WIKIPEDIA

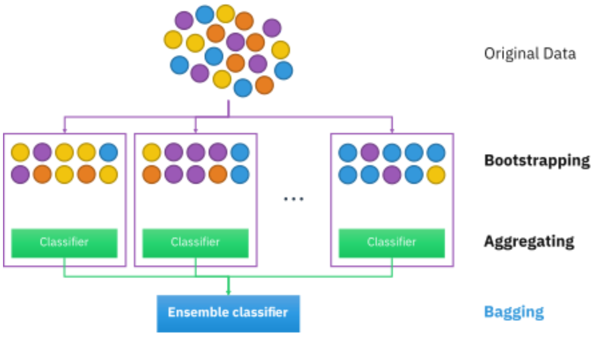
Bootstrap aggregating

Bootstrap aggregating, also called **bagging** (from **b**ootstrap **agg**regat**ing**), is a machine learning ensemble meta-algorithm designed to improve the stability and accuracy of machine learning algorithms used in statistical classification and regression. It also reduces variance and helps to avoid overfitting. Although it is usually applied to decision tree methods, it can be used with any type of method. Bagging is a special case of the model averaging approach.

Contents

Description of the technique

Given a standard training set D of size *n*, bagging generates *m* new training sets D_i, each of size *n′*, by sampling from *D* uniformly and with replacement. By sampling with replacement, some observations may be repeated in each D_i. If *n′*=*n*, then for large *n* the set D_i is expected to have the fraction (1 - 1/*e*) (≈63.2%) of the unique examples of *D*, the rest being duplicates.[1] This kind of sample is known as a bootstrap sample. Sampling with replacement ensures each bootstrap is independent from its peers, as it does not depend on previous chosen samples when sampling. Then, *m* models are fitted using the above *m* bootstrap samples and combined by averaging the output (for regression) or voting (for classification).



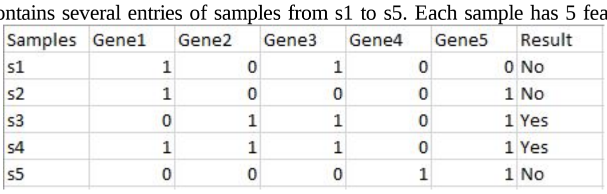
An illustration for the concept of bootstrap aggregating

Bagging leads to "improvements for unstable procedures",[2] which include, for example, artificial neural networks, classification and regression trees, and subset selection in linear regression.[3] Bagging was shown to improve preimage learning.[4][5] On the other hand, it can mildly degrade the performance of stable methods such as K-nearest neighbors.[2]

Process of the Algorithm

Original dataset

The original dataset contains several entries of samples from s1 to s5. Each sample has 5 features (Gene 1 to Gene 5). All samples are labeled as Yes or No for a classification problem.



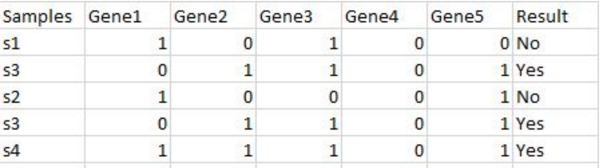
Samples	Gene1	Gene2	Gene3	Gene4	Gene5	Result
s1	1	0	1	0	0	No
s2	1	0	0	0	1	No
s3	0	1	1	0	1	Yes
s4	1	1	1	0	1	Yes
s5	0	0	0	1	1	No

Creation of Bootstrapped datasets

Given the table above to classify a new sample, first a bootstrapped dataset must be created using the data from the original dataset. This Bootstrapped dataset is typically the size of the original dataset, or smaller.

In this example, the size is 5 (s1 through s5). The Bootstrapped Dataset is created by randomly selecting samples from the original dataset. Repeat selections are allowed. Any samples that are not chosen for the bootstrapped dataset are placed in a separate dataset called the Out-of-Bag dataset.

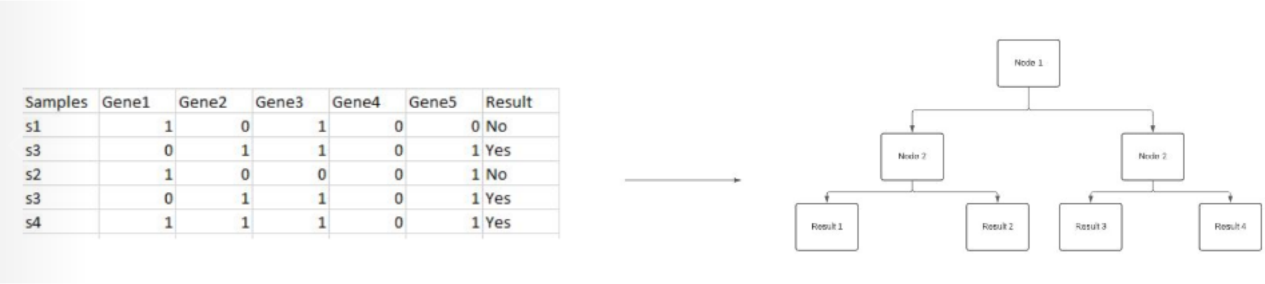
See an example bootstrapped dataset below. It has 5 entries (same size as the original dataset). There are duplicated entries such as two s3 since the entries are selected randomly with replacement.



Samples	Gene1	Gene2	Gene3	Gene4	Gene5	Result
s1	1	0	1	0	0	No
s3	0	1	1	0	1	Yes
s2	1	0	0	0	1	No
s3	0	1	1	0	1	Yes
s4	1	1	1	0	1	Yes

This step will repeat to generate m bootstrapped datasets.

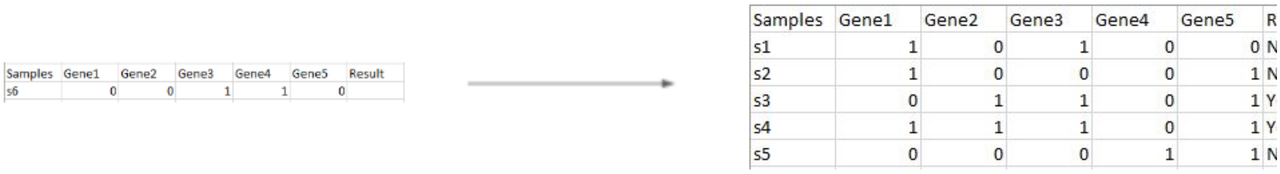
Creating of Decision Trees



Samples	Gene1	Gene2	Gene3	Gene4	Gene5	Result
s1	1	0	1	0	0	No
s3	0	1	1	0	1	Yes
s2	1	0	0	0	1	No
s3	0	1	1	0	1	Yes
s4	1	1	1	0	1	Yes

A Decision tree is created for each Bootstrapped dataset using randomly selected column values to split the nodes.

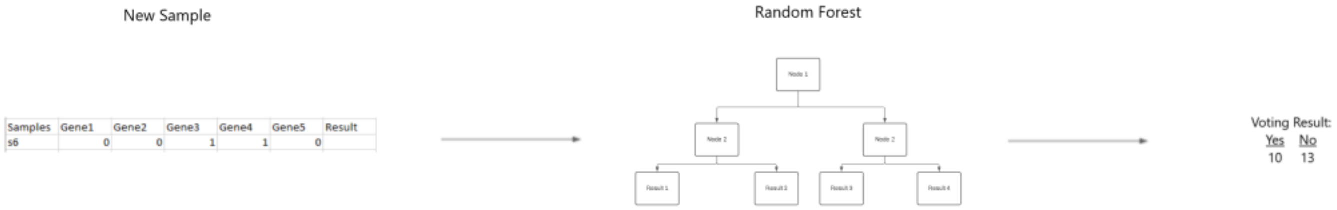
Predicting using Multiple Decision Trees



Samples	Gene1	Gene2	Gene3	Gene4	Gene5	Result
s6	0	0	1	1	0	

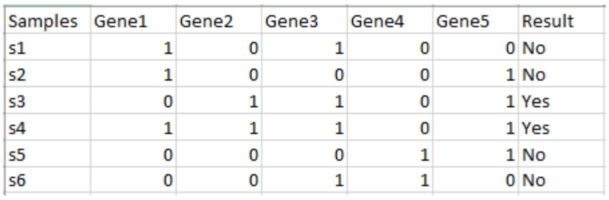
Samples	Gene1	Gene2	Gene3	Gene4	Gene5	R
s1	1	0	1	0	0	N
s2	1	0	0	0	1	N
s3	0	1	1	0	1	Y
s4	1	1	1	0	1	Y
s5	0	0	0	1	1	N

When a new sample is added to the table. The bootstrapped dataset is used to determine the new entry's clasifier value.



Samples	Gene1	Gene2	Gene3	Gene4	Gene5	Result
s6	0	0	1	1	0	

The new sample is tested in the random forest created by each bootstrapped dataset and each tree produces a classifier value for the new sample. For Classification, a process called voting is used to determine the final result, where the result produced the most frequently by the random forest is the given result for the sample. For Regression, the sample is assigned the average classifier value produced by the trees.



Samples	Gene1	Gene2	Gene3	Gene4	Gene5	Result
s1	1	0	1	0	0	No
s2	1	0	0	0	1	No
s3	0	1	1	0	1	Yes
s4	1	1	1	0	1	Yes
s5	0	0	0	1	1	No
s6	0	0	1	1	0	No

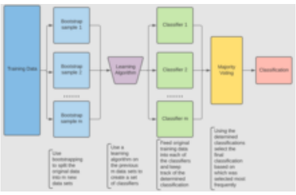
After the sample is tested in the random forest. A classifier value is assigned to the sample and it is added to the table.

Algorithm (Classification)

For Classification, use a training set D, Inducer I and the number of bootstrap samples m as input. Generate a classifier C^* as output[6]

1. Create m new training sets D_i, from D with replacement
2. Classifier C_i is built from each set D_i using I to determine the classification of set D_i
3. Finally classifier C^* is generated by using the previously created set of classifiers C_i on the original data set D, the classification predicted most often by the sub-classifiers C_i is the final classification

```
for i = 1 to m {
    D' = bootstrap sample from D    (sample with replacement)
    Ci = I(D')
}
C*(x) = argmax    Σ 1               (most often predicted label y)
         y∈Y   i:Ci(x)=y
```

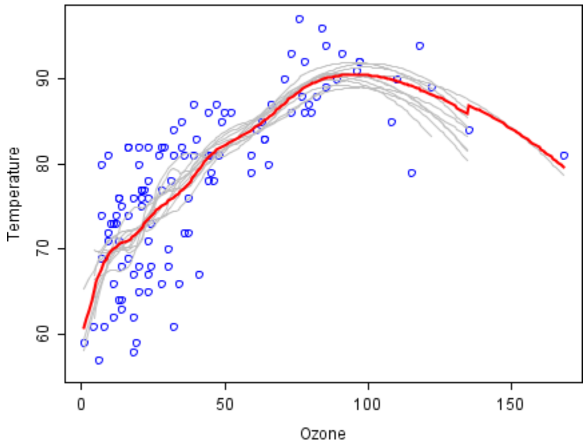

Training Data
Bootstrap sample 1
Bootstrap sample 2
Bootstrap sample m
Learning Algorithm
Classifier 1
Classifier 2
Classifier m
Majority Voting
Classification
Use bootstrapping to split the original data into m new data sets
Use a learning algorithm on the previous m data sets to create a set of classifiers
Feed original training data into each of the classifiers and keep track of the determined classification
Using the determined classifications select the final classification based on which was selected most frequently

Flow chart of the bagging algorithm when used for classification

Example: Ozone data

To illustrate the basic principles of bagging, below is an analysis on the relationship between ozone and temperature (data from Rousseeuw and Leroy (1986), analysis done in R).

The relationship between temperature and ozone appears to be nonlinear in this data set, based on the scatter plot. To mathematically describe this relationship, LOESS smoothers (with bandwidth 0.5) are used. Rather than building a single smoother for the complete data set, 100 bootstrap samples were drawn. Each sample is composed of a random subset of the original data and maintains a semblance of the master set's distribution and variability. For each bootstrap sample, a LOESS smoother was fit. Predictions from these 100 smoothers were then made across the range of the data. The black lines represent these initial predictions. The lines lack agreement in their predictions and tend to overfit their data points: evident by the wobbly flow of the lines.



By taking the average of 100 smoothers, each corresponding to a subset of the original data set, we arrive at one bagged predictor (red line). The red line's flow is stable and does not overly conform to any data point(s).

Advantages vs Disadvantages

Advantages:

- Many weak learners aggregated typically outperform a single learner over the entire set, and has less overfit
- Removes variance in high-variance low-bias data sets[7]
- Can be performed in parallel, as each separate bootstrap can be processed on its own before combination[8]

Disadvantages:

- In a data set with high bias, bagging will also carry high bias into its aggregate[7]
- Loss of interpretability of a model.
- Can be computationally expensive depending on the data set

History

The concept of Bootstrap Aggregating is derived from the concept of Bootstrapping which was developed by Bradley Efron.[9] Bootstrap Aggregating was proposed by Leo Breiman who also coined the abbreviated term "Bagging" (**B**ootstrap **agg**regat**ing**). Breiman developed the concept of bagging in 1994 to improve classification by combining classifications of randomly generated training sets. He argued, "If perturbing the learning set can cause significant changes in the predictor constructed, then bagging can improve accuracy."[3]

See also

- Boosting (meta-algorithm)
- Bootstrapping (statistics)
- Cross-validation (statistics)
- Random forest

- Random subspace method (attribute bagging)
- Resampled efficient frontier
- Predictive analysis: Classification and regression trees

References

1. Aslam, Javed A.; Popa, Raluca A.; and Rivest, Ronald L. (2007); *On Estimating the Size and Confidence of a Statistical Audit* (http://people.csail.mit.edu/rivest/pubs/APR07.pdf), Proceedings of the Electronic Voting Technology Workshop (EVT '07), Boston, MA, August 6, 2007. More generally, when drawing with replacement *n′* values out of a set of *n* (different and equally likely), the expected number of unique draws is $n(1 - e^{-n'/n})$.
2. Breiman, Leo (1996). "Bagging predictors". *Machine Learning*. **24** (2): 123–140. CiteSeerX 10.1.1.32.9399 (https://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.32.9399). doi:10.1007/BF00058655 (https://doi.org/10.1007%2FBF00058655). S2CID 47328136 (https://api.semanticscholar.org/CorpusID:47328136).
3. Breiman, Leo (September 1994). "Bagging Predictors" (https://www.stat.berkeley.edu/~breiman/bagging.pdf) (PDF). *Department of Statistics, University of California Berkeley*. Technical Report No. 421. Retrieved 2019-07-28.
4. Sahu, A., Runger, G., Apley, D., Image denoising with a multi-phase kernel principal component approach and an ensemble version (https://www.researchgate.net/profile/Anshuman_Sahu/publication/254023773_Image_denoising_with_a_multi-phase_kernel_principal_component_approach_and_an_ensemble_version/links/5427b5e40cf2e4ce940a4410/Image-denoising-with-a-multi-phase-kernel-principal-component-approach-and-an-ensemble-version.pdf), IEEE Applied Imagery Pattern Recognition Workshop, pp.1-7, 2011.
5. Shinde, Amit, Anshuman Sahu, Daniel Apley, and George Runger. "Preimages for Variation Patterns from Kernel PCA and Bagging (https://www.researchgate.net/profile/Anshuman_Sahu/publication/263388433_Preimages_for_variation_patterns_from_kernel_PCA_and_bagging/links/5427b3930cf26120b7b35ebd/Preimages-for-variation-patterns-from-kernel-PCA-and-bagging.pdf)." IIE Transactions, Vol.46, Iss.5, 2014
6. Bauer, Eric; Kohavi, Ron (1999). "An Empirical Comparison of Voting Classification Algorithms: Bagging, Boosting, and Variants" (https://link.springer.com/article/10.1023/A:1007515423169#article-info). *Machine Learning*. **36**: 108–109. doi:10.1023/A:1007515423169 (https://doi.org/10.1023%2FA%3A1007515423169). S2CID 1088806 (https://api.semanticscholar.org/CorpusID:1088806). Retrieved 6 December 2020.
7. "What is Bagging (Bootstrap Aggregation)?" (https://corporatefinanceinstitute.com/resources/knowledge/other/bagging-bootstrap-aggregation/). *CFI*. Corporate Finance Institute. Retrieved December 5, 2020.
8. Zoghni, Raouf (September 5, 2020). "Bagging (Bootstrap Aggregating), Overview" (https://medium.com/swlh/bagging-bootstrap-aggregating-overview-b73ca019e0e9). *Medium*. The Startup.
9. Efron, B. (1979). "Bootstrap methods: Another look at the jackknife" (https://doi.org/10.1214%2Faos%2F1176344552). *The Annals of Statistics*. **7** (1): 1–26. doi:10.1214/aos/1176344552 (https://doi.org/10.1214%2Faos%2F1176344552).

Further reading

- Breiman, Leo (1996). "Bagging predictors". *Machine Learning*. **24** (2): 123–140. CiteSeerX 10.1.1.32.9399 (https://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.32.9399). doi:10.1007/BF00058655 (https://doi.org/10.1007%2FBF00058655). S2CID 47328136 (https://api.semanticscholar.org/CorpusID:47328136).
- Alfaro, E., Gámez, M. and García, N. (2012). "adabag: An R package for classification with AdaBoost.M1, AdaBoost-SAMME and Bagging" (https://cran.r-project.org/package=adabag).
- Kotsiantis, Sotiris (2014). "Bagging and boosting variants for handling classifications problems: a survey". *Knowledge Eng. Review*. **29** (1): 78–100. doi:10.1017/S0269888913000313 (https://doi.org/10.1017%2FS0269888913000313).
- Boehmke, Bradley; Greenwell, Brandon (2019). "Bagging". *Hands-On Machine Learning with R*. Chapman & Hall. pp. 191–202. ISBN 978-1-138-49568-5.