature of ML methods

Simple tuning

Simplest way is to simply try a few values:

- In the case of LASSO, we might try $\lambda = \{0.1, 1, 10\}$
- Choose λ that yields lowest MSE from $MSE_{\lambda=0.1}, MSE_{\lambda=1}, MSE_{\lambda=10}$
- Use this value in the final model

But there are some limitations:

- You are "testing" your model on the same data that it was trained upon
- So this will inflate the actual accuracy of your model
- Goes against the train-test ethos of ML prediction

Holdout sample

As an alternative, we could create a holdout sample:

- Split our training data $\boldsymbol{X}$ into $\{\boldsymbol{X}^{\text{Train}}, \boldsymbol{X}^{\text{Holdout}}\}$
- Train our model for each value of λ on $\boldsymbol{X}^{\text{Train}}$
- Then test the predictive accuracy on $\boldsymbol{X}^{\text{Holdout}}$
- In other words, create a miniature version of the train-test split within our training data

But there are still limitations:

- By leaving out some observations, we lose predictive power

K-fold cross validation

We can generalise holdout sampling to incorporate all of our training data:

1. Randomly assign each *training* observation to one of k **folds**
2. Estimate the model k times, omitting one "fold" from training at a time
3. Calculate the prediction error using the fold not included in the data
4. Average the prediction errors across $k - folds$
5. Repeat 2-4 for each value of λ we want to test

Choose λ where the *average cross-validated MSE is lowest*

The choice of k will depend on:

- The time it takes to train the model
- The size of your training data

Grid search

LASSO hyperparameters are relatively “easy” to tune, as there is only one parameter

In a random forest, however, there are multiple hyperparameters so the number of models to test is relatively large (especially with cross-validation)

$$\{200, \ldots, 2000\}_{\text{Trees}} \times \{2, 3, \ldots, k-1\}_{m_{try}} \times \{\ldots\}_{\text{Tree Complexity}}$$

If we try every possible combination, we conduct a **grid search**

- Exhaustive
- Expensive

Alternative hyperparameter tuning regimes

One natural alternative is to **randomly search** each dimension, and try only these combinations:

- More efficient
- Not necessarily optimal
- Potential to repeatedly sample same area multiple times (randomly)

Latin Hypercube Sampling attempts to improve on the random search:

- Still an efficient search of the hyperparameter space
- Takes random samples but remembers where previous samples were
- Allows for a more efficient random search

Bayesian Additive Regression Trees

An alternative forest

Random forests are not the only type of multi-tree method:

- Suppose each tree is tasked with predicting a small part of the covariance between $\mathbf{X}$ and $\mathbf{y}$
- Averaging no longer makes sense
- But we can *sum* these trees if they focus on different parts of the covariance. Hence, $\hat{y}_i = \sum_t f_t(\mathbf{x}_i)$

Ideally, each constituent tree within the forest will adapt to meet the predictive needs of the forest as a whole!

- This intuition combines the constrained nature of CART models. . .
- . . . with the aggregate nature of random forests

Bayesian Additive Regression Trees

Bayesian Additive Regression Trees (BART; Chipman et al 2010) is a forest methods that sums a set of "weak learner" trees

- Each tree is constrained to predict only a small portion of the total outcome

$$f(\mathbf{X}) \approx \hat{f}(\mathbf{X}) = \sum_{j=1}^{m} g_j(\mathbf{X}, M_j, T_j),$$

where:

- $f(\mathbf{X})$ is the true functional relationship between $\mathbf{X}$ and $\mathbf{y}$
- m indicate the number of trees in the model
- g_j is the individual prediction from tree j
- M_j are the terminal node parameters of tree j
- T_j is the tree-structure of tree j (i.e. the decision rules of the tree)

BART regularisation

BART does not employ feature bagging or pruning to regularise the model

Instead we instantiate the model with a “prior” structure:

- A full (albeit bad) model exists prior to any training
- We instantiate M separate trees
- Each tree has a complete structure, including splits and terminal nodes

These priors act to *penalize* overly complex individual trees (more on why later)

BART algorithm

1. **Forest instantiation**
   - Tree structure prior over T_j sets probability that each split in the tree is non-terminal
   - The prior over each terminal node is denoted μ_{ij} and is drawn from a normal distribution
   - BART model also assumes random DGP $f(\mathbf{X})$ and so sets a prior over this variance – denoted σ

Note that these priors are drawn from **random** distributions. Hence, if we took multiple draws from the tree, we would get different values at the terminal nodes – this is a very convenient property.

Updating trees

2. Iterate through each individual tree

- Calculate the residual variance not explained by the remaining $m-1$ trees, i.e. $R_j = \mathbf{y} - \sum_{j' \neq j} f'_j(\mathbf{X})$
- The algorithm then proposes a new tree structure T^*_j by:
  - **Growing –** split a terminal node in two
  - **Pruning –** remove child nodes
  - **Swapping –** swap the split criteria for two non-terminal nodes
  - **Changing –** alter the criteria for a single non-terminal node
- Then decide whether to *accept* T^*_j
  - A probabilistic choice based on the extent of residual variance R_j and the initial tree T_j
- Proceed to the next tree in the forest

Constrained optimization

Since R_j encompasses the prediction of all but the tree under consideration, this updating procedure is constrained:

- Only focuses on a small portion of total variance
- I.e. that which *is not* explained by the remainder of the forest

3. Update σ and repeat

With all trees updated, the model then attempts to optimize the forest as a whole by revising the σ prior.

We then repeat steps 2-3 N times

- N is a hyperparameter chosen by the researcher

After N repetitions, we have a trained prediction function $\hat{f}$.

Predicting $\mathbf{y}$

To predict $\boldsymbol{y'}$ from $\boldsymbol{X'}$ we push each observation through the prediction function $\hat{f}$ *multiple* times

- Each time yields a different prediction given terminal nodes are random variables
- Typically we take 1000 draws from the prediction function

For every observation $\mathbf{x}_i$, we therefore have 1000 predicted values $\boldsymbol{\hat{y}_i}$:

- This is a distribution of the prediction for each y_i
- $\hat{y}_i = \frac{1}{N}\sum_k y_{ik} \sim \hat{f}(\mathbf{X})$

Similar to random forests, saving the full distribution gives us an idea of the uncertainty.

Comparing random forests and BART

$\hat{y}_i^{\mathsf{RF}}$ is the average over k trees in the forest:

- Each tree is a complete attempt to predict the outcome using bootstrapped data and feature bagging
- Therefore, we average over the individual tree predictions of the outcome

$\hat{y}_i^{\mathsf{BART}}$ is the average over k draws from the estimated function $\hat{f}$

- Each draw is the result of passing $\boldsymbol{x}_i'$ through the m constituent trees and *summed*
- Repeated k times to generate k predictions
- Averaging over individual draws from the *forest* not individual trees

Benefits of BART

One benefit of BART is that it is robust to the choice of hyperparameter values:

- Empirically we find that small changes in the hyperparameters do not yield drastically different predictions
- Good default estimator for predictive ML methods
- Default hyperparameter provided by Chipman et al (2010) are typically going to perform well