# Ensemble Methods: Bagging

One way to get a diverse set of classifiers is to use very different training algorithms, as we just described in the rationale of ensemble methods. Another approach is to use **the same training algorithm** for every feature, but to train them on different random subsets of the training set. This approach is called **bagging** (short for **bootstrap** (重複抽樣) **aggregating**) based on the **bootstrap**, a widely applicable and extremely powerful statistical tool.

The basic idea of **bootstrap** or **bootstrapping** is that inference about a population from sample data (sample → population) can be modelled by resampling the sample data and performing inference about a sample from resampled data (resampled → sample). In short, **bootstrap resamples the data with replacement as illustrated in the figure below**. When doing properly, we will have:

sample → population $\approx$ resampled → sample
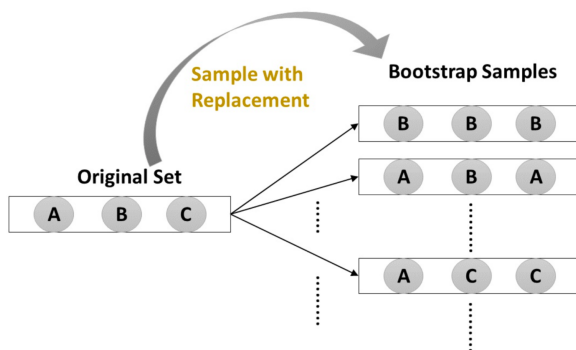
1. Theoretical Minimum for Bagging

Bagging is a general-purpose procedure for **reducing the variance of a statistical learning method**. Basically, we resample the data with replacement and then train a classifier on the newly sampled data. Then, we combine the outputs of each of the individual classifiers using a majority-voting scheme or other similar schemes.

Let us consider a given a set of *n* **independent** (or uncorrelated) observations $Z_1, Z_2, \cdots, Z_n$, each with variance σ^2. The variance of the mean $\bar{Z}$ of the observations is given by $\frac{\sigma^2}{n}$. **In other words, averaging a set of observations reduces variance.**

Hence a natural way to reduce the variance and hence increase the prediction accuracy of a statistical learning method is to take many training sets from the population, build a separate prediction model

using each training set, and average the resulting predictions. In other words, we could calculate $g^{(1)}(\mathbf{x})$, $g^{(2)}(\mathbf{x})$, …, $g^{(B)}(\mathbf{x})$ using B separate training sets, and average them in order to obtain a single low-variance statistical learning model,

$$g_{\text{avg}}(\mathbf{x}) = \frac{1}{B} \sum_{b=1}^{B} g^{(b)}(\mathbf{x})$$

Remark: $g_{\text{avg}}(\mathbf{x}) \approx \bar{g}(\mathbf{x})$ as we discussed in the note on bias and variance.

Fun Time: Is this (to take <u>many training sets from the population</u>) practical? (1) Yes (2) No

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Instead, we can **bootstrap**, by taking repeated samples from <u>the single training data set</u>. In this approach we generate B different bootstrapped training data sets. We then train our method on the bth bootstrapped training set in order to get $g^{(*b)}(x)$, and finally average all the predictions to obtain the *bootstrapped aggregated estimator* or *bagged estimator*:

$$g_{\text{bag}}(\mathbf{x}) = \frac{1}{B} \sum_{b=1}^{B} g^{(*b)}(\mathbf{x})$$

Remarks:

1. It is important to remember that g_{bag} is not exactly equal to g_{avg}. Thus g_{bag} might perform worse than the original estimator g.
2. The bagging procedure can be further enhanced by introducing random forests, which will be discussed next.

2. Python Example

Scikit-Learn offers a simple API for bagging with the BaggingClassifier class (or BaggingRegressor for regression). The following code trains an ensemble of 500 Decision Tree classifiers, each trained on 100 training instances, randomly sampled from the 500 data generated from make_moon with replacement. The n_jobs parameter tells Scikit-Learn the number of CPU cores to use for training and predictions (-1 tells Scikit-Learn to use all available cores):

```python
from sklearn.ensemble import BaggingClassifier
from sklearn.tree import DecisionTreeClassifier

bag_clf = BaggingClassifier(
    DecisionTreeClassifier(random_state=42), n_estimators=500,
```

```
    max_samples=100, bootstrap=True, n_jobs=-1, random_state=42)
bag_clf.fit(X_train, y_train)
y_pred = bag_clf.predict(X_test)
```

Figure below compares the decision boundary of a single Decision Tree with the decision boundary of a bagging ensemble of 500 trees (from the preceding code).
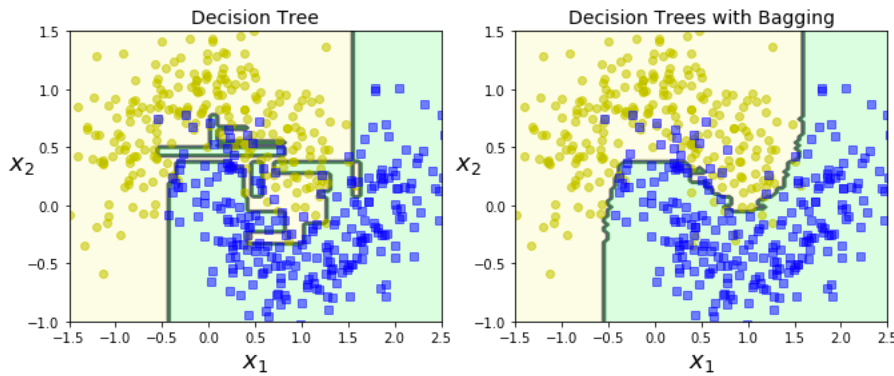
Q: what have you observed?

A:

As you can see, the decision boundary from the bagging ensemble is much smooth (low variance) and ensemble's predictions will likely generalize much better than the single Decision Tree's predictions (`0.904 vs 0.856`).

You can download the complete source code `Bagging.ipynb` from the course website.