Understanding variable importances in forests of randomized trees

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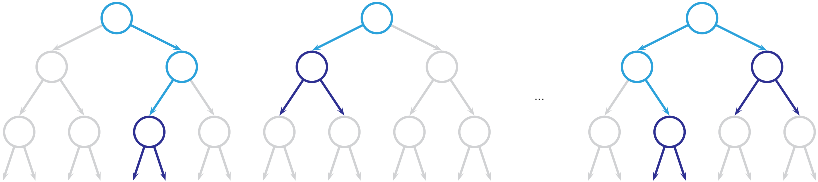
Random Forests are a well-tested, efficient and versatile tool.
Yet, they are still not fully **theoretically** understood.



Variable importances were first proposed as a heuristic to assess the influence of input variables.

$$Imp(X_m) = \frac{1}{N_T} \sum_T \sum_{t \in T : v(t) = X_m} p(t) \Delta i(t)$$

In the case of totally randomized trees, variable importances actually show sound and desirable **theoretical** properties.

✓ Variable importances provide **a three-level decomposition of the information jointly provided by all the input variables about the output**, accounting for all interaction terms in a fair and exhaustive way.

Thm. 1 :

$$Imp(X_m) = \underbrace{\sum_{k=0}^{p-1} \frac{1}{C_p^k} \frac{1}{p-k}}_{\text{ii) Decomposition along the degrees } k \text{ of interaction with the other variables}} \underbrace{\sum_{B \in \mathcal{P}_k(V^{-m})} I(X_m; Y|B)}_{\text{iii) Decomposition along all interaction terms } B \text{ of a given degree } k}$$

Thm. 2 :

$$\underbrace{\sum_{m=1}^{p} Imp(X_m)}_{\text{i) Decomposition in terms of the MDI importance of each input variable}} = \underbrace{I(X_1, \ldots, X_p; Y)}_{\text{Information jointly provided by all input variables about the output}}$$

✓ Variable importances **depend only on the relevant variables**.

Thm. 3 : A variable is irrelevant if and only if its importance is 0.

Thm. 5 : The importance of a relevant variable is insensitive to the addition or the removal of irrelevant variables.