Decision Trees & Extensions

Why decision trees

Several related reasons

- they are known to perform very well on **structured/rectangular** data: typically the type of financial data (if we exclude alt-data)
- they (i.e., their **extensions**) are probably the most popular solutions among winning solutions in Kaggle competitions
- they are often easy to understand and to **interpret** (at least through variable importance)

Agenda

1. Principle & Examples
2. Extensions
3. Variable importance
4. Wrap-up

Introduction

Difference with linear approaches

Linear approach:

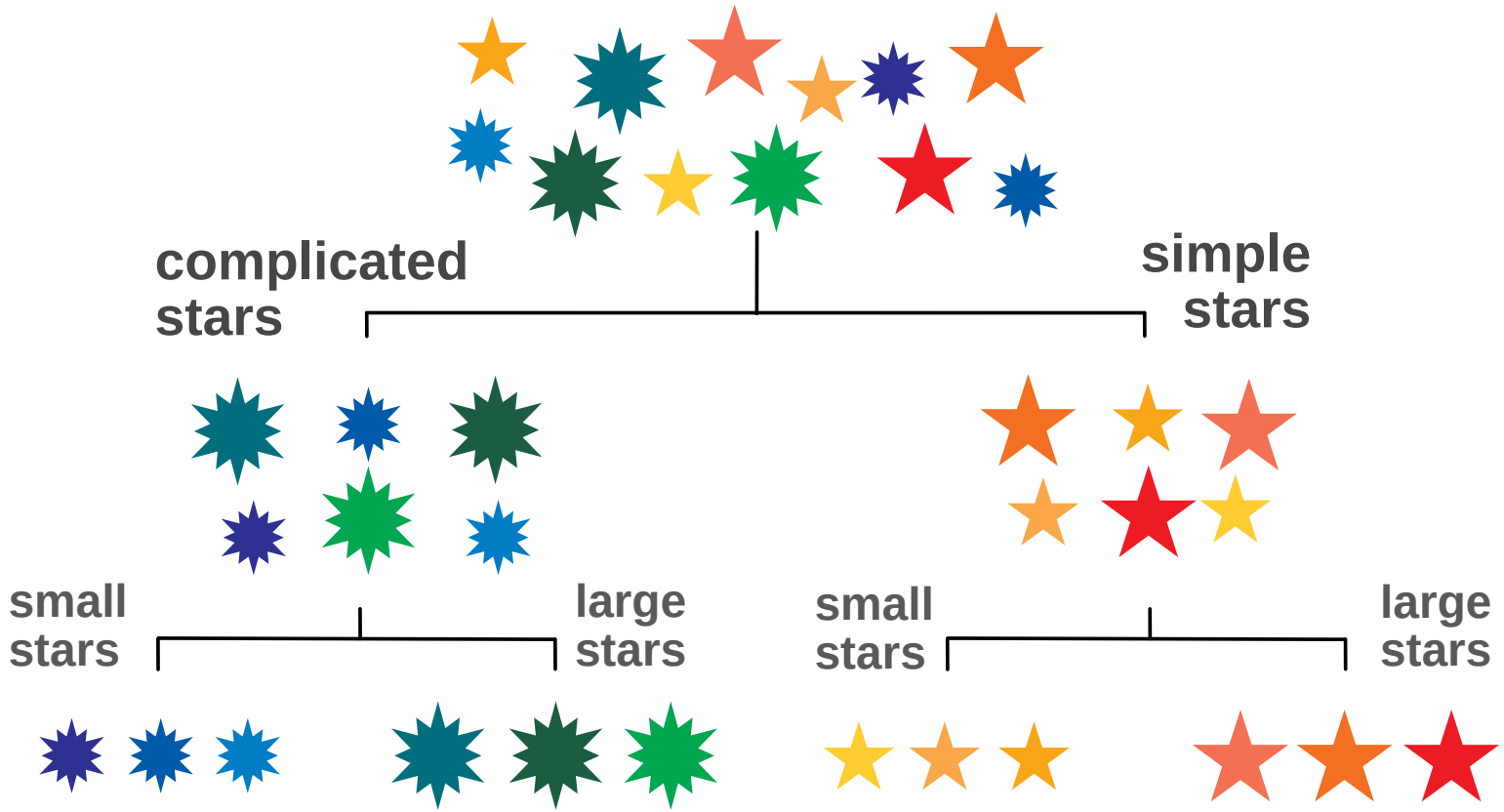
$$y_i = \alpha + \beta^{(1)} x_i^{(1)} + \cdots + \beta^{(K)} x_i^{(K)} + \epsilon_i$$

There are **much more complicated functions** $y_i = f(\boldsymbol{x}_i) + \epsilon_i$!
Trees are models that form clusters based on $\boldsymbol{x}$ such that the clusters are homogeneous in y.
In portfolio management, y is related to performance, say, return.
Hence depending on $\boldsymbol{x}$, some clusters will have low average y (e.g., return) and others high average y. Those are the ones we will want to invest in!

Usual non-financial example: Obama-Clinton votes from NY Times

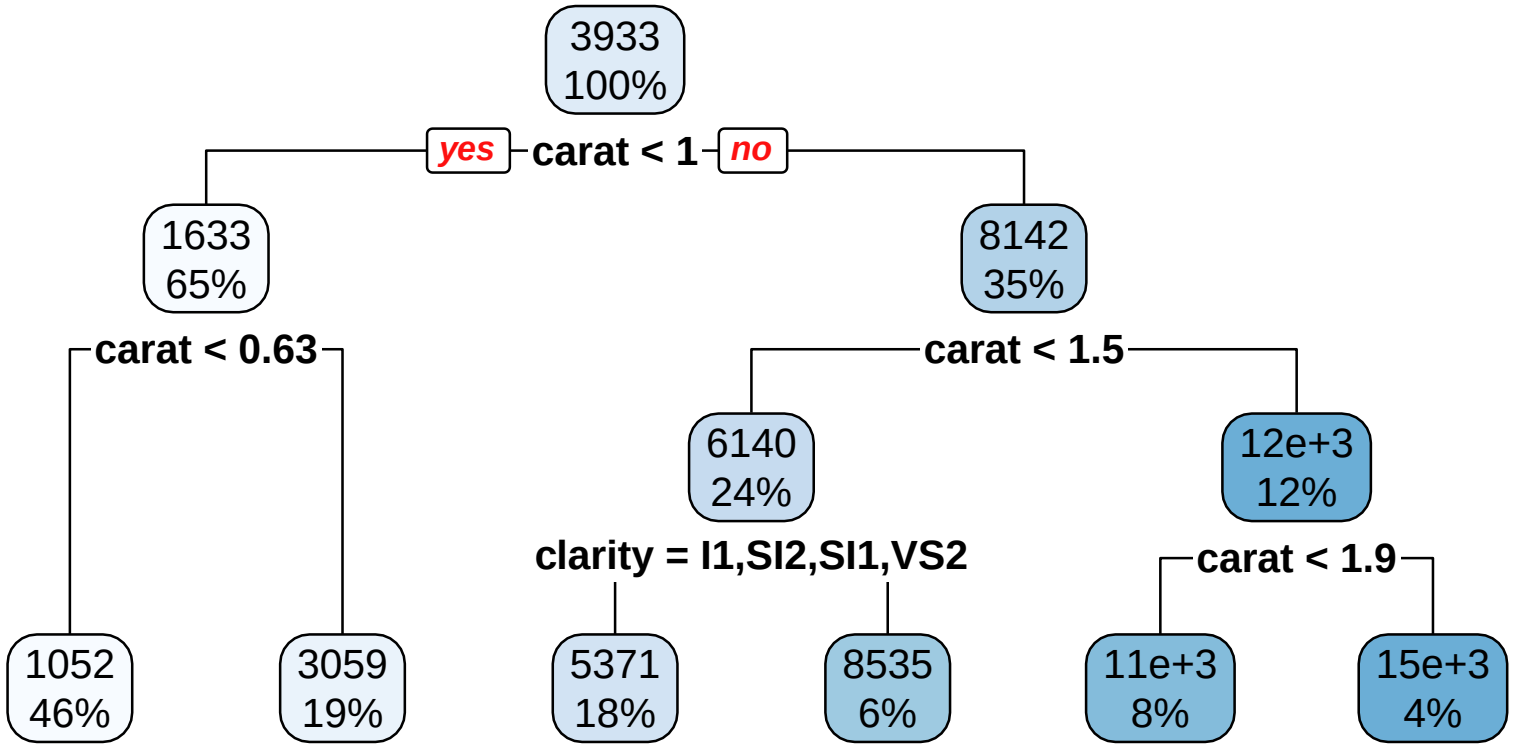
A basic example

y is the colour of the star (to be predicted), $\mathbf{x}^{(1)}$ is the size of the star, $\mathbf{x}^{(2)}$ is the shape (complexity) of the star.



Diamonds

Splits, **splits**, it'a all about splits!
What are the **drivers** of their prices? Cut, colour, clarity... size?



The **size**, of course, but not only!
→ in rpart, from the condition under the node, it's always: TRUE to the left and FALSE to the right.

Process (1/3)

A large majority of trees work with binary splits (so will we).

A simplified case: how to choose splitting points?

Imagine we work with only one explanatory variable x. In the case of diamonds, let's assume we only consider the size (weight in carats). What's the best possible (initial) split?
Since we seek **homogeneous clusters**, total quadratic variation/dispersion is a good start:

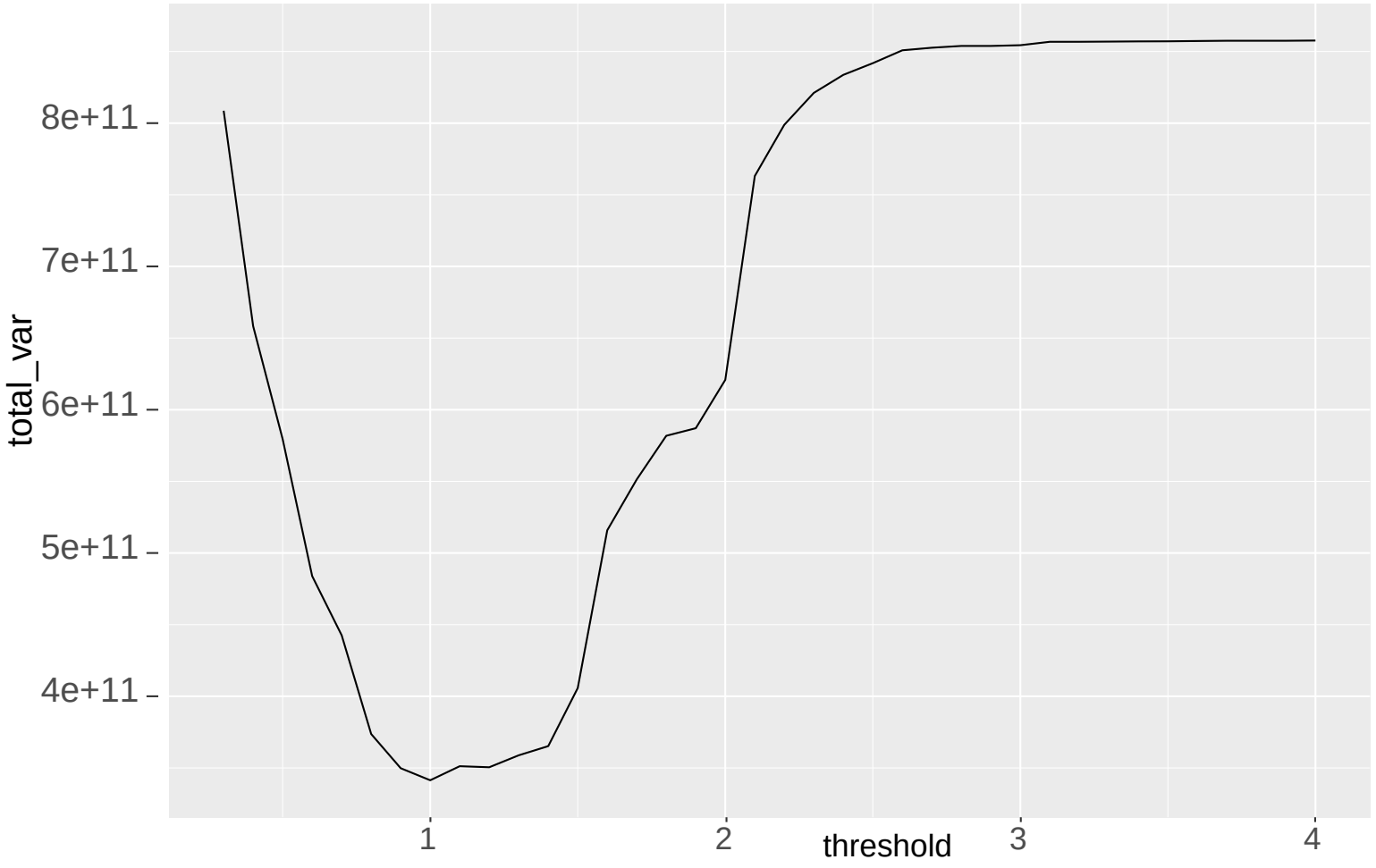
$$V(c) = \underbrace{\sum_{i:carat>c} (p_i - \bar{p}_{carat>c})^2}_{\text{large diamond cluster } (>c)} + \underbrace{\sum_{i:carat<c} (p_i - \bar{p}_{carat<c})^2}_{\text{small diamond cluster } (<c)}$$

$\bar{p}_{carat>c}$ is the average price of all diamonds with weight larger than c.

This split yields a decomposition that is smaller than the original total variation (scaled variance): $TV = \sum_i (p_i - \bar{p})^2$. The gain is

$$G(c) = TV - V(c)$$

Process (2/3)



Minimum point at 1 carat. **No other feature** can achieve this low level of total dispersion.

Process (3/3)

The full splitting process can be described as:

For each node / cluster:

1. Find the best splitting point for each variable.
2. Determine which variable achieves the **highest gain** (reduction in loss or objective)
3. Split according to this variable $\rightarrow$ two **new clusters**!

This is performed until some condition is met (improvement of gain becomes too small or sufficient depth is reached).

Categorical output

When working with numerical outputs, the variance is the natural dispersion metrics: it measures how (in-)**homogeneous** a cluster is. Things are more complicated for categorical data and several solutions exist. All metrics are based on the **proportions of classes** within a node: p_k.

Examples:

- the Gini impurity index: $1 - \sum_{k=1}^{K} p_k^2$
- the misclassification error: $1 - \max_k p_k$
- cross-entropy: $-\sum_{k=1}^{K} \log(p_k) p_k$

The tree is built by **minimising** one of these values at each split. [1]
It is also possible to weight loss according to categories (some errors are sometimes more costly than others) $\rightarrow$ loss matrix.

[1] **Note**: the Gini index is related to the Herfindahl index (portfolio diversification)

Categorical features

Test all configurations!

- Splitting is only computationally feasible for a small number of classes.
- Indeed, given q classes, there are $2^{q-1} - 1$ ways to split the data.
- 10 classes imply $\sim$500 partitions - this is probably already too much, especially if there are many predictors.

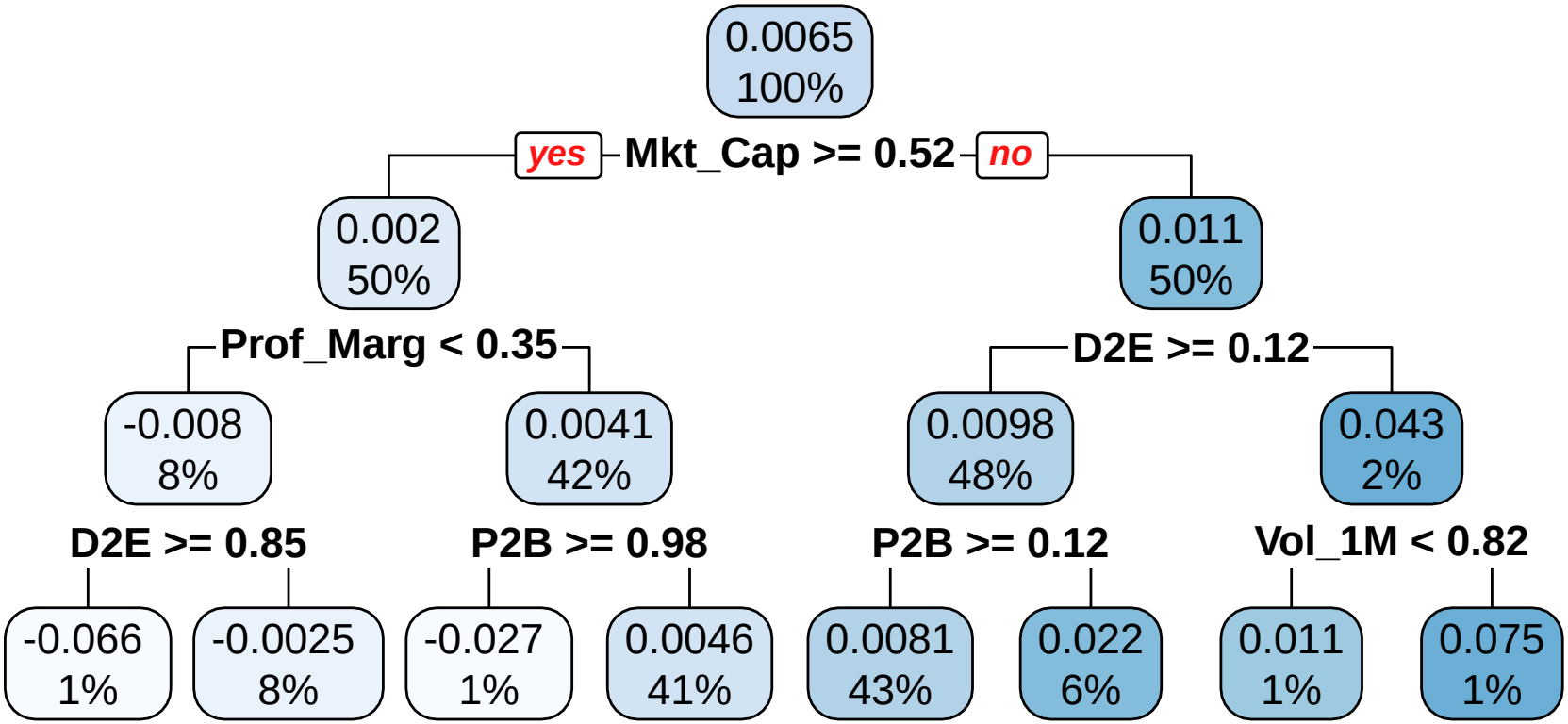
In fact, there are some tricks to speed up the computation when y is numerical. The idea is to **rank** classes according to their mean in the output variable and to treat them as an ordered variable (the number of splits is greatly reduced: linear in q!).[2]

(for multiclass output, there is no simple way out)

[2] See Sec. 9.2.4 in the *Elements of Statistical Learning* for more details.

Financial data

On rescaled features



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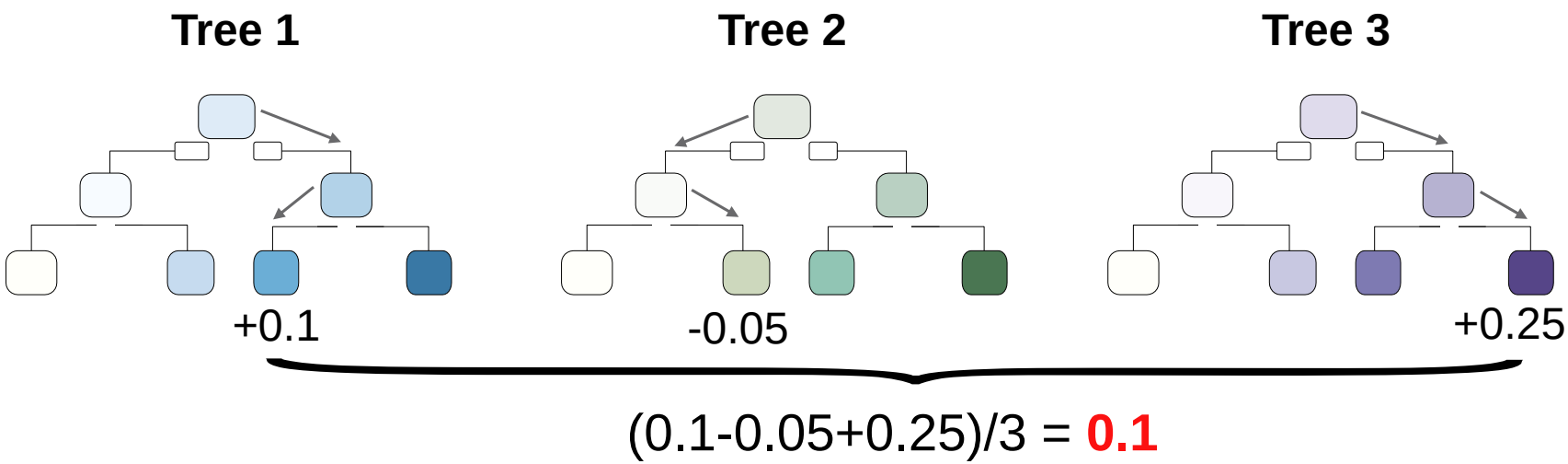
Random forests (1/2)

- Given one splitting rule and one dataset, there is only one optimal tree.
- RF pick random combinations of features to build aggregations of trees. This technique is called '**bagging**'.
- Each output value is the average of the outputs obtained over all trees.



(or **majority voting** if categorical output)

Random forests (2/2)

Options when building the forests:

- fix the **depth** / **complexity** of the tree (just as for simple trees);
- select the **number of features** to retain for each individual learner (tree);
- determine the **sample size** required to train the learners.

Random forests are more complex and richer than simple trees. One cool feature: RFs don't have a huge tendency to **overfit**. Thus, most of the time, their performance is higher.

Boosted trees: principle (1/6)

Idea

Like RFs, **boosted trees** aggregate trees. The model can be written as:

$$\tilde{y}_i = m_J(\boldsymbol{x}_i) = \sum_{j=1}^{J} T_j(\boldsymbol{x}_i),$$

where i is the index of the occurrence (e.g., stock-date pair) and J is the **number of trees**. We thus has the following simple relationship when we add trees to the model:

$$m_J(\boldsymbol{x}_i) = \underbrace{m_{J-1}(\boldsymbol{x}_i)}_{\text{old trees}} + \underbrace{T_J(\boldsymbol{x}_i)}_{\text{new tree}}$$

When the previous model is built, how do we choose the new tree?
$\rightarrow$ the model is constructed **iteratively**.

Boosted trees: principle (2/6)

We follow the approach of **XGBoost** (Chen & Guestrin (2016)).

Objective

What we seek to minimise is

$$O = \underbrace{\sum_{i=1}^{I} \text{loss}(y_i, \tilde{y}_i)}_{\text{error term}} + \underbrace{\sum_{j=1}^{J} \Omega(T_j)}_{\text{regularisation term}}$$

The first term (over all instances) measures the distance between the true label and the output from the model. The second term (over all trees) penalises models that are too complex.

For simplicity, we will work with $\text{loss}(y, \tilde{y}) = (y - \tilde{y})^2$:

$$O = \sum_{i=1}^{I} (y_i - m_{J-1}(\boldsymbol{x}_i) - T_J(\boldsymbol{x}_i))^2 + \sum_{j=1}^{J} \Omega(T_j)$$

Boosted trees: principle (3/6)

We have built tree T_{J-1} (and hence model m_{J-1}): how to choose tree T_J?
Decompose the objective:

$$
\begin{aligned}
O &= \sum_{i=1}^{I} (y_i - m_{J-1}(\boldsymbol{x}_i) - T_J(\boldsymbol{x}_i))^2 + \sum_{j=1}^{J} \Omega(T_j) \\
&= \sum_{i=1}^{I} \left\{ y_i^2 + m_{J-1}(\boldsymbol{x}_i)^2 + T_J(\boldsymbol{x}_i)^2 \right\} + \sum_{j=1}^{J-1} \Omega(T_j) + \Omega(T_J) \\
&\quad - 2 \sum_{i=1}^{I} \{ y_i m_{J-1}(\boldsymbol{x}_i) + y_i T_J(\boldsymbol{x}_i) - m_{J-1}(\boldsymbol{x}_i) T_J(\boldsymbol{x}_i)) \} \quad \text{cross terms} \\
&= \sum_{i=1}^{I} \left\{ -2 y_i T_J(\boldsymbol{x}_i) + 2 m_{J-1}(\boldsymbol{x}_i) T_J(\boldsymbol{x}_i)) + T_J(\boldsymbol{x}_i)^2 \right\} + \Omega(T_J) + c
\end{aligned}
$$

The red terms are known at step J!
$\rightarrow$ things are simple with quadratic loss. For more complicated loss functions, **Taylor expansions** are used.

supervised **learning factor** investing

Boosted trees: principle (4/6)

We need to take care of the **penalisation** now. For a given tree T, we specify tree $T(x) = w_{q(x)}$, where w is the output value of some leaf and $q(\cdot)$ is the function that maps an input to its final leaf. We write $l = 1, \ldots, L$ for the indices of the leafs of the tree. In XGBoost, complexity is defined as:

$$\Omega(T) = \gamma L + \frac{\lambda}{2} \sum_{l=1}^{L} w_l^2,$$

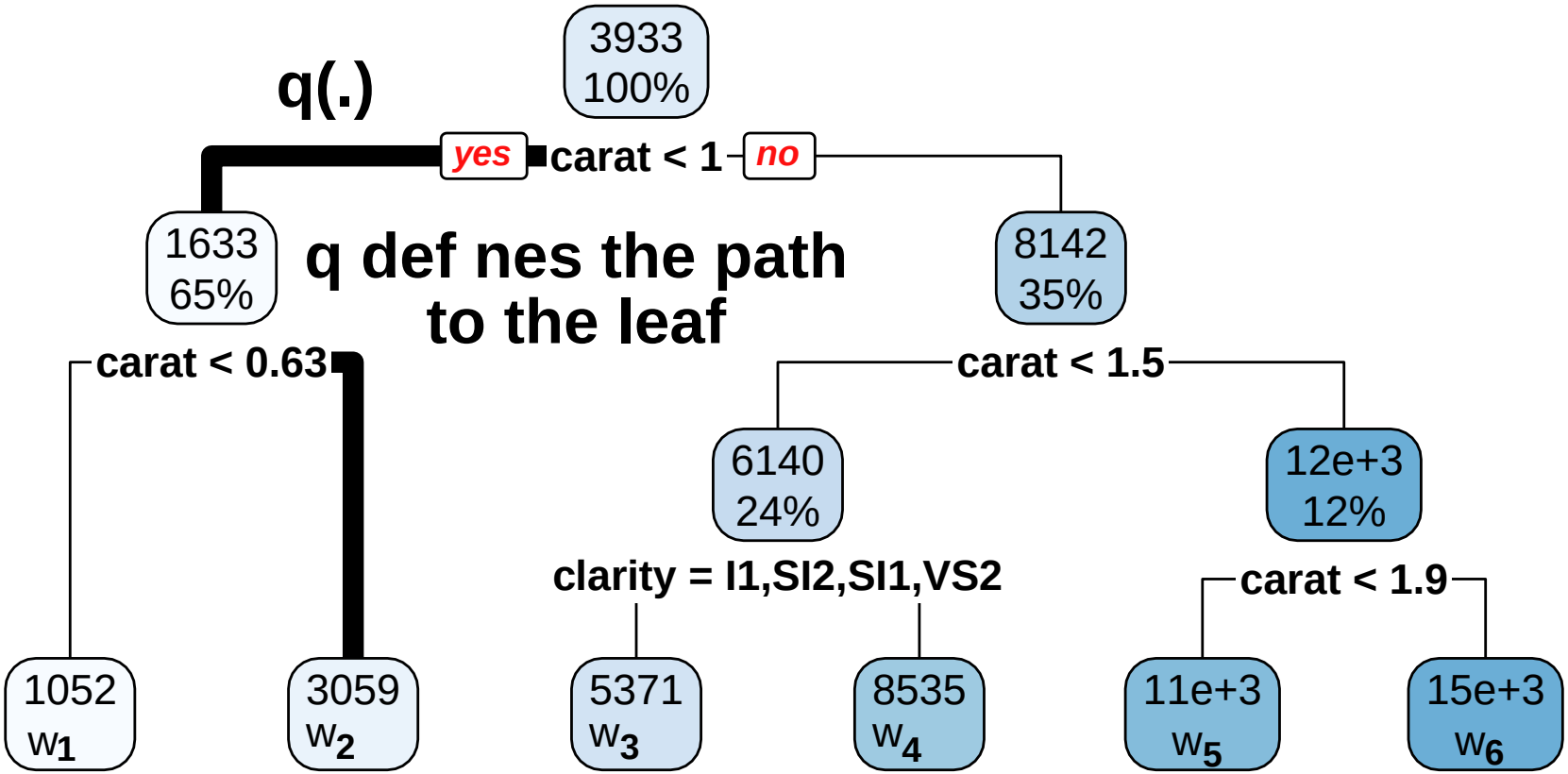
where

- the first term penalises the **total number of leaves**
- the second term penalises the **magnitude of output values** (this helps reduce variance).

Below, we omit the index (J) of the tree of interest (i.e., the last one). Moreover, we write I_l for the set of the indices of the instances belonging to leaf l.

Boosted trees: principle (4b/6)

Illustration of *q* and *w*:



Boosted trees: principle (5/6)

We aggregate both sections of the objective:

$$
\begin{aligned}
O &= 2\sum_{i=1}^{I}\left\{ y_i T_J(\boldsymbol{x}_i) - m_{J-1}(\boldsymbol{x}_i) T_J(\boldsymbol{x}_i)) + \frac{T_J(\boldsymbol{x}_i)^2}{2} \right\} + \gamma L + \frac{\lambda}{2}\sum_{l=1}^{L} w_l^2 \\
&= 2\sum_{i=1}^{I}\left\{ y_i w_{q(\boldsymbol{x}_i)} - m_{J-1}(\boldsymbol{x}_i) w_{q(\boldsymbol{x}_i)}) + \frac{w_{q(\boldsymbol{x}_i)}^2}{2} \right\} + \gamma L + \frac{\lambda}{2}\sum_{l=1}^{L} w_l^2 \\
&= 2\sum_{l=1}^{L}\left(w_l \sum_{i\in I_l}(y_i - m_{J-1}(\boldsymbol{x}_i)) + \frac{w_l^2}{2}\sum_{i\in I_l}\left(1+\frac{\lambda}{2}\right)\right) + \gamma L
\end{aligned}
$$

$$
\rightarrow \quad w_l^* = -\frac{\sum_{i\in I_l}(y_i - m_{J-1}(\boldsymbol{x}_i))}{\left(1+\frac{\lambda}{2}\right)\#\{i\in I_l\}},
$$

$$
O_L(q) = -\frac{1}{2}\sum_{l=1}^{L}\frac{\left(\sum_{i\in I_l}(y_i - m_{J-1}(\boldsymbol{x}_i))\right)^2}{\left(1+\frac{\lambda}{2}\right)\#\{i\in I_l\}} + \gamma L
$$

which gives the optimal weights (or leaf scores) and objective value.[3]

[3] $f(x) = ax + \frac{b}{2}x^2$: min at $x^* = -a/b$, min value = $-a^2/(2b)$.

Boosted trees: principle (6/6)

Final problem: the **tree structure**! This is the q function essentially. For instance: what's the best depth? Do we continue to grow the tree or not?

- we proceed node by node
- for each node, we look at whether a split is useful (in terms of objective) or not:

$$\text{Gain} = \frac{1}{2}\left(\text{Gain}_L + \text{Gain}_R - \text{Gain}_O\right) - \gamma$$

- each gain is computed with respect to the instances in each bucket:

$$\text{Gain}_{\mathcal{X}} = \frac{\left(\sum_{i \in I_{\mathcal{X}}} (y_i - m_{J-1}(\boldsymbol{x}_i))\right)^2}{\left(1 + \frac{\lambda}{2}\right) \#\{i \in I_{\mathcal{X}}\}},$$

  where $I_{\mathcal{X}}$ is the set of instances within cluster $\mathcal{X}$.

Gain_O is the original gain (no split).
$-\gamma$: one unit of new leaves: two minus one!
NOTE: XGBoost also applies a learning rate: each new tree weight is multiplied by η.

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Interpretability!

Definition = gain allocation!

- Each time a split is performed according to one variable/**feature**, the objective function is reduced
- This **gain** is entirely attributed to the variable
- If we sum the gains obtained by all variables over all trees and normalise them in the cross-section of features, we get the **relative importance** of each feature!

$$V_f \propto \sum_{n=1}^{N} G_n(f),$$

where f is the index of the feature and $G_n(f)$ the gain associated to feature f at node n (positive if the split is performed according to f and zero otherwise).

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Key takeaways

Trees are powerful

- they organise the data into **homogeneous clusters** in a highly nonlinear fashion
- extensions help improve the predictive performance by **aggregating several trees**
- variable importance is a first step towards **interpretability** (global in this case)

Thank you for your attention

Any questions?