Lecture 09

Model Evaluation 2:
Confidence Intervals and Resampling Methods

STAT 451: Machine Learning, Fall 2020
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http://stat.wisc.edu/~sraschka/teaching/stat451-fs2020/
1. **Introduction**

2. Holdout method for model evaluation

3. Holdout method for model selection

4. Confidence intervals -- normal approximation

5. Resampling & repeated holdout

6. Empirical confidence intervals via Bootstrap

7. The 0.632 and 0.632+ Bootstrap
Overview

Model Eval Lectures

Basics
- Bias and Variance
- Overfitting and Underfitting
- Holdout method
- Confidence Intervals

Resampling methods
- Repeated holdout
- Empirical confidence intervals

Cross-Validation
- Hyperparameter tuning
- Model selection
- Algorithm Selection

Statistical Tests
- Evaluation Metrics

This Lecture
Main points why we evaluate the predictive performance of a model:
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1. Want to estimate the generalization performance, the predictive performance of our model on future (unseen) data.
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2. Want to increase the predictive performance by tweaking the learning algorithm and selecting the best performing model from a given hypothesis space.
Main points why we evaluate the predictive performance of a model:

1. Want to estimate the generalization performance, the predictive performance of our model on future (unseen) data.

2. Want to increase the predictive performance by tweaking the learning algorithm and selecting the best performing model from a given hypothesis space.

3. Want to identify the ML algorithm that is best-suited for the problem at hand; thus, we want to compare different algorithms, selecting the best-performing one as well as the best performing model from the algorithm’s hypothesis space.
Some unfortunate facts about test sets

- Training set error is an optimistically biased estimator of the generalization error

- Test set error is an unbiased estimator of the generalization error (test sample and hypothesis chosen independently)

- (In practice, the test set error is actually pessimistically biased; why?)
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- (in practice, the test set error is actually pessimistically biased; why?)
Holdout Method

2-Fold Cross-Validation

Repeated Holdout

Training  Evaluation

1 2 3 4 5 6 7 8 9 10

Holdout Method
Often, using the holdout method is not a good idea ...
Often using the holdout method is not a good idea ...

Test set error as generalization error estimator is ____imistically biased (not so bad)

But it does not account for variance in the training data (bad)
Why is pessimistic bias not "so bad"?

Suppose we have the following ranking based on accuracy:

\[ h_2: 75\% > h_1: 70\% > h_3: 65\% , \]

we would still rank them the same way if we add a 10% pessimistic bias:

\[ h_2: 65\% > h_1: 60\% > h_3: 55\% . \]
Test set errors can also be optimistically biased
Do CIFAR-10 Classifiers Generalize to CIFAR-10?

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Ludwig Schmidt  
MIT  

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UC Berkeley

June 4, 2018

Abstract

Machine learning is currently dominated by largely experimental work focused on improvements in a few key tasks. However, the impressive accuracy numbers of the best performing models are questionable because the same test sets have been used to select these models for multiple years now. To understand the danger of overfitting, we measure the accuracy of CIFAR-10 classifiers by creating a new test set of truly unseen images. Although we ensure that the new test set is as close to the original data distribution as possible, we find a large drop in accuracy (4% to 10%) for a broad range of deep learning models. Yet, more recent models with higher original accuracy show a smaller drop and better overall performance, indicating that this drop is likely not due to overfitting based on adaptivity. Instead, we view our results as evidence that current accuracy numbers are brittle and susceptible to even minute natural variations in the data distribution.

The CIFAR-10 dataset

CIFAR -> Canadian Institute For Advanced Research

- 60,000 32x32 color images in 10 classes
- 6,000 images per class
- 50,000 training images and 10,000 test images

https://www.cs.toronto.edu/~kriz/cifar.html
After collecting a sufficient number of high-quality images for each keyword, we sampled a random subset from our pruned candidate set. The sampling procedure was such that the keyword-level distribution of our new dataset matches the keyword-level distribution of CIFAR-10 (see Appendix E). In the final stage, we again proceeded similar to the original CIFAR-10 dataset creation process and used $k$-nearest neighbors to filter out near duplicates. In particular, we removed near-duplicates within our new dataset and also images that had a near duplicate in the original CIFAR-10 dataset (train or test). The latter aspect is particularly important since our reproducibility study is only interesting if we evaluate on truly unseen data. Hence we manually reviewed the top-10 nearest neighbors for each image in our new test set. After removing near-duplicates in our dataset, we re-sampled the respective keywords until this process converged to our final dataset.

We remark that we did not run any classifiers on our new dataset during the data collection phase of our study. In order to ensure that the new data does not depend on the existing classifiers, it is important to strictly separate the data collection phase from the following evaluation phase.

4 Model Performance Results

After we completed the new test set, we evaluated a broad range of image classification models. The main question was how the accuracy on the original CIFAR-10 test set compares to the accuracy on our new test set. To this end, we experimented with a broad range of classifiers spanning multiple years of machine learning research. The models include widely used convolutional networks (VGG and ResNet\textsuperscript{7,18}), more recent architectures (ResNeXt, PyramidNet, DenseNet\textsuperscript{6,10,20}), the published state-of-the-art (Shake-Drop\textsuperscript{21}), and a model derived from RL-based hyperparameter search (NASNet\textsuperscript{23}). In addition, we also evaluated “shallow” approaches based on random features\textsuperscript{2,16}. Overall, the accuracies on the original CIFAR-10 test set range from about 80% to 97%. For all deep architectures, we used code previously published online (see Appendix A for a list).

To avoid bias due to specific model repositories or frameworks, we also evaluated two widely used (a) Test Set A
(b) Test Set B

Figure 1: Class-balanced random draws from the new and original test sets.$^{1}$

Figure 2: Model accuracy on new test set vs. model accuracy on original test set.

(a) All models

(b) High accuracy models

Table 1: Model accuracy on the original CIFAR-10 test set and the new test set, with the gap reported as the difference between the two accuracies. Δ Rank is the relative difference in the ranking from the original test set to the new test set. For example, ΔRank = -2 means a model dropped in the rankings by two positions on the new test set.

<table>
<thead>
<tr>
<th>Model Name</th>
<th>Original Accuracy</th>
<th>New Accuracy</th>
<th>Gap</th>
<th>Δ Rank</th>
</tr>
</thead>
<tbody>
<tr>
<td>shake_shake_64d_cutout [3, 4]</td>
<td>97.1 [96.8, 97.4]</td>
<td>93.0 [91.8, 94.0]</td>
<td>4.1</td>
<td>0</td>
</tr>
<tr>
<td>shake_shake_64d [4]</td>
<td>97.0 [96.6, 97.3]</td>
<td>91.4 [90.1, 92.6]</td>
<td>5.6</td>
<td>-2</td>
</tr>
<tr>
<td>wide_resnet_28_10_cutout [3, 22]</td>
<td>97.0 [96.6, 97.3]</td>
<td>92.0 [90.7, 93.1]</td>
<td>5</td>
<td>+1</td>
</tr>
<tr>
<td>shake_drop [21]</td>
<td>96.9 [96.5, 97.2]</td>
<td>92.3 [91.0, 93.4]</td>
<td>4.6</td>
<td>+3</td>
</tr>
<tr>
<td>shake_shake_32d [4]</td>
<td>96.6 [96.2, 96.9]</td>
<td>89.8 [88.4, 91.1]</td>
<td>6.8</td>
<td>-2</td>
</tr>
<tr>
<td>darc [11]</td>
<td>96.6 [96.2, 96.9]</td>
<td>89.5 [88.1, 90.8]</td>
<td>7.1</td>
<td>-4</td>
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<tr>
<td>resnext_29_4x64d [20]</td>
<td>96.4 [96.0, 96.7]</td>
<td>89.6 [88.2, 90.9]</td>
<td>6.8</td>
<td>-2</td>
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<td>96.3 [96.0, 96.7]</td>
<td>90.5 [89.1, 91.7]</td>
<td>5.9</td>
<td>+3</td>
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<tr>
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<td>96.2 [95.8, 96.6]</td>
<td>90.0 [88.6, 91.2]</td>
<td>6.3</td>
<td>+3</td>
</tr>
<tr>
<td>wide_resnet_28_10 [22]</td>
<td>95.9 [95.5, 96.3]</td>
<td>89.7 [88.3, 91.0]</td>
<td>6.2</td>
<td>+2</td>
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<tr>
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<td>89.3 [87.8, 90.6]</td>
<td>6.5</td>
<td>0</td>
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<tr>
<td>densenet_BC_100_12 [10]</td>
<td>95.5 [95.1, 95.9]</td>
<td>87.6 [86.1, 89.0]</td>
<td>8</td>
<td>-2</td>
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<td>neural_architecture_search [23]</td>
<td>95.4 [95.0, 95.8]</td>
<td>88.8 [87.4, 90.2]</td>
<td>6.6</td>
<td>+1</td>
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<tr>
<td>wide_resnet_tf [22]</td>
<td>95.0 [94.6, 95.4]</td>
<td>88.5 [87.0, 89.9]</td>
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<td>+1</td>
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<td>85.9 [84.3, 87.4]</td>
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<td>-1</td>
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<tr>
<td>vgg16_keras [14, 18]</td>
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<td>85.3 [83.6, 86.8]</td>
<td>8.3</td>
<td>-1</td>
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<tr>
<td>resnet_basic_110 [7]</td>
<td>93.5 [93.0, 93.9]</td>
<td>85.2 [83.5, 86.7]</td>
<td>8.3</td>
<td>-1</td>
</tr>
<tr>
<td>resnet_v2_basic_110 [8]</td>
<td>93.4 [92.9, 93.9]</td>
<td>86.5 [84.9, 88.0]</td>
<td>6.9</td>
<td>+3</td>
</tr>
<tr>
<td>resnet_basic_56 [7]</td>
<td>93.3 [92.8, 93.8]</td>
<td>85.0 [83.3, 86.5]</td>
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<td>resnet_basic_44 [7]</td>
<td>93.0 [92.5, 93.5]</td>
<td>84.2 [82.6, 85.8]</td>
<td>8.8</td>
<td>-3</td>
</tr>
<tr>
<td>vgg_15_BN_64 [14, 18]</td>
<td>93.0 [92.5, 93.5]</td>
<td>84.9 [83.2, 86.4]</td>
<td>8.1</td>
<td>+1</td>
</tr>
<tr>
<td>resnet_preact_tf [7]</td>
<td>92.7 [92.2, 93.2]</td>
<td>84.4 [82.7, 85.9]</td>
<td>8.3</td>
<td>0</td>
</tr>
<tr>
<td>resnet_basic_32 [7]</td>
<td>92.5 [92.0, 93.0]</td>
<td>84.9 [83.2, 86.4]</td>
<td>7.7</td>
<td>+3</td>
</tr>
<tr>
<td>cudaconvnet [13]</td>
<td>88.5 [87.9, 89.2]</td>
<td>77.5 [75.7, 79.3]</td>
<td>11</td>
<td>0</td>
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<tr>
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<td>73.1 [71.1, 75.1]</td>
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<tr>
<td>random_features_32k_aug [2]</td>
<td>85.0 [84.3, 85.7]</td>
<td>71.9 [69.9, 73.9]</td>
<td>13</td>
<td>0</td>
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<tr>
<td>random_features_256k [2]</td>
<td>84.2 [83.5, 84.9]</td>
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<td>14</td>
<td>0</td>
</tr>
<tr>
<td>random_features_32k [2]</td>
<td>83.3 [82.6, 84.0]</td>
<td>67.9 [65.9, 70.0]</td>
<td>15</td>
<td>-1</td>
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<tr>
<td>alexnet_tf</td>
<td>82.0 [81.2, 82.7]</td>
<td>68.9 [66.8, 70.9]</td>
<td>13</td>
<td>+1</td>
</tr>
</tbody>
</table>

Often using the holdout method is not a good idea ...

- Test set error as generalization error estimator is pessimistically biased (not so bad)
- Does not account for variance in the training data (bad)
Issues with Subsampling (Independence Violation)

The Iris dataset consists of 50 Setosa, 50 Versicolor, and 50 Virginica flowers; the flower species are distributed uniformly:
- 33.3% Setosa
- 33.3% Versicolor
- 33.3% Virginica

If our random function assigns 2/3 of the flowers (100) to the training set and 1/3 of the flowers (50) to the test set, it may yield the following:
- training set → 38 x Setosa, 28 x Versicolor, 34 x Virginica
- test set → 12 x Setosa, 22 x Versicolor, 16 x Virginica
Holdout evaluation

1. Data
   - Labels
   - Training Data
   - Training Labels
   - Test Data
   - Test Labels

2. Learning Algorithm
   - Hyperparameter Values
   - Model

3. Prediction
   - Test Data
   - Test Labels
   - Performance

4. Data
   - Labels
   - Hyperparameter Values
   - Learning Algorithm
   - Final Model
1. Introduction

2. Holdout method for model evaluation

3. Holdout method for model selection

4. Confidence intervals -- normal approximation

5. Resampling & repeated holdout

6. Empirical confidence intervals via Bootstrap

7. The 0.632 and 0.632+ Bootstrap
Holdout evaluation

1. Data
   - Labels
   - Training Data
   - Training Labels
   - Test Data
   - Test Labels

2. Training Data
   - Training Labels
   - Hyperparameter Values
   - Learning Algorithm
   - Model

3. Test Data
   - Prediction
   - Performance
   - Test Labels
   - Model

4. Data
   - Labels
   - Hyperparameter Values
   - Learning Algorithm
   - Final Model
Can we use the holdout method for model selection?
Holdout validation (hyperparam. tuning)
Holdout validation (hyperparam. tuning)

1. Data
   - Training Data
   - Validation Data
   - Test Data

   Labels
   - Training Labels
   - Validation Labels
   - Test Labels

2. Learning Algorithm
   - Hyperparameter values
     - Model
     - Model
     - Model
Holdout validation (hyperparam. tuning)

3.

Validation Data → Prediction → Performance → Best Model

4.

Training Data → Validation Data → Model

Training Labels → Validation Labels
Holdout validation
(hyperparam. tuning)

5.

Test Data \rightarrow Prediction \rightarrow Performance

6.

Data
Labels

Best Hyperparameter Values
Learning Algorithm

Final Model
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Binomial distribution

<table>
<thead>
<tr>
<th>Notation</th>
<th>$B(n, p)$</th>
</tr>
</thead>
</table>
| Parameters | $n \in \mathbb{N}_0$ — number of trials  
$p \in [0, 1]$ — success probability in each trial |
| Support | $k \in \{0, \ldots, n\}$ — number of successes |
| pmf | $\binom{n}{k} p^k (1 - p)^{n-k}$ |
| CDF | $I_{1-p}(n - k, 1 + k)$ |
| Mean | $np$ |
| Median | $\lfloor np \rfloor$ or $\lceil np \rceil$ |
| Mode | $\lfloor (n + 1)p \rfloor$ or $\lceil (n + 1)p \rceil - 1$ |
| Variance | $np(1 - p)$ |

(Image credit: Screenshot from https://en.wikipedia.org/wiki/Binomial_distribution)
Binomial distribution \[ Pr(k) = \frac{n!}{k!(n-k)!} p^k (1-p)^{n-k} \].

**Coin Flip (Bernoulli Trial)**
- coin lands on head ("success")
- probability of success \( p \)
- \( \frac{k}{n} \), estimator of \( p \)
- mean, number of successes \( \mu_k = np \)

**0-1 Loss**
- example misclassified (0-1 loss)
- true error \( ERR_\mathcal{D}(h) = Pr \left[ f(x) \neq h(x) \right] \)
- sample (test set) error
  \[ ERR_\mathcal{S}(h) = \frac{1}{n} \sum_{x \in \mathcal{S}} \delta(f(x), h(x)) \]
Binomial distribution  

\[ Pr(k) = \frac{n!}{k!(n-k)!} p^k(1-p)^{n-k}. \]

**Coin Flip (Bernoulli Trial)**

- mean, number of successes  
  \[ \mu_k = np \]

- variance  \[ \sigma_k^2 = np(1-p) \]

- standard deviation  \[ \sigma_k = \sqrt{np(1-p)} \]

**0-1 Loss**

We are interested in proportions

\[ ERR_S = \frac{1}{n} \sum_{x \in S} \delta(f(x), h(x)) \]

\[ \sigma^2 = p(1-p) \]

\[ \sigma = \sqrt{p(1-p)} \]

\[ SE = \frac{\sqrt{ERR_S(1-ERR_S)}}{\sqrt{n}} = \sqrt{\frac{ERR_S(1-ERR_S)}{n}} \]
Confidence Intervals

A XX% confidence interval of some parameter $p$ is an interval that is expected to contain $p$ with probability XX%.*

* the more precise definition is "In an infinite long series of trials in which repeated samples of n are taken from the same distribution, the 95% Confidence Interval is calculated using the same method, the proportion of intervals covering the true parameter $p$ is xx%."
```python
import matplotlib.pyplot as plt
import numpy as np

np.random.seed(123)

std_norm_sample = np.random.randn(1000000)
plt.hist(std_norm_sample, bins=np.arange(-4, 4, 0.01), density=True)
plt.show()

binom_sample = np.random.binomial(n=100, p=0.2, size=1000000)
plt.hist(binom_sample, bins=np.arange(0, 40, 0.5), density=True)
plt.show()
```
Normal Approximation Interval

- Less tedious than confidence interval for Binomial distribution and hence often used in (ML) practice for large $n$

- Rule of thumb: if $n$ larger than 40, the Binomial distribution can be reasonably approximated by a Normal distribution; and $np$ and $n(1 - p)$ should be greater than 5

$$CI = ERR_S \pm z \sqrt{\frac{ERR_S(1 - ERR_S)}{n}}$$
The z constant for different confidence intervals:

- 99%: $z=2.58$
- 95%: $z=1.96$
- 90%: $z=1.64$
Code

```python
clf.fit(X_train, y_train)
acc_test_na = clf.score(X_test, y_test)
ci_test_na = 1.96 * np.sqrt((acc_test_na*(1-acc_test_na)) / y_test.shape[0])

test_na_lower = acc_test_na-ci_test_na
test_na_upper = acc_test_na+ci_test_na

print(test_na_lower, test_na_upper)
0.8731774862637585 1.0398659919971112
```

https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L09/code/09-eval2-ci__4-confidence-intervals_iris.ipynb
Later in this lecture we will construct confidence intervals using different Bootstrap Techniques.
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Proportionally large test sets increase the pessimistic bias if a model has not reached its full capacity, yet.

To produce the plot above, I took 500 random samples of each of the ten classes from MNIST.

The sample was then randomly divided into a 3500-example training subset and a test set (1500 examples) via stratification.

Even smaller subsets of the 3500-sample training set were produced via randomized, stratified splits, and I used these subsets to fit softmax classifiers and used the same 1500-sample test set to evaluate their performances; samples may overlap between these training subsets.

```python
from mlxtend.plotting import plot_learning_curves
import matplotlib.pyplot as plt
from mlxtend.data import iris_data
from mlxtend.preprocessing import shuffle_arrays_unison
from sklearn.neighbors import KNeighborsClassifier
import numpy as np

# Loading some example data
X, y = iris_data()
X, y = shuffle_arrays_unison(arrays=[X, y], random_seed=123)
X_train, X_test = X[:100], X[100:]
y_train, y_test = y[:100], y[100:]

clf = KNeighborsClassifier(n_neighbors=5)

plot_learning_curves(X_train, y_train, X_test, y_test, clf)
plt.show()
```

**Learning Curves**

*KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
metric_params=None, n_jobs=1, n_neighbors=5, p=2,
weights='uniform')*

[Image of learning curve graph]
Decreasing the size of the test set brings up another problem: It may result in a substantial variance increase of our model’s performance estimate.

The reason is that it depends on which instances end up in training set, and which particular instances end up in test set. Keeping in mind that each time we resample our data, we alter the statistics of the distribution of the sample.
Repeated Holdout: Estimate Model Stability

(also called Monte Carlo Cross-Validation)

Average performance over $k$ repetitions

$$\text{ACC}_{avg} = \frac{1}{k} \sum_{j=1}^{k} \text{ACC}_j,$$

where $\text{ACC}_j$ is the accuracy estimate of the $j$th test set of size $m$,

$$\text{ACC}_j = 1 - \frac{1}{n} \sum_{i=1}^{n} L(h(x[i]), f(x[i])).$$
Repeated Holdout: Estimate Model Stability

How repeated holdout validation may look like for different training-test split using the Iris dataset to fit to 3-nearest neighbors classifiers:

Left: I performed 50 stratified training/test splits with 75 samples in the test and training set each; a K-nearest neighbors model was fit to the training set and evaluated on the test set in each repetition.

Right: Here, I repeatedly performed 90/10 splits, though, so that the test set consisted of only 15 samples.

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Circa 1900, to pull (oneself) up by (one’s) bootstraps was used figuratively of an impossible task (Among the “practical questions” at the end of chapter one of Steele’s “Popular Physics” schoolbook (1888) is, “30. Why can not a man lift himself by pulling up on his boot-straps?”). By 1916 its meaning expanded to include “better oneself by rigorous, unaided effort.” The meaning “fixed sequence of instructions to load the operating system of a computer” (1953) is from the notion of the first-loaded program pulling itself, and the rest, up by the bootstrap.

(Source: Online Etymology Dictionary)
The Bootstrap Method and Empirical Confidence Intervals

- The bootstrap method is a resampling technique for estimating a sampling distribution.
- Here, we are particularly interested in estimating the uncertainty of our performance estimate.
- The bootstrap method was introduced by Bradley Efron in 1979 [1].
- About 15 years later, Bradley Efron and Robert Tibshirani even devoted a whole book to the bootstrap, “An Introduction to the Bootstrap” [2].
- In brief, the idea of the bootstrap method is to generate new data from a population by repeated sampling from the original dataset with replacement — in contrast, the repeated holdout method can be understood as sampling without replacement.


The Bootstrap Method and Empirical Confidence Intervals

Using the bootstrap, we can estimate sample statistics and compute the standard error of the mean and confidence intervals as if we have drawn a number of samples from an infinite population. In a nutshell, the bootstrap procedure can be described as follows:

1. Draw a sample with replacement
2. Compute the sample statistic
3. Repeat step 1-2 n times
4. Compute the standard deviation (standard error of the mean of the statistic)
5. Compute the confidence interval
The Bootstrap Method and Empirical Confidence Intervals For Evaluating Classifier Performance

1. We are given a dataset of size $n$.

2. For $b$ bootstrap rounds:
   1. We draw one single instance from this dataset and assign it to our $j$th bootstrap sample. We repeat this step until our bootstrap sample has size $n$ (the size of the original dataset). Each time, we draw samples from the same original dataset so that certain samples may appear more than once in our bootstrap sample and some not at all.
   2. We fit a model to each of the $b$ bootstrap samples and compute the resubstitution accuracy.
   3. We compute the model accuracy as the average over the $b$ accuracy estimates

   $\text{ACC}_{\text{boot}} = \frac{1}{b} \sum_{j=1}^{b} \frac{1}{n} \sum_{i=1}^{n} \left( 1 - L(h(x^{[i]}), f(x^{[i]})) \right)$. 
The Bootstrap Method and Empirical Confidence Intervals

• As we discussed previously, the resubstitution accuracy usually leads to an extremely optimistic bias, since a model can be overly sensible to noise in a dataset.

• Originally, the bootstrap method aims to determine the statistical properties of an estimator when the underlying distribution was unknown and additional samples are not available.

• So, in order to exploit this method for the evaluation of predictive models, such as hypotheses for classification and regression, we may prefer a slightly different approach to bootstrapping using the so-called Leave-One-Out Bootstrap (LOOB) technique.

• Here, we use out-of-bag samples as test sets for evaluation instead of evaluating the model on the training data. Out-of-bag samples are the unique sets of instances that are not used for model fitting.
Bootstrap Sampling

Original Dataset

| $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ | $x_7$ | $x_8$ | $x_9$ | $x_{10}$ |

Bootstrap 1

| $x_8$ | $x_6$ | $x_2$ | $x_9$ | $x_5$ | $x_8$ | $x_1$ | $x_4$ | $x_8$ | $x_2$ |

Bootstrap 2

| $x_{10}$ | $x_1$ | $x_3$ | $x_5$ | $x_1$ | $x_7$ | $x_4$ | $x_2$ | $x_1$ | $x_8$ |

Bootstrap 3

| $x_6$ | $x_5$ | $x_4$ | $x_1$ | $x_2$ | $x_4$ | $x_2$ | $x_6$ | $x_9$ | $x_2$ |

Out-of-bag samples

| $x_3$ | $x_7$ | $x_{10}$ |

| $x_6$ | $x_9$ |

| $x_3$ | $x_7$ | $x_8$ | $x_{10}$ |
The Bootstrap Method and Empirical Confidence Intervals

We can compute the 95% confidence interval of the bootstrap estimate as

\[ \text{ACC}_{\text{boot}} = \frac{1}{b} \sum_{i=1}^{b} \text{ACC}_i \]

and use it to compute the standard error

\[ \text{SE}_{\text{boot}} = \sqrt{\frac{1}{b-1} \sum_{i=1}^{b} (\text{ACC}_i - \text{ACC}_{\text{boot}})^2} . \]

Finally, we can then compute the confidence interval around the mean estimate as

\[ \text{ACC}_{\text{boot}} \pm t \times \text{SE}_{\text{boot}} . \]

For instance, given a sample with n=100, we find that \( t_{\alpha=0.05,99} = 1.984 \) (95% CI)

(In practice, at least 200 bootstrap rounds are recommended)
4.1 Iris Simulation

```python
from mlxtend.data import iris_data
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import train_test_split

X, y = iris_data()

X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                      test_size=0.15,
                                                      random_state=12345,
                                                      stratify=y)

clf = KNeighborsClassifier(n_neighbors=3,
                            weights='uniform',
                            algorithm='kd_tree',
                            leaf_size=30,
                            p=2,
                            metric='minkowski',
                            metric_params=None,
                            n_jobs=1)
```

Code: https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L09/code/09-eval2-ci_4-confidence-intervals_iris.ipynb
4.1.1 Out-of-Bag (OOB) Bootstrap; Bootstrapping Training Sets -- Setup Step

- If you don't tune your model on the training set, you actually don’t need a test set for this approach

```python
import numpy as np

rng = np.random.RandomState(seed=12345)
idx = np.arange(y_train.shape[0])

bootstrap_train_accuracies = []

for i in range(200):
    train_idx = rng.choice(idx, size=idx.shape[0], replace=True)
    test_idx = np.setdiff1d(idx, train_idx, assume_unique=False)

    boot_train_X, boot_train_y = X_train[train_idx], y_train[train_idx]
    boot_test_X, boot_test_y = X_train[test_idx], y_train[test_idx]

    clf.fit(boot_train_X, boot_train_y)
    acc = clf.score(boot_test_X, boot_test_y)
    bootstrap_train_accuracies.append(acc)

bootstrap_train_mean = np.mean(bootstrap_train_accuracies)
bootstrap_train_mean

: 0.9552421700709434
```

Code: https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L09/code/09-eval2-ci_4-confidence-intervals_iris.ipynb
### 4.1.2 Bootstrap 1-sample Confidence Interval (Based on OOB Estimates)

```python
se = np.sqrt((1. / (200-1)) * np.sum([(acc - bootstrap_train_mean)**2 for acc in bootstrap_train_accuracies]))

ci = 1.97 * se  # 1.97 based on T distribution

bootstrap_na_lower = bootstrap_train_mean-ci
bootstrap_na_upper = bootstrap_train_mean+ci

print(bootstrap_na_lower, bootstrap_na_upper)
```

```
0.900528306142954 1.0099560339989329
```

The Bootstrap Method and Empirical Confidence Intervals

And if our samples do not follow a normal distribution? A more robust, yet computationally straight-forward approach is the **percentile method** as described by B. Efron (Efron, 1981). Here, we pick our lower and upper confidence bounds as follows:

\[
\text{ACC}_{\text{lower}} = \alpha_1 \text{th} \text{ percentile of the } \text{ACC}_{\text{boot}} \text{ distribution}
\]

\[
\text{ACC}_{\text{upper}} = \alpha_1 \text{th} \text{ percentile of the } \text{ACC}_{\text{boot}} \text{ distribution}
\]

where \( \alpha_1 = \alpha \) and \( \alpha_2 = 1 - \alpha \) and \( \alpha \) is our degree of confidence to compute the \( 100 \times (1 - 2 \times \alpha) \) confidence interval.

For instance, to compute a 95% confidence interval, we pick \( \alpha = 0.025 \) to obtain the 2.5th and 97.5th percentiles of the \( b \) bootstrap samples distribution as our upper and lower confidence bounds.
4.1.3 Bootstrap Percentile Method

```python
bootstrap_percentile_lower = np.percentile(bootstrap_trainaccuracies, 2.5)
bootstrap_percentile_upper = np.percentile(bootstrap_trainaccuracies, 97.5)
print(bootstrap_percentile_lower, bootstrap_percentile_upper)
```

0.8977324263038549 1.0

Code: https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L09/code/09-eval2-ci_4-confidence-intervals_iris.ipynb
4.1.5 Bootstrapping the Test Set predictions

- Avoids retraining the model

```python
clf.fit(X_train, y_train)

predictions_test = clf.predict(X_test)
acc_test = np.mean(predictions_test == y_test)

rng = np.random.RandomState(seed=12345)
idx = np.arange(y_test.shape[0])

test_accuracies = []

for i in range(200):
    pred_idx = rng.choice(idx, size=idx.shape[0], replace=True)
    acc_test_boot = np.mean(predictions_test[pred_idx] == y_test[pred_idx])
    test_accuracies.append(acc_test_boot)

mean_test_accuracies = np.mean(test_accuracies)
bootstrap_lower_test = np.percentile(test_accuracies, 2.5)
bootstrap_upper_test = np.percentile(test_accuracies, 97.5)

print(bootstrap_lower_test, bootstrap_upper_test)
```

0.8695652173913043 1.0

Iris dataset
3-NN classifier

95% confidence intervals

- .632+ Bootstrap, percentile method
- .632 Bootstrap, percentile method
- Bootstrap, percentile method
- Bootstrap, sample CI
- Bootstrapping the test set, percentile method
- Normal approx. sample CI (test set, no bootstrap)

Prediction Accuracy

0.86 0.88 0.90 0.92 0.94 0.96 0.98 1.00

Code: https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L09/code/09-eval2-ci_4-confidence-intervals_iris.ipynb
1. Introduction
2. Holdout method for model evaluation
3. Holdout method for model selection
4. Confidence intervals -- normal approximation
5. Resampling & repeated holdout
6. Empirical confidence intervals via Bootstrap
7. The 0.632 and 0.632+ Bootstrap
Bootstrap Sampling

Original Dataset

\[ x_1 \ x_2 \ x_3 \ x_4 \ x_5 \ x_6 \ x_7 \ x_8 \ x_9 \ x_{10} \]

Bootstrap 1

\[ x_8 \ x_6 \ x_2 \ x_9 \ x_5 \ x_8 \ x_1 \ x_4 \ x_8 \ x_2 \]

Bootstrap 2

\[ x_{10} \ x_1 \ x_3 \ x_5 \ x_1 \ x_7 \ x_4 \ x_2 \ x_1 \ x_8 \]

Bootstrap 3

\[ x_6 \ x_5 \ x_4 \ x_1 \ x_2 \ x_4 \ x_2 \ x_6 \ x_9 \ x_2 \]

Out-of-bag samples

\[ x_3 \ x_7 \ x_{10} \]

\[ x_6 \ x_9 \]

\[ x_3 \ x_7 \ x_8 \ x_{10} \]
OOB Bootstrap
Object Oriented API

In this section, we are going to look at the OOB bootstrap method, which I recently implemented in mlxtend.

```python
from mlxtend.evaluate import BootstrapOutOfBag
import numpy as np

oob = BootstrapOutOfBag(n_splits=3, random_seed=1)
for train, test in oob.split(np.array([1, 2, 3, 4, 5])):
    print(train, test)
```

```
[3 4 0 1 3] [2]
[0 0 1 4 4] [2 3]
[1 2 4 2 4] [0 3]
```

The reason why I chose a object-oriented implementation is that we can plug it into scikit-learn's `cross_val_score` function, which is super convenient.

from mlxtend.data import iris_data
from sklearn.tree import DecisionTreeClassifier
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import train_test_split

X, y = iris_data()

X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.4, random_state=123, stratify=y)

model = DecisionTreeClassifier(random_state=123)

bootstrap_scores = \
    cross_val_score(model, X_train, y_train,
                    cv=BootstrapOutOfBag(n_splits=200, random_seed=123))

print('Mean Bootstrap score', np.mean(bootstrap_scores))
print('Score Std', np.std(bootstrap_scores))

Mean Bootstrap score 0.9483980861793887
Score Std 0.039817322453014004

lower = np.percentile(bootstrap_scores, 2.5)
upper = np.percentile(bootstrap_scores, 97.5)
print('95% Confidence interval: [%2f, %2f]' % (100*lower, 100*upper))

95% Confidence interval: [83.33, 100.00]

**OOB Bootstrap**

**Functional API**

### 4.1.5 OOB Bootstrap with Percentile Method

Same as "4.1.2 Normal Approximation-based Bootstrap Interval (Based on OOB Estimates)" but using mlxtend

```python
from mlxtend.evaluate import bootstrap_point632_score

bootstrap_scores = bootstrap_point632_score(clf,
                                            X_train, y_train,
                                            n_splits=200,
                                            method='oob',
                                            random_seed=12345)

bootstrap_oob_mean = np.mean(bootstrap_scores)
print('Mean Bootstrap score', bootstrap_oob_mean)
print('Score Std', np.std(bootstrap_scores))

bootstrap_oob_percentile_lower = np.percentile(bootstrap_scores, 2.5)
bootstrap_oob_percentile_upper = np.percentile(bootstrap_scores, 97.5)

Mean Bootstrap score 0.9552421700709434
Score Std 0.027704014141397008

print(bootstrap_oob_percentile_lower, bootstrap_oob_percentile_upper)

0.8977324263038549 1.0
```

The 0.632 Bootstrap Method

• In 1983, Bradley Efron described the .632 Estimate, a further improvement to address the pessimistic bias of the bootstrap [1].

• The pessimistic bias in the “classic” bootstrap method can be attributed to the fact that the bootstrap samples only contain approximately 63.2% of the unique samples from the original dataset.

Bootstrap Sampling

\[ P(\text{not chosen}) = \left( 1 - \frac{1}{n} \right)^n, \]
\[ \frac{1}{e} \approx 0.368, \quad n \to \infty. \]
$P(\text{not chosen}) = \left(1 - \frac{1}{n}\right)^n,$

$\frac{1}{e} \approx 0.368, \quad n \to \infty.$

$P(\text{chosen}) = 1 - \left(1 - \frac{1}{n}\right)^n \approx 0.632$
The .632 Bootstrap Method

The .632 Estimate, is computed via the following equation:

\[
\text{ACC}_{\text{boot}} = \frac{1}{b} \sum_{i=1}^{b} \left( 0.632 \cdot \text{ACC}_{h,i} + 0.368 \cdot \text{ACC}_{r,i} \right),
\]

where

- \( \text{ACC}_{r,i} \) is the resubstitution accuracy
- \( \text{ACC}_{h,i} \) is the accuracy on the out-of-bag sample.

4.1.6 .632 Bootstrap

The .632 Bootstrap is the default setting of bootstrap_point632_score; it tends to be overly optimistic.

```python
bootstrap_scores = bootstrap_point632_score(clf, 
    X_train, y_train, 
    n_splits=200, 
    random_seed=12345)

bootstrap_632_mean = np.mean(bootstrap_scores)
print('Mean Bootstrap score', bootstrap_632_mean)
print('Score Std', np.std(bootstrap_scores))

bootstrap_632_percentile_lower = np.percentile(bootstrap_scores, 2.5)
bootstrap_632_percentile_upper = np.percentile(bootstrap_scores, 97.5)

Mean Bootstrap score 0.967105807390348
Score Std 0.016625361563867836

print(bootstrap_632_percentile_lower, bootstrap_632_percentile_upper)
```

0.930974050743657 0.9942047244094488

The .632+ Bootstrap Method

Now, while the .632 Bootstrap attempts to address the pessimistic bias of the estimate, an optimistic bias may occur with models that tend to overfit so that Bradley Efron and Robert Tibshirani proposed the The .632+ Bootstrap Method [1].

Instead of using a fixed “weight” $\omega = 0.632$ in

$$\text{ACC}_{\text{boot}} = \frac{1}{b} \sum_{i=1}^{b} \left( \omega \cdot \text{ACC}_{h,i} + (1 - \omega) \cdot \text{ACC}_{r,i} \right),$$

we compute the weight as

$$\omega = \frac{0.632}{1 - 0.368 \times R},$$

where $R$ is the relative overfitting rate

$$R = \frac{(-1) \times (\text{ACC}_{h,i} - \text{ACC}_{r,i})}{\gamma - (1 - \text{ACC}_{h,i})}.$$ 

The .632+ Bootstrap Method

$R$ is the relative overfitting rate

$$R = \frac{(-1) \times (\text{ACC}_{h,i} - \text{ACC}_{r,i})}{\gamma - (1 - \text{ACC}_{h,i})}.$$ 

Now, we need to determine the no-information rate $\gamma$ in order to compute $R$.

For instance, we can compute $\gamma$ by fitting a model to a dataset that contains all possible combinations between the examples and target class labels:

$$\gamma = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{i'=1}^{n} \left(1 - L(h(x_i), f(x_{i'}))\right).$$

4.1.7 .632+ Bootstrap

The .632+ Bootstrap method attempts to address the optimistic bias of the regular .632 Bootstrap.

```python
bootstrap_scores = bootstrap_point632_score(clf, X_train, y_train,
                                            n_splits=200,
                                            method='\.632+',
                                            random_seed=12345)

bootstrap_632plus_mean = np.mean(bootstrap_scores)
print('Mean Bootstrap score', bootstrap_632plus_mean)
print('Score Std', np.std(bootstrap_scores))

Mean Bootstrap score 0.9663500334312962
Score Std 0.01757293812762708

bootstrap_632plus_percentile_lower = np.percentile(bootstrap_scores, 2.5)
bootstrap_632plus_percentile_upper = np.percentile(bootstrap_scores, 97.5)

print(bootstrap_632plus_percentile_lower, bootstrap_632plus_percentile_upper)

0.9282626011381683 0.9941168892152473
```

Code: https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L09/code/09-eval2-ci_4-confidence-intervals_iris.ipynb
Iris dataset
3-NN classifier

MNIST 5k subset
DT classifier

Code: https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L09/code/09-eval2-ci_4-confidence-intervals_iris.ipynb