Ensembles: Bagging, Random Forests, Boosting

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December 2020

Overview

- What is an ensemble?
- Bagging
- Random Forests
- Boosting
- Why trees?

What is an ensemble?

- **Imagine**
  - A project evaluation committee
  - A juri in a court
  - The government of a country
  - The referees in a VAR decision
- A **Committee** of experts
  - Each model is one expert
  - Each expert has a **different view**
  - The final decision is a combination of the decisions of the experts

What is an ensemble?

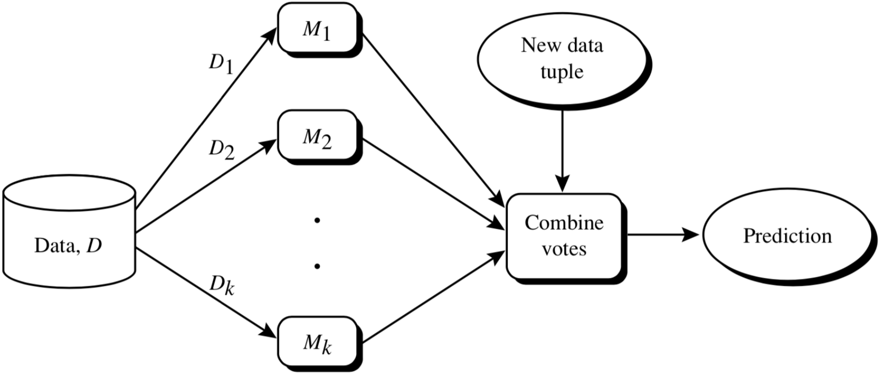


Figure 1: Simplified generic ensemble architecture (Han et al.)

Why ensembles?

- Robustness
  - individual errors are **compensated** by the other experts
    - a judge that overlooks a piece of evidence
- Consistency
  - collective decisions are more **stable**
- Power and accuracy
  - the collective may be **better** than each individual

More formally: learning

- **Given**
  - a dataset D with labelled examples
- **Produce**
  - k models $M_1, \ldots, M_k$ from D
- **Issues**
  - how **different** must the models be?
  - **how many** models do we need?
  - how do we **obtain** the models from data?

More formally: classification and regression

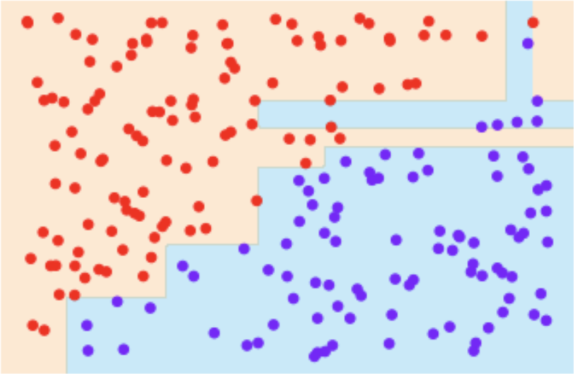
- **Given**
  - an ensemble of k models
  - an example x to classify/predict
- **Do**
  - **obtain** the decision $\hat{y}_i = M_i(x)$ for each model M_i
    - each M_i is a **base** model
  - **combine** the decisions into $\hat{y} = Aggreg_i(\hat{y}_i)$
- **Issues**
  - how to **combine** the decisions
    - voting, averaging, ...

Famous Ensemble methods (families)

- Bagging
  - using different sub-samples of D for each M_i
- Random Forests
  - sub-sample D and use different attributes in each (step of) M_i
- Boosting
  - build each M_i to correct the errors of other models
- **Note**
  - these methods are **mostly** for decision trees
    - we will see why
  - but **not only**

Simple Example

- A classification problem
  - 2 inputs
  - linear diagonal boundary
- Result with a single tree (unpruned)



Simple Example

The model

Figure 3: Single Decision Tree model

Result of an ensemble

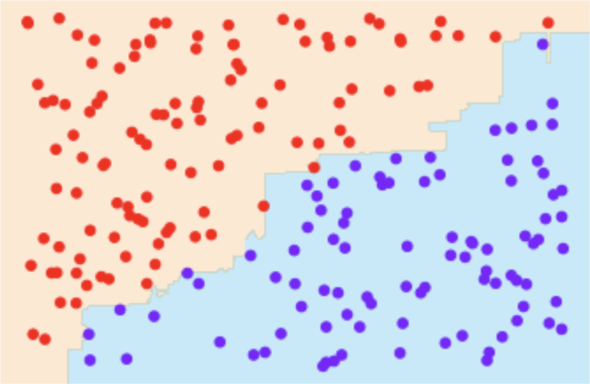


Figure 4: Ensemble of trees boundary

Bagging

- **Bootstrap Aggregation**
  - aggregate models obtained from bootstrap
- **Bootstrap Sampling**
  - Sample from D **with replacement**
  - Example: $D = \{1, 2, 3, 4, 5, 6\}$
  - Bootstrap sample of D is for example $\{1, 2, 2, 4, 6, 6\}$

Bagging

- **Given**
  - a dataset D with labelled examples
  - a number k of models
  - a learning algorithm A
- **For each** $1 \leq i \leq k$
  - S_i = bootstrap sample from D
  - $M_i = A(S_i)$
- **Notes**
  - typically A is a decision tree learner

Bagging

- **Classification**
  - Majority vote
    - $\hat{y}(x) = mode\{M_1(x), \ldots, M_k(x)\}$
- **Regression**
  - Average
    - $\hat{y}(x) = mean\{M_1(x), \ldots, M_k(x)\}$

Why Bagging?

- Models are **different** from each other
  - each model is learned from a different sample
  - an ensemble of similar models adds nothing
- **Why** are they different?
  - each sample misses less representative cases
    - noise, rare situations
  - each sample has repeated cases
    - tends to give importance to more likely cases
- Bootstrapping **simulates** having more data
  - you can obtain multiple views from one D and one A
  - very data efficient

Why Bagging?

- Learning agorithms have two main **error components**
  - Bias
  - Variance
- **Bias**
  - the error caused by the assumptions of the algorithm
- **Variance**
  - the error caused by important random processes
    - sample
    - random initialization

Why Bagging?

- **Error decomposition**
- Expected prediction error
  - $Error(x) = IrreducibleError + Bias^2 + Variance$
- **Bias-Variance tradeoff**
  - variance can be reduced by increasing bias
    - e.g. linear models are stable but have strong assumptions
  - reducing bias ususally leads to increase in variance
    - e.g. decision trees are sensitive to changes in data

Why Bagging?

- Bagging and the tradeoff
  - **reduces** variance
  - does not affect (much) bias
- Bagging **works better** when the base models have
  - low bias (more expressive)
  - high variance (sensitive to changes)
  - low computational cost
- Bagging is popular with **Decision Trees**

Random Forests

- In bagging models are different
  - but we can **reduce the correlation** of models in an ensemble
  - less correlated models may **improve predictive performance**
- RF: a **generalization** of Bagging
  - a bootstrap sample for each base model
  - a different set of attributes for each base model
    - or in each step of the model construction
- RF: designed for decision trees
  - but principles can be used with other models
- RF were introduced by Leo Breiman (1928-2005)

Random Forests

- **Given**
  - a dataset D with labelled examples
  - a number k of models (or tries)
  - a number m of attributes to use in each split
  - a decision tree learning algorithm DT
- **For each** $1 \leq i \leq k$
  - S_i = bootstrap sample from D
  - M_i is learned with DT but sampling m attributes in each split
- **Notes**
  - typically A is a decision tree learner

Random Forests

- **Example:** build a RF base tree for *Iris* with $m = 2$
    - attributes are
        - SL=Sepal Length, SW=Sepal Width,
        - PL=Petal Length, PW=Petal Width,
    - take a bootstrap sample S from *Iris*
        - S has the same size of *Iris*
        - some examples are repeated
        - some are missing
    - Randomly sample 2 attributes
        - e.g. SL and PW
    - Make the top split using only these
    - Build the rest of the tree
        - allways sample $m = 2$ attributes for each split

Random Forests

- Reduce variance
- More accurate than Bagging (in general)
- Robust to errors and outliers
- Base models are less correlated
  - if m is low
  - suggested $m = log_2(|D|) + 1$
- Improves as k increases
  - does not tend to overfit
- Faster than Bagging

Random Forests

Random Forests boundary

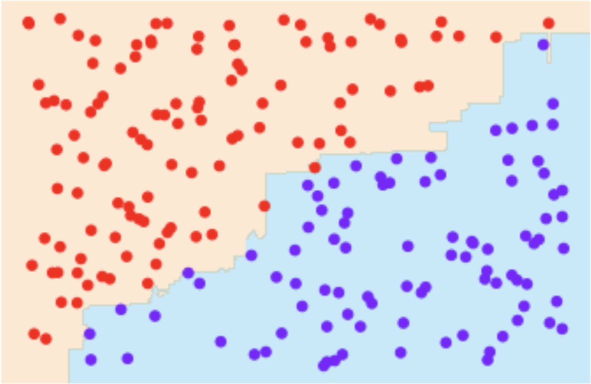


Figure 5: Random Forests boundary

Boosting

- Boosting is a very **powerful idea**
  - found in many different variants
- Boosting is building an ensemble by
  - minimizing the error
  - using **optimization** based search

Boosting

- Questions:
  - can we build a **strong model** from weak base models?
  - can it be **iterativelly** improved?
- A weak model
  - slightly better than random guessing
    - e.g. a tree of depth 1
- Overall idea (intuitively)
  - obtain a first model
  - identify **difficult cases**
  - obtain a new model that **corrects these errors**
  - **iterate** until convergence or a maximum number of models
  - apply models with **weighted** aggregation

AdaBoost (Yoav Freund and Robert Schapire)

- A popular boosting algorithm
  - Adaptive Boosting
- Overall idea
  - start with D and give equal weights to all cases
  - in each iteration
    - get a sample S from D **using the weights**
    - build a model from S
    - **increase the weights** of cases with wrong decisions

AdaBoost: in detail

- **Given**
  - a dataset D with n class-labelled examples
  - a number k of models (or tries)
  - a learning algorithm A
- **Assign** equal weights $w_i = 1/n$
- **For each** $1 \leq i \leq k$
  - $S_i =$ sample D with replacement using w_i
  - $M_i = A(S_i)$
  - $e_i =$ error rate of M_i on S_i
  - if $e_i < 0.5$ repeat previous steps
  - for each example x_i update weights
    - $w_i = w_i.e_i/(1 - e_i)$
    - high e_i -> low w_i
  - max-normalize the weigths

Weight as a function of error

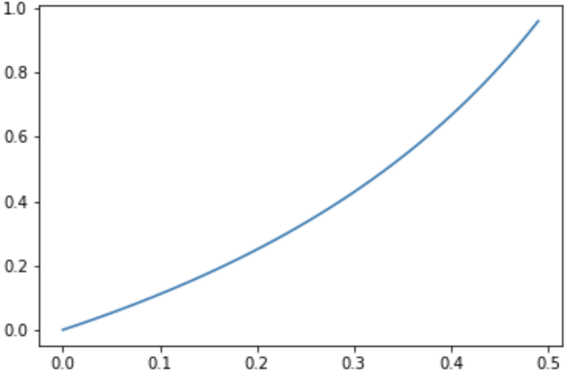


Figure 6: Example weight as a function of error

The boundary for AdaBoost

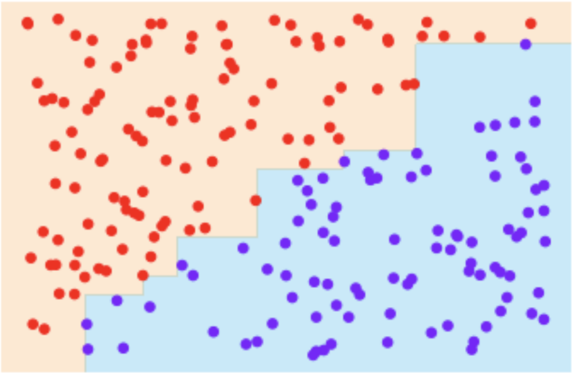


Figure 7: AdaBoost boundary

Boosting

- Computational **efficiency**
  - base learners are very simple
- **one parameter** (k)
  - better “off-the-shelf” algorithm
- Can be stated as an **optimization** approach
  - very powerful paradigm
- Tends to beat Bagging and RF
- May **overfit**
  - by focusing “too much” on recovering errors
  - Bagging and RF are not prone to overfitting

Other tasks

- Regression
    - These approaches are directly adapted
- Recommender systems
- Clustering and non-supervised learning

Interpretability

- Decision trees are **highly interpretable**
  - transparency
  - explainability
- Ensembles complicate **interpretability**
  - e.g. aggregation of 100 models
- But we can obtain a rank of important features
  - Features that are more common in the trees
  - Features in the top split
  - Mean decrease impurity (normalised)
    - how much a feature decreases impurity in a tree
- An overview of feature importance
  - https://machinelearningmastery.com/calculate-feature-importance-with-python/

References

- Books
  - Han, Kamber & Pei, Data Mining Concepts and Techniques, Morgan Kaufman.
  - Jake VanderPlas, Data Science Handbook, O'Reilly
  - Tibshirani et al., Elements of Statistical Learning