

Bootstrapping

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Overview

- 1 Bias-Variance trade-off and Cross Validation
- 2 Bootstrapping
- 3 Little Bag of Bootstraps

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Bias-Variance Trade-off

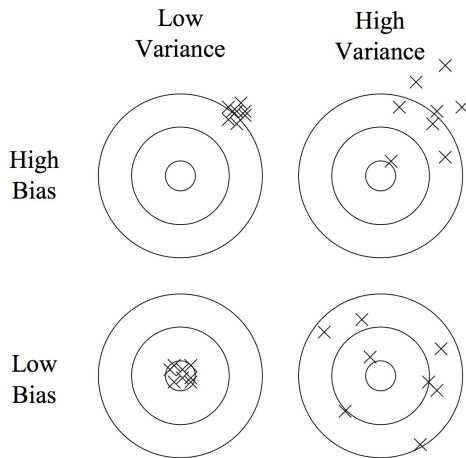


Figure: Image showing Bias Variance Trade-off - courtesy Quora

Bias-Variance Trade-off

- In machine learning, we are trying to learn $y = f(x) + \epsilon$
- In addition to intrinsic noise, ϵ , the models have their own sources of error
- Bias: The tendency of the algorithm to be consistently incorrect
- Variance: The algorithm's tendency to fit to the noise in the data in addition to the signal
- Models with high bias tend to **underfit**. E.g. represent a linear relationship with the mean
- Models with high variance tend to **overfit** E.g. represent a linear relationship with a higher-order polynomial

Bias-Variance Trade-off: Mathematical definition

Bias Variance Mathematical definition

We can represent the error of a model as $Err(x) = E[(y - \hat{f}(x))^2]$.

Decompose this down as $(E[\hat{f}(x)] - f(x))^2 + E[(\hat{f}(x) - E[\hat{f}(x)])^2] + \epsilon^2$.

In other words, $Err(x) = Bias^2 + Variance + Noise$.

Given infinite data, we can construct models that drive both bias and variance down to zero. However, we live in an imperfect world with finite data, noisy measurement tools, and finite resources. Typically there is a trade-off between Bias and Variance and we try to find the best balance between the two.

Bias Variance Trade-off example

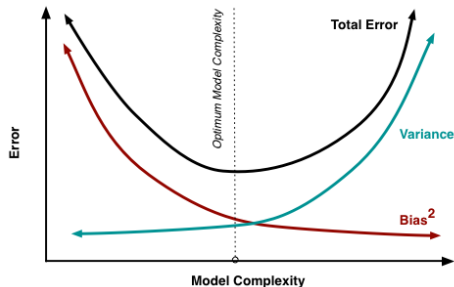


Figure: Bias and Variance vs Model Complexity

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Some ways to understand and work with bias-variance trade-off

- Cross-validation
- Bootstrapping
- Little Bag of Bootstraps

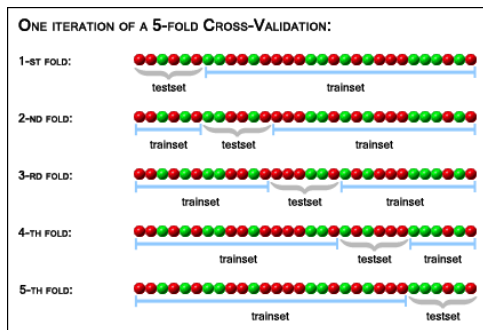


Figure: Cross Validation of a Model

Cross-validation

- Doesn't use the entire training set
- Typically the error is *biased* upwards
- Variance estimates of Θ is not strictly correct (K splits are not *independent*)

Cross-validation mistakes

Cross-validation

Consider a simple classifier applied to some two-class data:

- 1 Starting with 5000 predictors and 50 samples, find the 100 predictors having the largest correlation with the class labels.
- 2 We then apply a classifier such as logistic regression, using only these 100 predictors.
- 3 How do we estimate the test set performance of this classifier?

Can we apply cross-validation in step 2, forgetting about step 1?

Cross-validation mistakes

- **Wrong:** Running CV only on Step 2
- **Right:** Running CV on both Step 1 and 2

Bootstrap

- Powerful technique for estimating Bias and Variance
- Very simple, applies to most situations (e.g. except for Power Law/non-finite variance)
- Make inference about the population from a single sample
- Approximate population distribution by empirical distribution

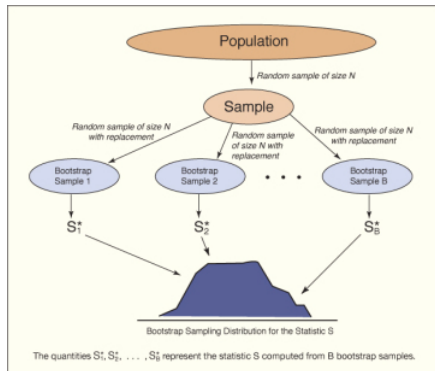


Figure: The Bootstrap Method

The Bootstrap

- The bootstrap is a flexible and powerful statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical learning method.
- For example, it can provide an estimate of the standard error of a coefficient, or a confidence interval for that coefficient.

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- Sample **with replacement** from the original data set and derive as many copies of the data as you want
- Estimate coefficients on each sample independently and use that to derive variance, and standard error estimates

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Little Bag of Bootstraps

- Approximately 63.2% samples covered in each bootstrap round
- When N , the sample size, is large this can be a severe limitation
- 1TB of data \rightarrow 632GB per bootstrap round
- You need to perform several rounds to get good estimates
- Difficult to parallelize when you have to move that much data around

Little Bag of Bootstraps

The Bag of Little Bootstraps (BLB)

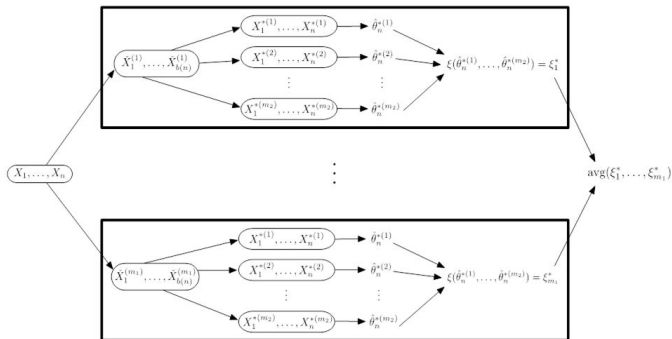


Figure: The Little Bag of Bootstraps Method

Little Bag of Bootstraps

- From your sample of N data points, create s samples (without replacement) of size $\approx N^{0.6}$
- On each of these s samples, run r bootstrap iterations
- In the inner bootstraps (r iterations), data is sampled with replacement and resampled back to size N
- Take average of averages and return that as your estimate. Also return confidence intervals

Little Bag of Bootstraps

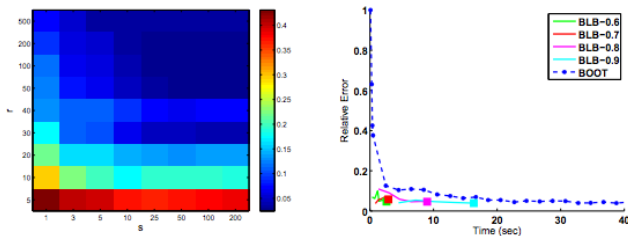


Figure: Little Bag of Bootstraps Performance

