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Machine Learning

Session 12 - T

Tree-Based Models – Part 2

Degree in Applied Data Science

2024/2025

Why are Decision Trees poor predictors?

- Decision trees tend to have **high variance**. A small change in the training data can produce big changes in the estimated Tree.

- To improve the performance:
  - **Pruning (last session):** grow deep trees (small bias, high variance) which then are pruned into smaller ones (reduce variance);
  - **Ensemble methods (today's session):** combine multiple simple trees.
    - Bagging and Random Forests
    - Boosted trees

Bagging

- Let's revisit the concept of **Cross-Validation** and why it performs better than the **Holdout** method!

- The Holdout method often overestimates the error and **provides highly different error estimates** if you alter the test split.

- On the other hand, K-fold Cross-Validation generates more **consistent error estimates by averaging across K distinct estimates of error** (one for each fold).

- **Bagging** (Bootstrap AGGregatING) operates with a similar objective: **reducing the variance** of a predictor prone to high variance by **averaging across multiple estimates**.

Bagging

- In other words, averaging a set of observations reduces variance.

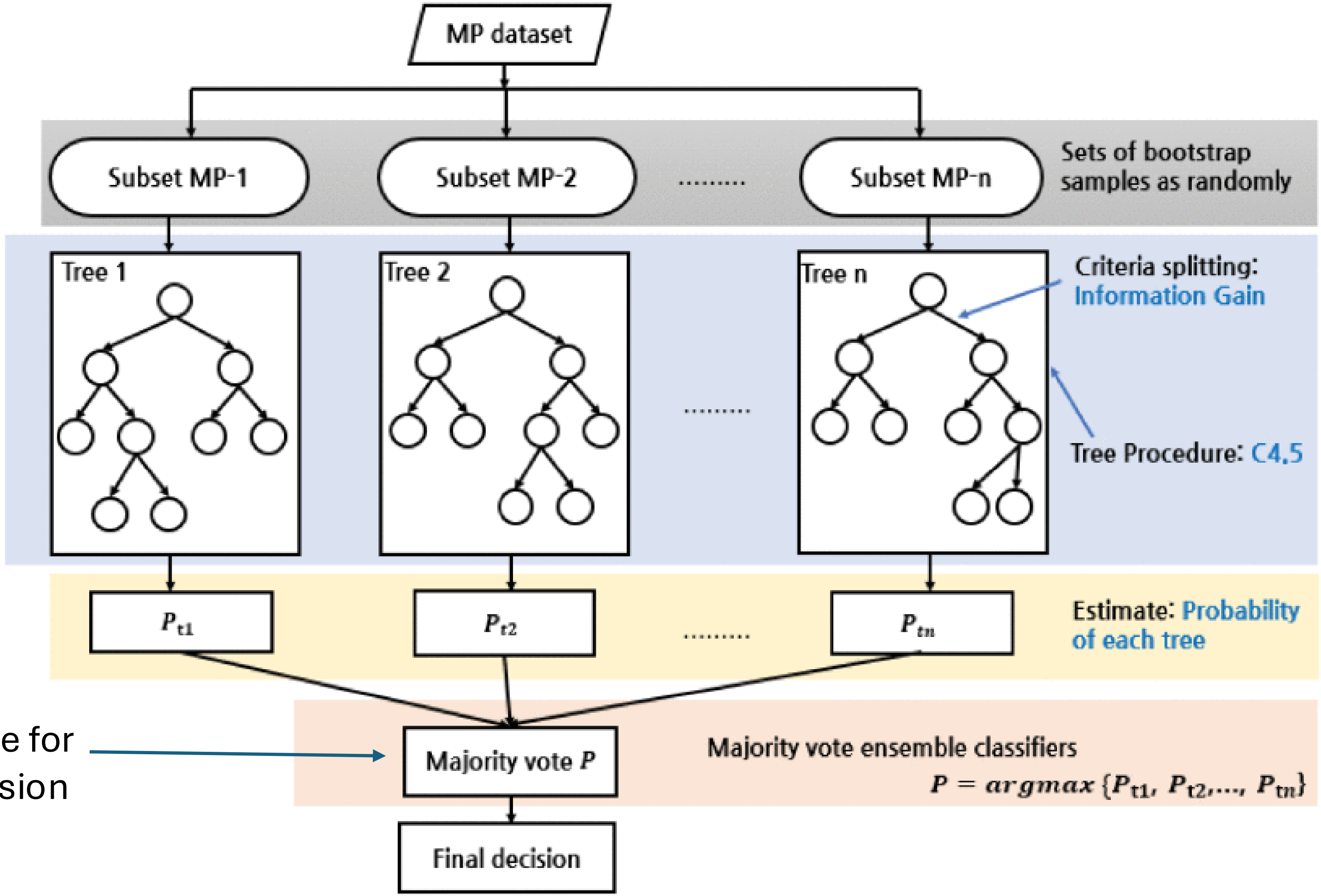
- **Obvious problem:** We only have access to one training dataset.

- **Solution:** Bootstrap the data!
  - Sample n times with replacement from the original training data;
  - Repeat B times to generate B ”bootstrapped” training datasets.

- For each bootstrapped dataset train a decision tree.

- Averaging the predictions of each tree trained with different bootstrapped datasets is called bootstrap aggregation (Bagging).

Bagging



Average for regression

Le, T.-T.-H., Kang, H., & Kim, H. (2020). Household Appliance Classification Using Lower Odd-Numbered Harmonics and the Bagging Decision Tree. In IEEE Access (Vol. 8, pp. 55937–55952). Institute of Electrical and Electronics Engineers (IEEE). https://doi.org/10.1109/access.2020.2981969

Out-of-Bag (OOB) Error Estimation

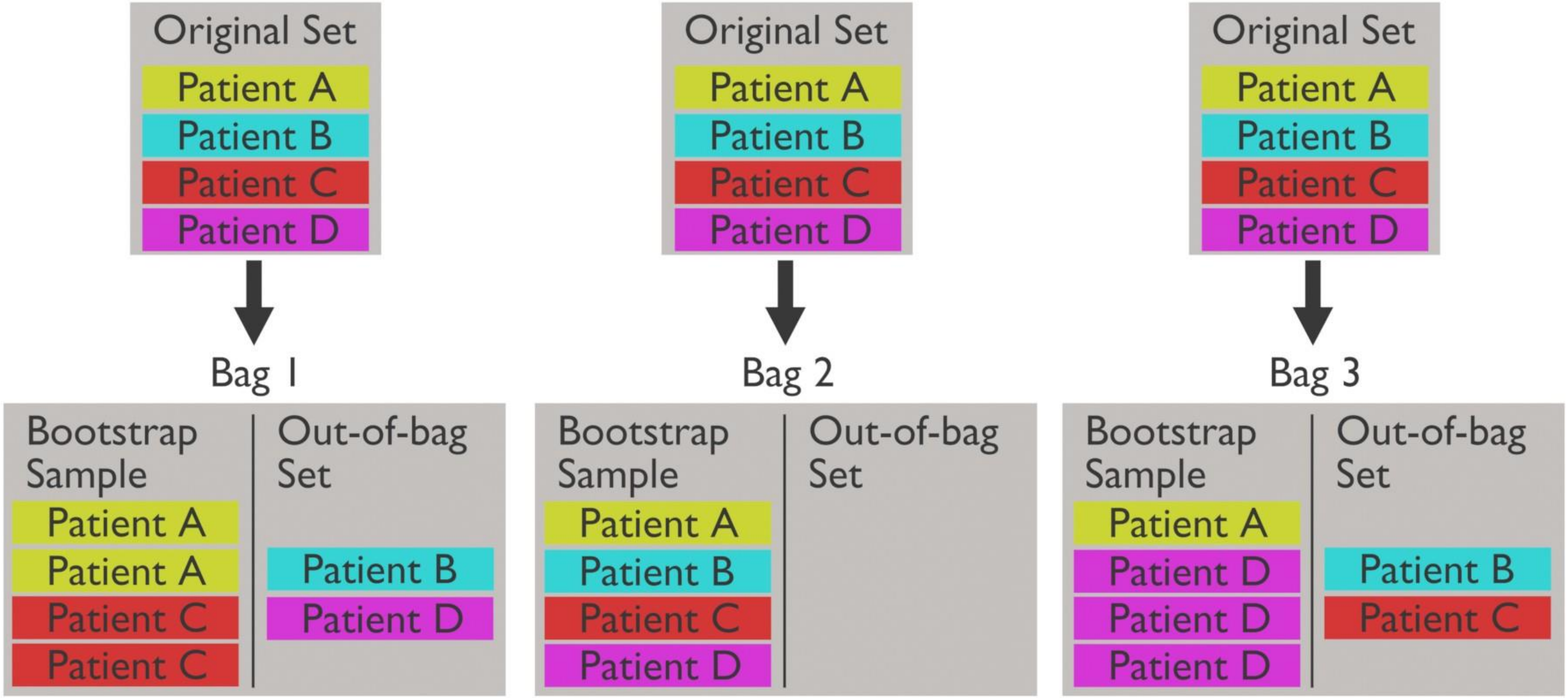
- **Not all** of the training points will appear in each sample;

- Each bootstrap sample contains roughly **63.2%** of the observed data points;

- The remaining observations not used to fit a given bagged tree are called the **out-of-bag (OOB)** observations

- Another way of thinking about it: Each observation is OOB for roughly B/3 of the trees. We can treat observation i as a test point each time it is OOB.

Out-of-Bag (OOB) Error Estimation



Out-of-Bag (OOB) Error Estimation

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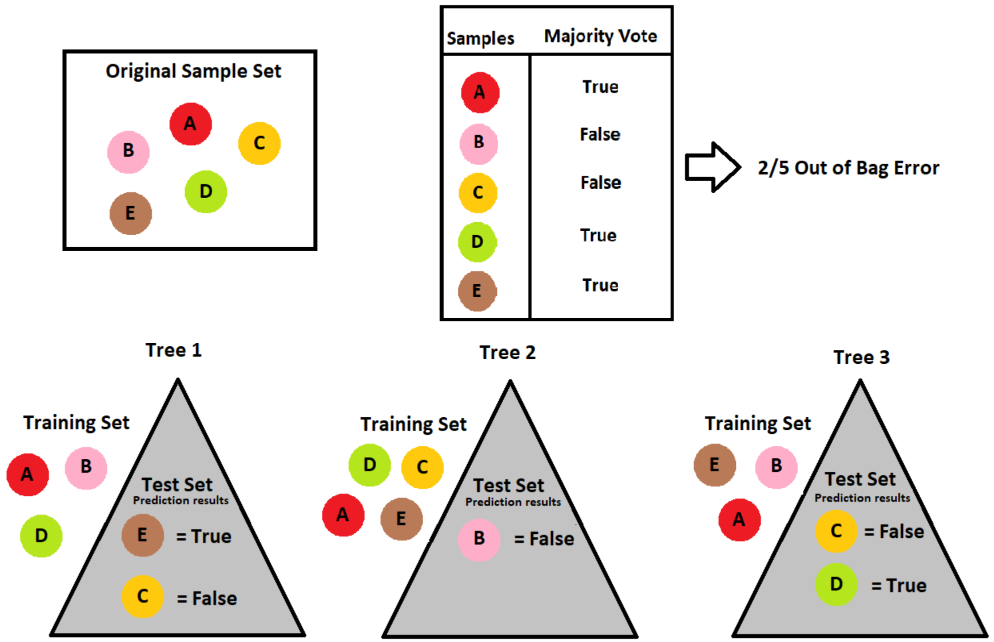
- To form the OOB estimate of test error:
  - Predict the response for the ith observation using each of the trees for which i was OOB. This gives us roughly B/3 predictions for each observation;
  - Calculate the error of each OOB prediction;
  - Average all of the errors.



Random Forests

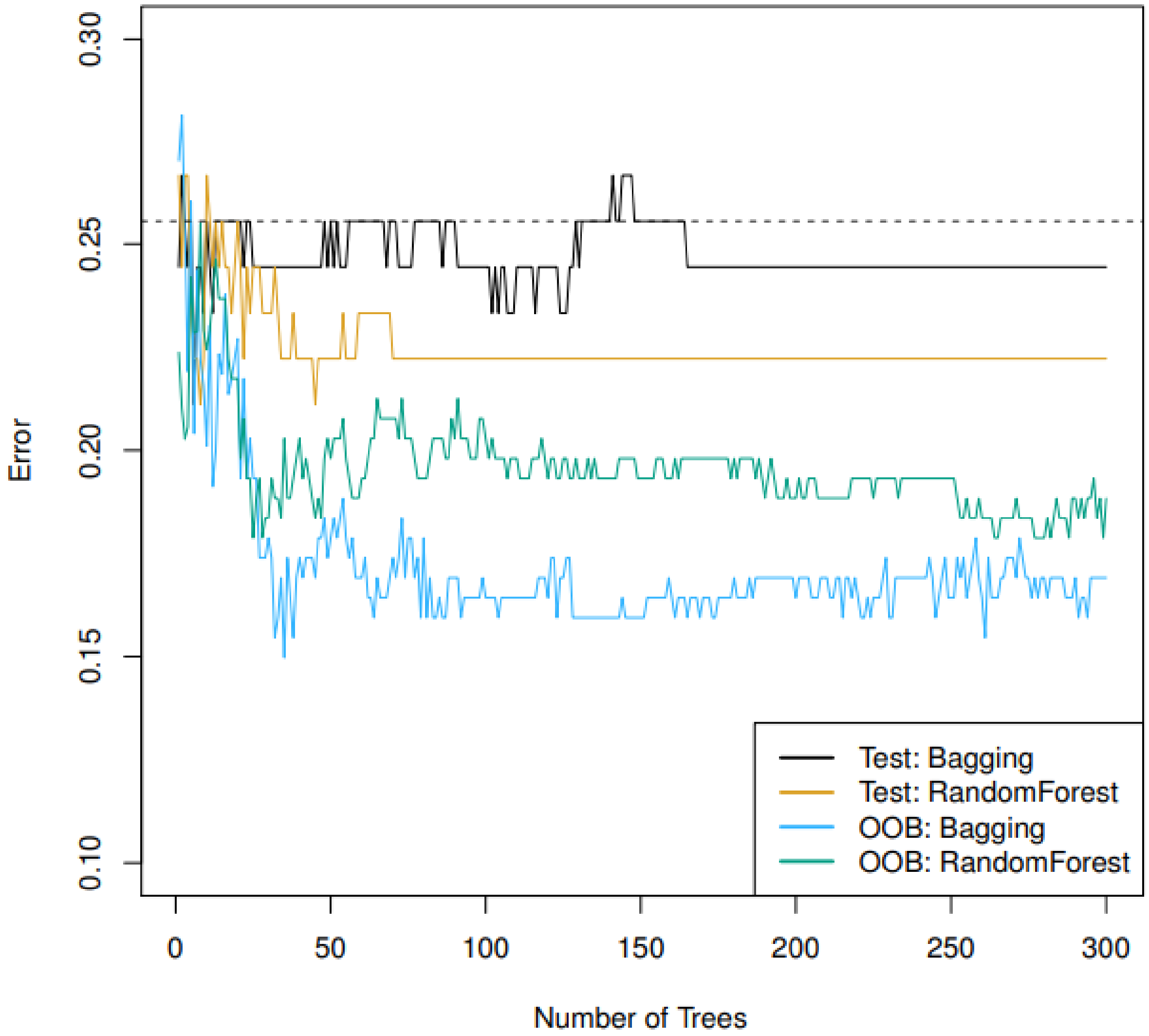
- However, the B **bootstrapped dataset are correlated**!
  - the variance reduction due to averaging is diminished.

- **Random forests** provide an improvement over **bagged trees** by **de-correlate** the B trees by **randomly perturbing each tree**.

- A **random forest** is constructed by **bagging**, but for each split in each tree only a **random subset of features** are considered as splitting variables.

- Rule of thumb: **$\sqrt{p}$ for classification trees** and **p/3 for regression trees** (p is the number of features).

Bagging vs Random Forests



Advantages of Random Forests

- **Reduced Overfitting:** Random forests mitigate overfitting by aggregating the predictions of multiple decision trees.

- **Improved Performance:** Random forests often provide higher performance compared to individual decision trees, especially for complex datasets.

- **Reduced Bias:** The ensemble nature of random forests reduces bias that may be present in individual decision trees.

- **Parallelization:** Training of individual decision trees within a random forest can be easily parallelized, leading to faster computation.

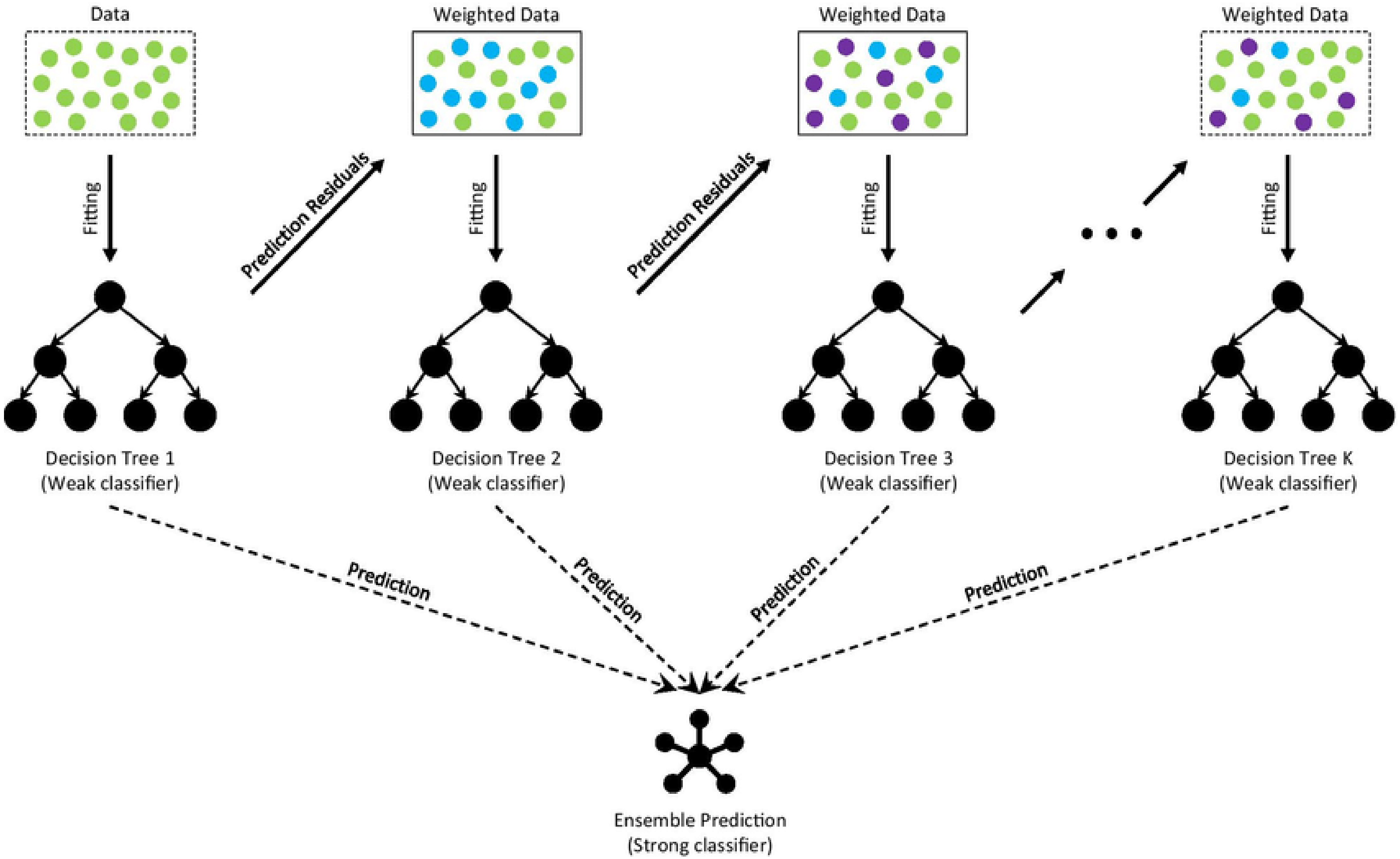
Boosting

- **Boosting** works in a similar way to bagging, except that the **trees are grown sequentially**: each tree is grown using **information from previously grown trees**.

- Each subsequent tree focus on the **training examples that the previous ones got wrong**.

- To focus on specific examples, boosting uses a **weighted training set**.

Boosting



Data
Weighted Data
Weighted Data
Weighted Data
Fitting
Fitting
Fitting
Fitting
Prediction Residuals
Prediction Residuals
Decision Tree 1
(Weak classifier)
Decision Tree 2
(Weak classifier)
Decision Tree 3
(Weak classifier)
Decision Tree K
(Weak classifier)
Prediction
Prediction
Prediction
Prediction
Ensemble Prediction
(Strong classifier)

AdaBoost

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- Given a base classifier, the key steps of **AdaBoost** are:
  - At each iteration, re-weight the training samples by assigning larger weights to samples that were classified incorrectly.
  - Train a new base classifier based on the re-weighted samples.
  - Add it to the ensemble of classifiers with an appropriate weight.
  - Repeat the process many times.

- Requirements for base classifier:
  - Needs to minimize weighted error.
  - Ensemble may get very large, so base classifier must be fast. It turns out that any so-called weak learner/classifier suffices (e.g. decison trees).

- Individually, **weak learners** may have **high bias** (underfit). By making each classifier focus on previous mistakes, AdaBoost **reduces bias**.

Bagging and Boosting Recap

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- Bagging and boosting are **ensemble learning methods** that can improve performance;

- **Bagging:**
  - Reduces variance;
  - Bias is not changed (much);
  - Parallel;
  - Want to minimiza correlation between ensemble elements.

- **Boosting:**
  - Reduces bias;
  - Increases variance;
  - Sequential;
  - High fependency between ensemble elements.

Resources

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- Collins, R. (2018). Machine learning with bagging and boosting. Independently Published.
- https://www.youtube.com/watch?v=J4Wdy0Wc_xQ
- https://www.youtube.com/watch?v=sQ870aTKqiM
- https://www.youtube.com/watch?v=Xz0x-8-cgaQ
- https://www.youtube.com/watch?v=tjy0yL1rRRU