Data Science
Bagging – Random Forest

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BAGGING (M2...)

Idea of Bagging

Make a *vote* from B trees built from bootstrap samples.

Learning

Input number of models B, learning algorithme $ALGO$, data $\Omega = \{\{X_p\}, Y\}$, $|\Omega| = \text{n}$

Iteration

$MODELS = \{\}$

For b in 1 to B, do

   Draw n samples (with replacement), Ω_b

   Built a model M_b on Ω_b with $ALGO$

   Add M_b to $MODELS$

end For

Output $MODELS$

Classifying

For $i^\star$ to be classified

   Apply each model to get an ensemble of $\hat{y}_b(i^\star)$

   Make a simple vote $\hat{y}_{bag}(i^\star) = argmax_k \left[\sum_b^B I\Big(\hat{y}_b(i^\star) = y_k\Big) \right]$

Bagging - Pros

- **Cooperation** Multiple models with *various* predictions are cooperating (Caution: you should not use too similar models)
- **Variance** Individual variance is compensated by the cooperation of the ensemble
- **No overfitting** A large B does not imply overfitting (In practice: $B \geq 100$)

Bagging - Cons

- **Bias** Bagging does not manage the underfitting (but, you can reduce the bias with deep trees)
- You should avoid **weak classifiers** (cf. Boosting)

We want to estimate an a posteriori probability for $Y \in \{+, -\}$, ie. $P(Y = +|\mathbf{X})$

Using the vote frequency

$$P(Y = +|\mathbf{X}) = \frac{\sum_{b=1}^{B} I(\hat{y}_b = +)}{B}$$

Using the probability P_b of each model M_b

$$P(Y = +|\mathbf{X}) = \frac{\sum_{b=1}^{B} \hat{P}_b(Y = +|\mathbf{X})}{B}$$

NB: Better when only few models

Issue

We have now B models

$\Rightarrow$ cannot inspect all trees to identify the most important features

Straightforward solution

Averaging the measure (eg., Tschuprow T, Gini) over all M_b models for all attributes.

Out-of-bag (OOB) error estimation

The error can be measured **during** the bootstrap **training**.

Each model M_b is based on n samples drawn **with replacement**.
Hence, some samples are not used.

$\rightarrow$ We can use these samples as test set ($\approx 36.8\%$ of the samples).

Why the tests set can be estimated to 36.8%

Sampling with replacement $\sim$ sequence of binomial trials with success $=$ being chosen

For n samples, $P(success) = 1/n$ and $P(failure) = (n-1)/n$

For a subsample of size b, the odds of selecting a sample x times are

$$P(x, b, n) = \left(\frac{1}{n}\right)^x \left(\frac{n-1}{n}\right)^{b-x} \binom{b}{x}$$

For bootstrap, $b = n$; if we have enough samples ($n \rightarrow +\inf$),

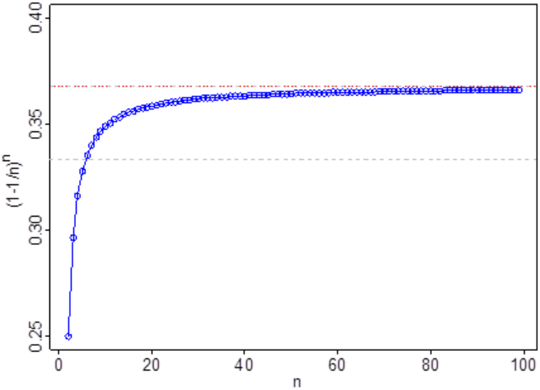
$$P(x, b, n) = \lim_{n \rightarrow +\infty} \left(\frac{1}{n}\right)^x \left(\frac{n-1}{n}\right)^{n-x} \binom{n}{x} = \frac{1}{ex!}$$

Finally, if $x = 0$ (never selected),

$$P(x = 0, b = n, n) = \lim_{n \rightarrow +\infty} \left(\frac{n-1}{n}\right)^n = \frac{1}{e} \approx 0.368$$

So, with the bootstrap approach, each model M_b is learnt on $\approx 63.2\%$ of the dataset.

What is a large n?



For $n \geq 11$, you already reach $1/3$

Definition of margin (for bagging)

The margin is the difference between the proportion of *vote* for the true class and the proportion of *vote* for another. When $Y \in \{+,-\}$,
For one sample $Y(i) = y_{k^\star}$

$$m = \frac{\sum_{b=1}^{B} I(\hat{y}_b(i) = k^\star)}{B} - max_{k \neq k^\star} \frac{\sum_{b=1}^{B} I(\hat{y}_b(i) = k)}{B}$$

A **large margin** means a **sharp decision** and a **small variance**
$\Rightarrow$ the ensemble approaches increase the margin

RANDOM FOREST (M2...)

Efficient bagging

- Individually efficient trees
- Deep trees (weak bias) – min leaf size $= 1$
- **Decorrelated trees** – strongly different trees that be complementary

The idea of Random Forest

Introduce a stochastic perturbation when learning the models M_b by considering only m variables out of p, randomly selected for each split.

Learning *(modified bagging)*

Input number of models B, learning algorithme $ALGO$, data $\Omega = \{\{X_p\}, Y\}$, $|\Omega| = n$, m (default: $m = \sqrt{(p)}$)

Iteration

$MODELS = \{\}$
For b in 1 to B, do
  Draw n samples (with replacement), Ω_b
  Built a model M_b on Ω_b with $ALGO$
  For each split, do
    Choose m variables **at random** among $\{X_p\}$
    Split with the best variables among m
  Add M_b to $MODELS$
end For

Output $MODELS$

Classifying *(same as bagging)*

For $i^\star$ to be classified
  Apply each model to get an ensemble of $\hat{y}_b(i^\star)$
  Make a simple vote $\hat{y}_{bag}(i^\star) = argmax_k \left[\sum_b^B I\left(\hat{y}_b(i^\star) = y_k\right)\right]$

Pros

- Good prediction performance in general
- Few parameters (B and m)
- When large B, no overfitting
- Variables ranking
- Error evaluation while learning (OOB)
- Parallelization

Cons

- Bad performance if few good predictors X ($\Rightarrow$ each M_b might be bad...)

Bibliography

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