Review Model_evaluation_classification

COSC 3337: Data Science I
Instructor: Nouhad Rizk

1 Model Evaluation 2 – Confidence Intervals and Bootstrapping

[2]:
```
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
```

2 Iris Feature by Class Distribution in Random Subsampling

[3]:
```
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from mlxtend.data import iris_data
from mlxtend.preprocessing import shuffle_arrays_unison

X, y = iris_data()

X, y = shuffle_arrays_unison([X, y], random_seed=123)
X_train, X_test = X[:100], X[100:150]
y_train, y_test = y[:100], y[100:150]
```

[4]:
```
np.bincount(y)
```

[4]: array([50, 50, 50])

[5]:
```
np.bincount(y_train)
```

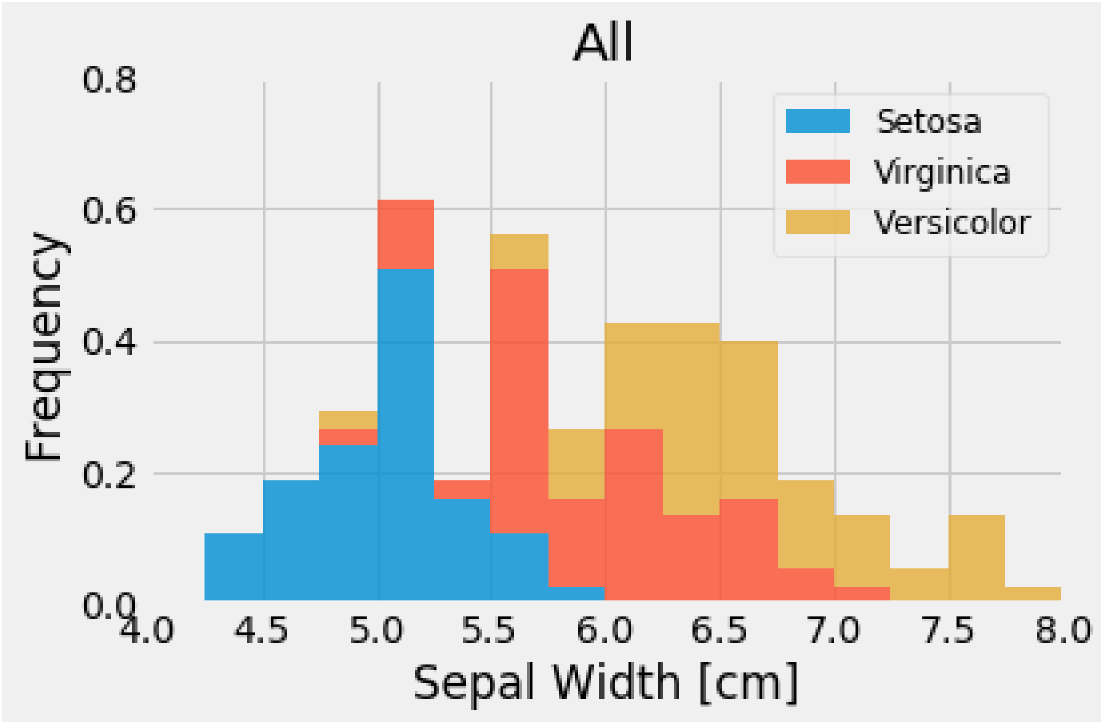
[5]: array([38, 28, 34])

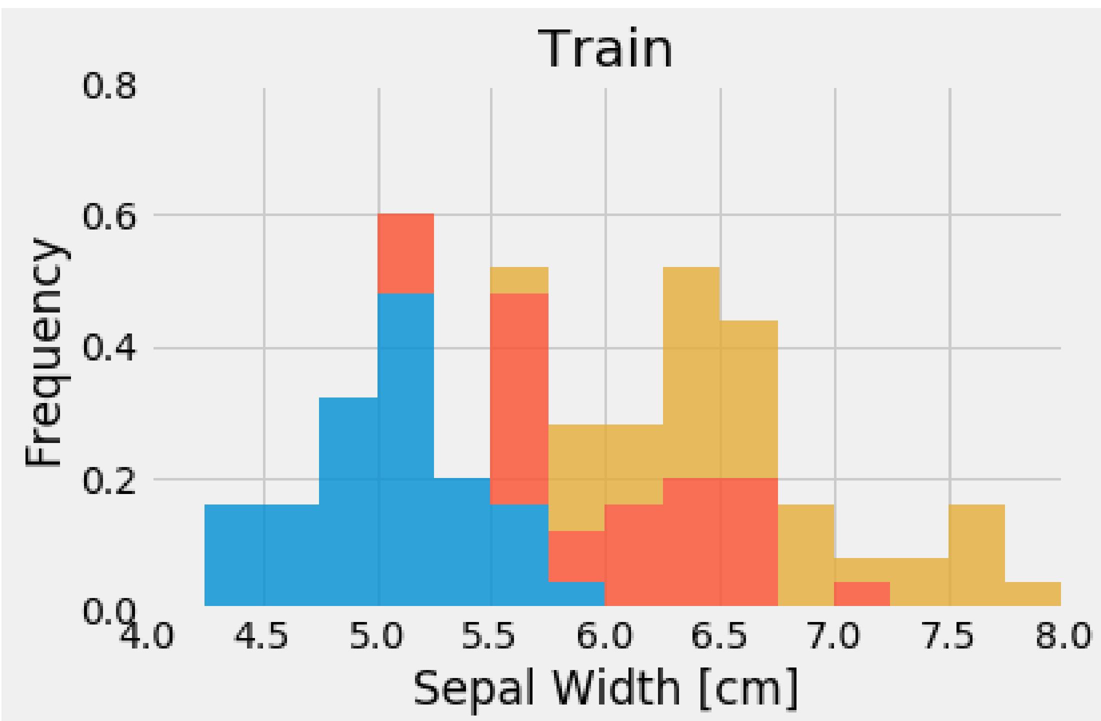
[6]:
```
np.bincount(y_test)
```

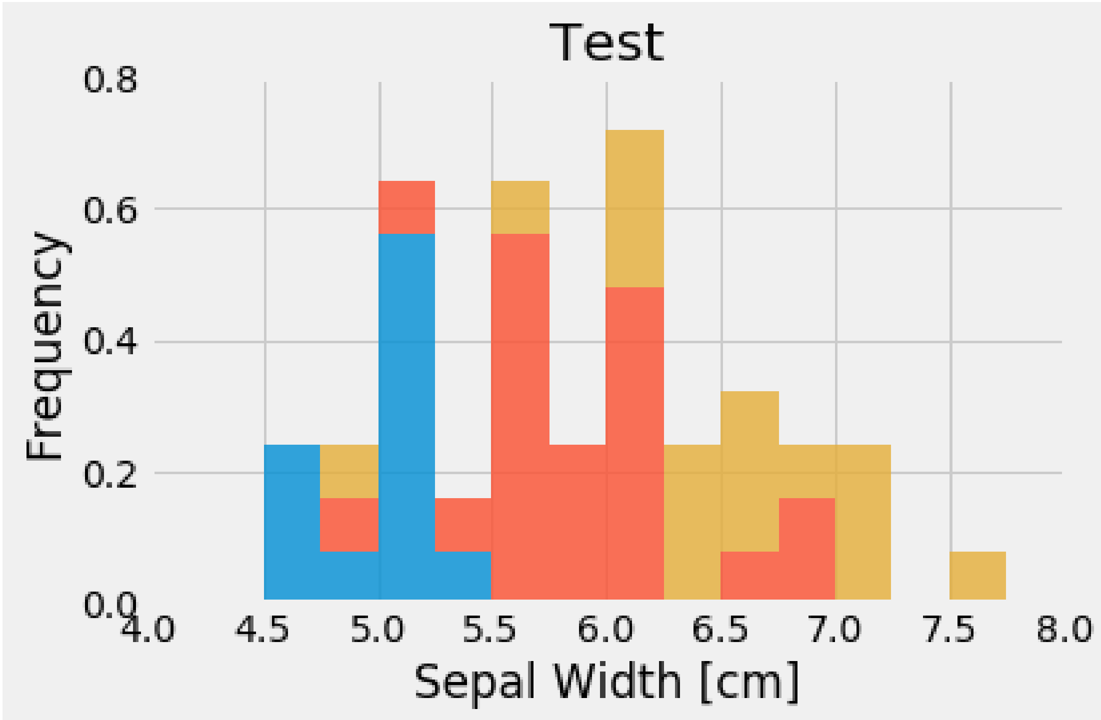
[6]: array([12, 22, 16])

[7]:
```
df = pd.DataFrame(X)
df['class'] = y

df_train = pd.DataFrame(X_train)
df_train['class'] = y_train

df_test = pd.DataFrame(X_test)
df_test['class'] = y_test
```

[8]:
```
def stackhist(x, y, **kws):
    grouped = x.groupby(y)
    data = [d for _, d in grouped]
    labels = [l for l, _ in grouped]
    plt.hist(data,
             histtype="barstacked",
             label=labels,
             alpha=0.8,
             density=True,
             bins=np.arange(4.0, 8.1, 0.25))
    plt.ylim([0, 0.8])
    plt.xlim([4, 8])
    plt.xlabel('Sepal Width [cm]')
    plt.ylabel('Frequency')


with plt.style.context('fivethirtyeight'):

    stackhist(df[0], df['class'])
    plt.legend(['Setosa', 'Virginica', 'Versicolor'], fontsize=12)
    plt.title('All')
    plt.tight_layout()
    #plt.savefig('./all.svg')
    plt.show()

    stackhist(df_train[0], df_train['class'])
    plt.title('Train')
    plt.tight_layout()
    #plt.savefig('./train.svg')
    plt.show()

    stackhist(df_test[0], df_test['class'])
    plt.title('Test')
    plt.tight_layout()
    #plt.savefig('./test.svg')
    plt.show()
```


All
0.8
0.6
0.4
0.2
0.0
Frequency
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
Sepal Width [cm]
Setosa
Virginica
Versicolor


Train
0.8
0.6
0.4
0.2
0.0
Frequency
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
Sepal Width [cm]



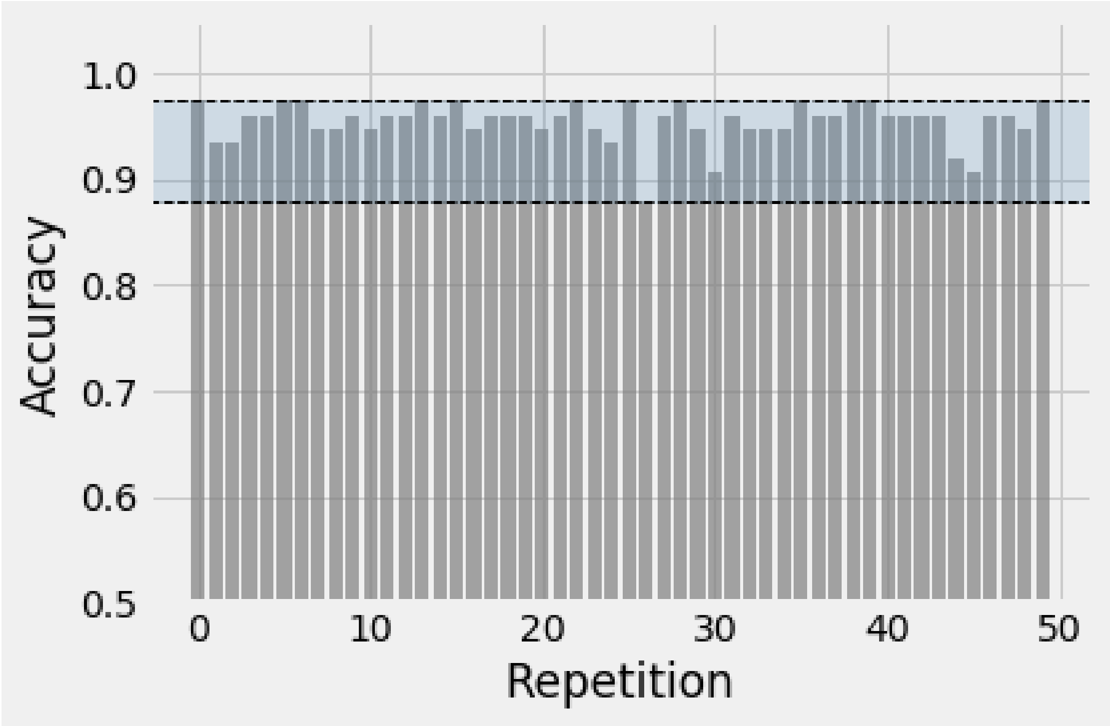
3 Holdout method and repeated sampling

[9]:
```
from mlxtend.data import iris_data
from sklearn.model_selection import train_test_split
from sklearn.neighbors import KNeighborsClassifier

X, y = iris_data()

clf_1 = KNeighborsClassifier(n_neighbors=3,
                             weights='uniform',
                             algorithm='kd_tree',
                             leaf_size=30,
                             p=2,
                             metric='minkowski',
                             metric_params=None,
                             n_jobs=1)
```

[10]:
```
rng = np.random.RandomState(seed=12345)
seeds = np.arange(10**5)
rng.shuffle(seeds)
seeds = seeds[:50]

pred_2 = []
```

```
for i in seeds:
    X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                        test_size=0.5,
                                                        random_state=i,
                                                        stratify=y)
    y_pred_i = clf_1.fit(X_train, y_train).predict(X_test)
    y_pred_i_acc = np.mean(y_test == y_pred_i)
    pred_2.append(y_pred_i_acc)

pred_2 = np.asarray(pred_2)
print('Average: %.2f%%' % (pred_2.mean()*100))

with plt.style.context(('fivethirtyeight')):
    plt.bar(range(0, pred_2.shape[0]), pred_2, color='gray', alpha=0.7)
    plt.axhline(pred_2.max(), color='k', linewidth=1, linestyle='--')
    plt.axhline(pred_2.min(), color='k', linewidth=1, linestyle='--')
    plt.axhspan(pred_2.min(), pred_2.max(), alpha=0.2, color='steelblue')
    plt.ylim([0, pred_2.max() + 0.1])
    plt.xlabel('Repetition')
    plt.ylabel('Accuracy')
    plt.ylim([0.5, 1.05])
    plt.tight_layout()
    #plt.savefig('figures/model-eval-iris_0.svg')
    plt.show()
```

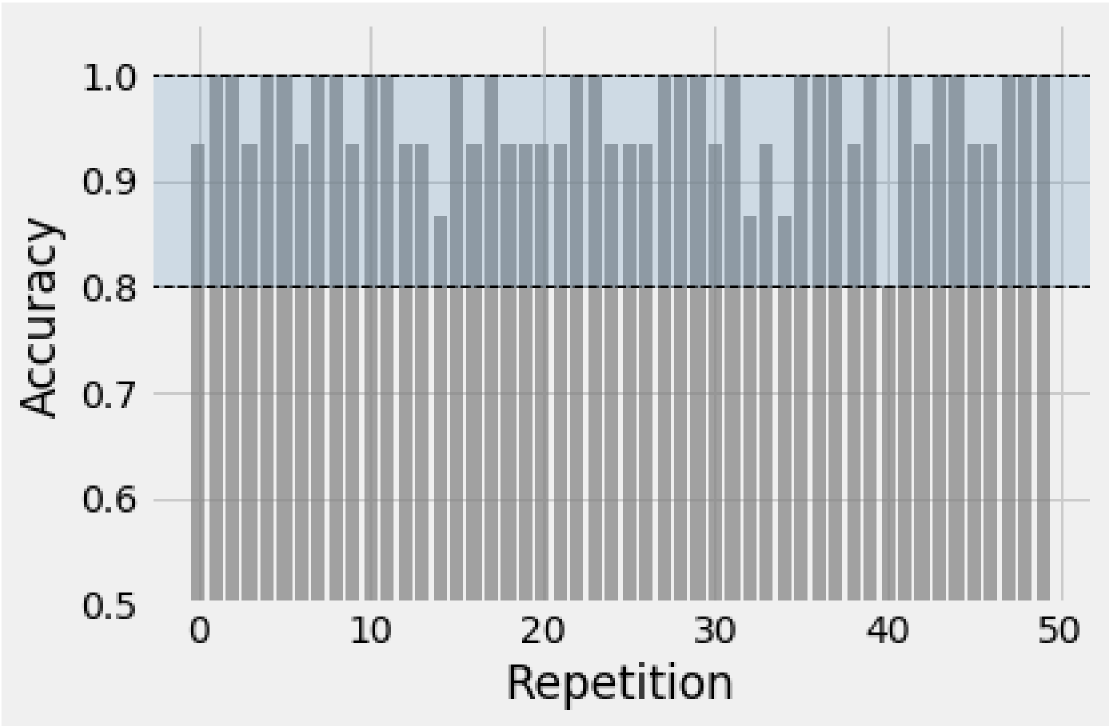
```
Average: 95.41%
```



[11]:
```
rng = np.random.RandomState(seed=12345)
seeds = np.arange(10**5)
rng.shuffle(seeds)
seeds = seeds[:50]

pred_2 = []

for i in seeds:
    X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                        test_size=0.1,
                                                        random_state=i,
                                                        stratify=y)
    y_pred_i = clf_1.fit(X_train, y_train).predict(X_test)
    y_pred_i_acc = np.mean(y_test == y_pred_i)
    pred_2.append(y_pred_i_acc)

pred_2 = np.asarray(pred_2)
print('Average: %.2f%%' % (pred_2.mean()*100))

with plt.style.context(('fivethirtyeight')):
    plt.bar(range(0, pred_2.shape[0]), pred_2, color='gray', alpha=0.7)
    plt.axhline(pred_2.max(), color='k', linewidth=1, linestyle='--')
    plt.axhline(pred_2.min(), color='k', linewidth=1, linestyle='--')
    plt.axhspan(pred_2.min(), pred_2.max(), alpha=0.2, color='steelblue')
```

```
    plt.ylim([0, pred_2.max() + 0.1])
    plt.xlabel('Repetition')
    plt.ylabel('Accuracy')
    plt.ylim(0.5, 1.05)
    plt.tight_layout()
    #plt.savefig('figures/model-eval-iris_0_2.svg')
    plt.show()
```

```
Average: 96.13%
```



3.1 Pessimistic Bias in Holdout

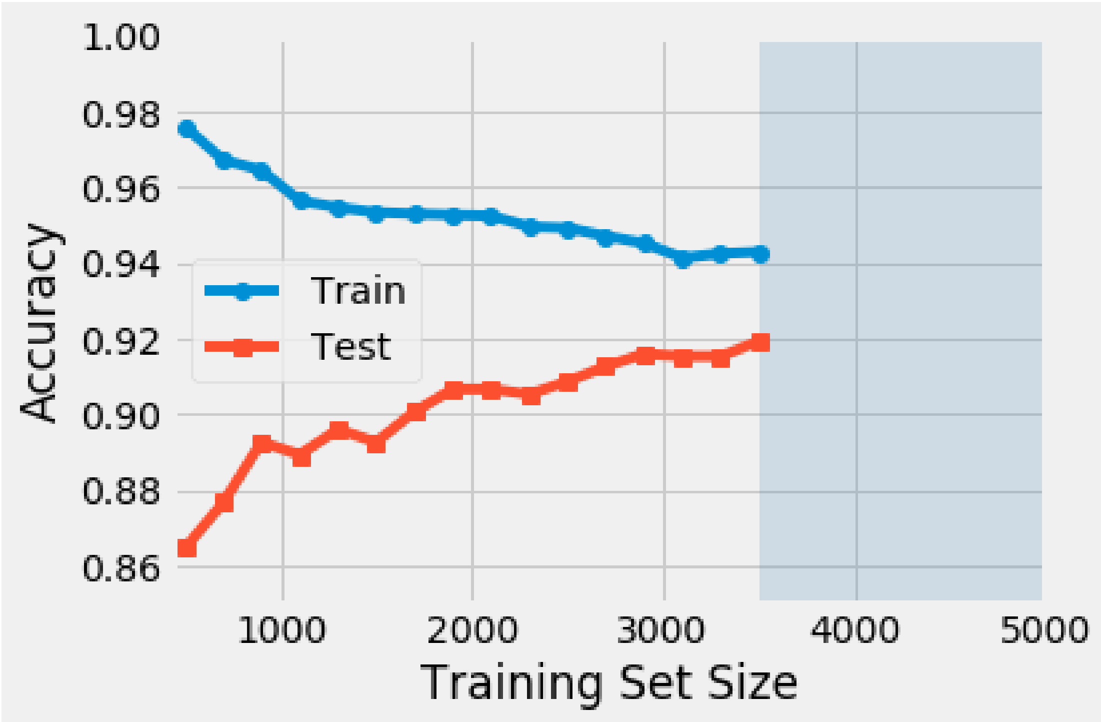
[12]:
```
from mlxtend.data import mnist_data

X2, y2 = mnist_data()
X_train2, X_test2, y_train2, y_test2 = train_test_split(X2, y2,
                                                        test_size=0.3,
                                                        random_state=12,
                                                        stratify=y2)
print('Number of train examples:', y_train2.shape[0])
print('Number of test examples:', y_test2.shape[0])
print('Labels:', y_train2)
```

```
Number of train examples: 3500
```

```
Number of test examples: 1500
Labels: [8 8 7 … 6 9 8]
```

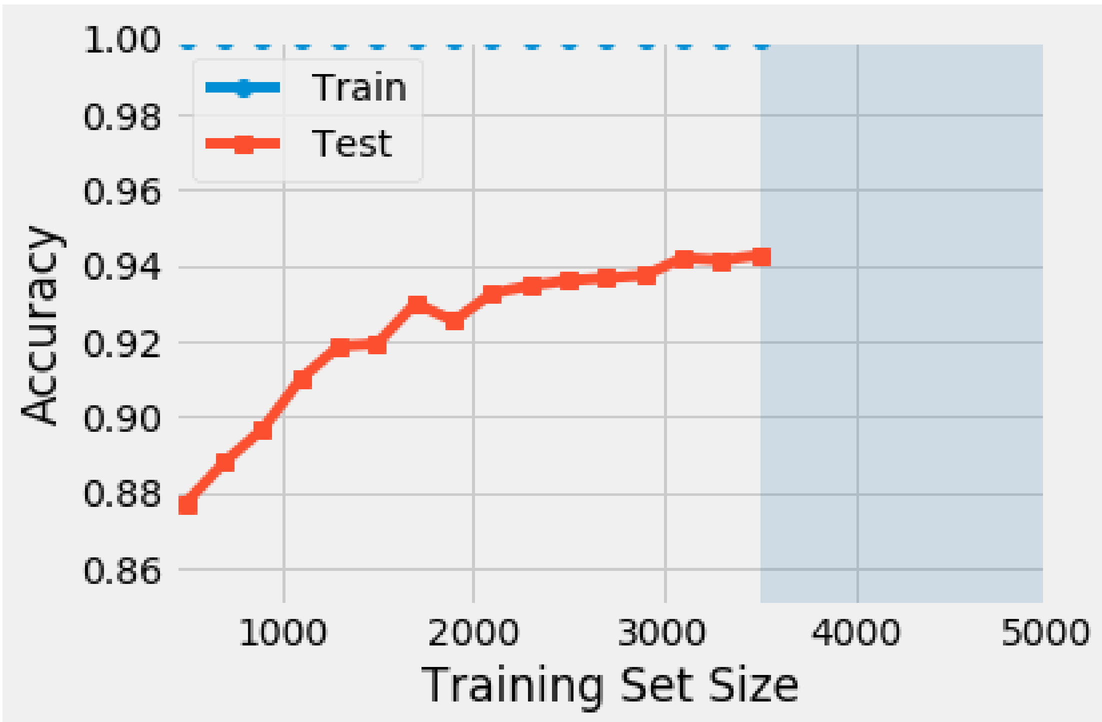
[13]:

```python
from sklearn.linear_model import LogisticRegression

clf_2 = LogisticRegression(penalty='l2',
                           dual=False,
                           tol=0.0001,
                           C=0.000001,
                           fit_intercept=True,
                           intercept_scaling=1,
                           class_weight=None,
                           random_state=12,
                           solver='lbfgs',
                           max_iter=1000,
                           multi_class='multinomial',
                           verbose=0,
                           warm_start=False,
                           n_jobs=1)

pred_train, pred_test = [], []

intervals = np.arange(500, X_train2.shape[0] + 1, 200)

for i in intervals:
    clf_2.fit(X_train2[:i], y_train2[:i])
    p_train = clf_2.score(X_train2[:i], y_train2[:i])
    p_test = clf_2.score(X_test2, y_test2)
    pred_train.append(p_train)
    pred_test.append(p_test)


with plt.style.context(('fivethirtyeight')):
    plt.plot(intervals, pred_train, marker='o', label='Train')
    plt.plot(intervals, pred_test, marker='s', label='Test')
    plt.legend(loc='best', numpoints=1)
    plt.xlim([430, X_train2.shape[0] + X_test2.shape[0]])
    plt.axvspan(X_train2.shape[0],
                X_train2.shape[0] + X_test2.shape[0],
                alpha=0.2,
                color='steelblue')
    plt.ylim([0.85, 1.0])
    plt.xlabel('Training Set Size')
    plt.ylabel('Accuracy')
    plt.tight_layout()
    #plt.savefig('figures/model-eval-mnist_0.svg')
```



[14]:
```
from sklearn.ensemble import RandomForestClassifier


clf_2 = RandomForestClassifier(n_estimators=100, random_state=123)

pred_train, pred_test = [], []

intervals = np.arange(500, X_train2.shape[0] + 1, 200)

for i in intervals:
    clf_2.fit(X_train2[:i], y_train2[:i])
    p_train = clf_2.score(X_train2[:i], y_train2[:i])
    p_test = clf_2.score(X_test2, y_test2)
    pred_train.append(p_train)
    pred_test.append(p_test)


with plt.style.context(('fivethirtyeight')):
    plt.plot(intervals, pred_train, marker='o', label='Train')
    plt.plot(intervals, pred_test, marker='s', label='Test')
    plt.legend(loc='best', numpoints=1)
    plt.xlim([430, X_train2.shape[0] + X_test2.shape[0]])
    plt.axvspan(X_train2.shape[0],
                X_train2.shape[0] + X_test2.shape[0],
```

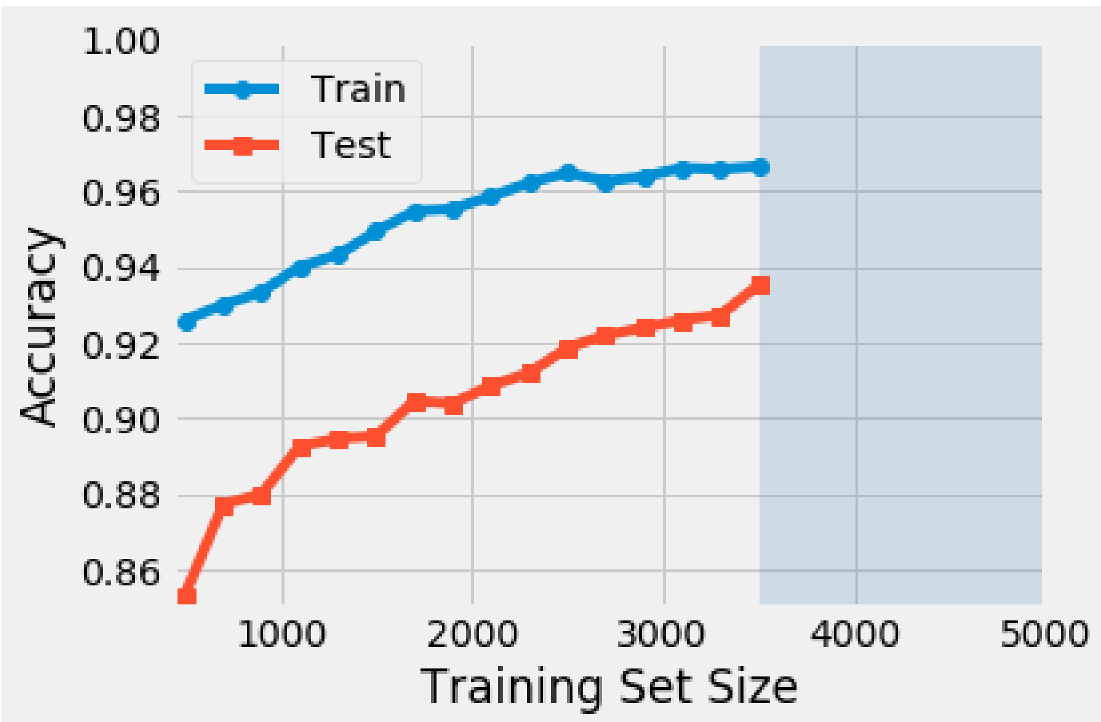
```
                alpha=0.2,
                color='steelblue')
    plt.ylim([0.85, 1.0])
    plt.xlabel('Training Set Size')
    plt.ylabel('Accuracy')
    plt.tight_layout()
    #plt.savefig('figures/model-eval-mnist_0.svg')
```



[15]:

```
from sklearn.neighbors import KNeighborsClassifier


clf_2 = KNeighborsClassifier(n_neighbors=3)

pred_train, pred_test = [], []

intervals = np.arange(500, X_train2.shape[0] + 1, 200)

for i in intervals:
    clf_2.fit(X_train2[:i], y_train2[:i])
    p_train = clf_2.score(X_train2[:i], y_train2[:i])
    p_test = clf_2.score(X_test2, y_test2)
    pred_train.append(p_train)
    pred_test.append(p_test)
```

```
with plt.style.context(('fivethirtyeight')):
    plt.plot(intervals, pred_train, marker='o', label='Train')
    plt.plot(intervals, pred_test, marker='s', label='Test')
    plt.legend(loc='best', numpoints=1)
    plt.xlim([430, X_train2.shape[0] + X_test2.shape[0]])
    plt.axvspan(X_train2.shape[0],
                X_train2.shape[0] + X_test2.shape[0],
                alpha=0.2,
                color='steelblue')
    plt.ylim([0.85, 1.0])
    plt.xlabel('Training Set Size')
    plt.ylabel('Accuracy')
    plt.tight_layout()
    #plt.savefig('figures/model-eval-mnist_0.svg')
```



3.2 Bootstrapping

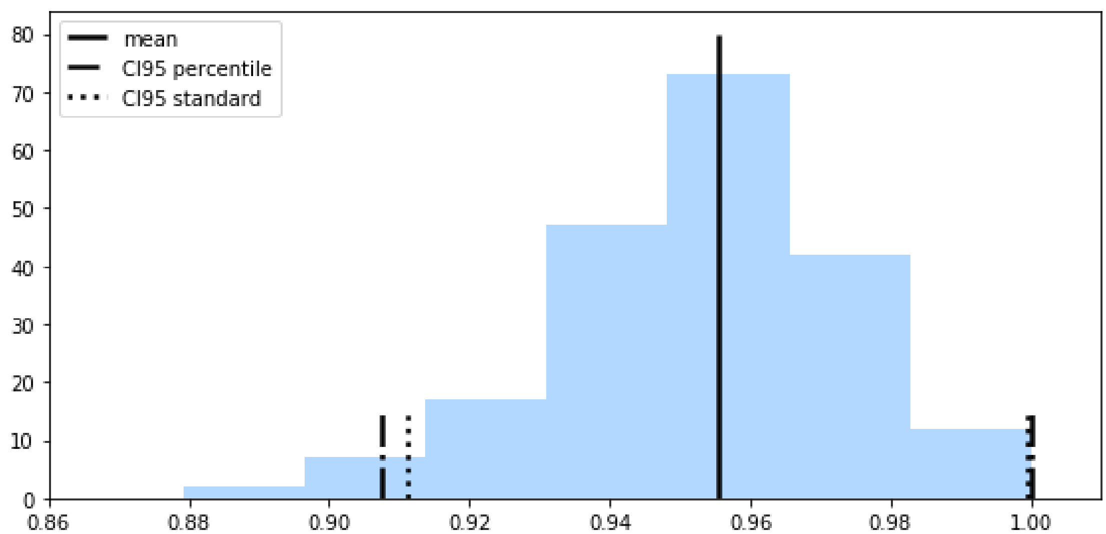
3.2.1 Iris

[16]:
```
from sklearn.neighbors import KNeighborsClassifier

rng = np.random.RandomState(seed=12345)
```

```
X, y = iris_data()

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


idx = np.arange(y.shape[0])

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_idx], y[train_idx]
    boot_test_X, boot_test_y = X[test_idx], y[test_idx]

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

[17]:
```
mean = np.mean(accuracies)

#se = np.sqrt( (1. / (100-1)) * np.sum([(acc - mean)**2 for acc in␣
↪accuracies]))
#ci = 1.984 * se

se = np.sqrt( (1. / (200-1)) * np.sum([(acc - mean)**2 for acc in accuracies]))
ci = 1.97 * se

lower = np.percentile(accuracies, 2.5)
upper = np.percentile(accuracies, 97.5)

fig, ax = plt.subplots(figsize=(8, 4))
ax.vlines(mean, [0], 80, lw=2.5, linestyle='-', label='mean')
#ax.vlines(med, [0], 60, lw=2.5, linestyle='--', label='median')
ax.vlines(lower, [0], 15, lw=2.5, linestyle='-.', label='CI95 percentile')
ax.vlines(upper, [0], 15, lw=2.5, linestyle='-.')

ax.vlines(mean + ci, [0], 15, lw=2.5, linestyle=':', label='CI95 standard')
```

```
ax.vlines(mean - ci, [0], 15, lw=2.5, linestyle=':')


ax.hist(accuracies, bins=7,
        color='#0080ff', edgecolor="none",
        alpha=0.3)
plt.legend(loc='upper left')

plt.xlim([0.86, 1.01])
plt.tight_layout()
#plt.savefig('figures/bootstrap-histo-1.svg')

plt.show()
```



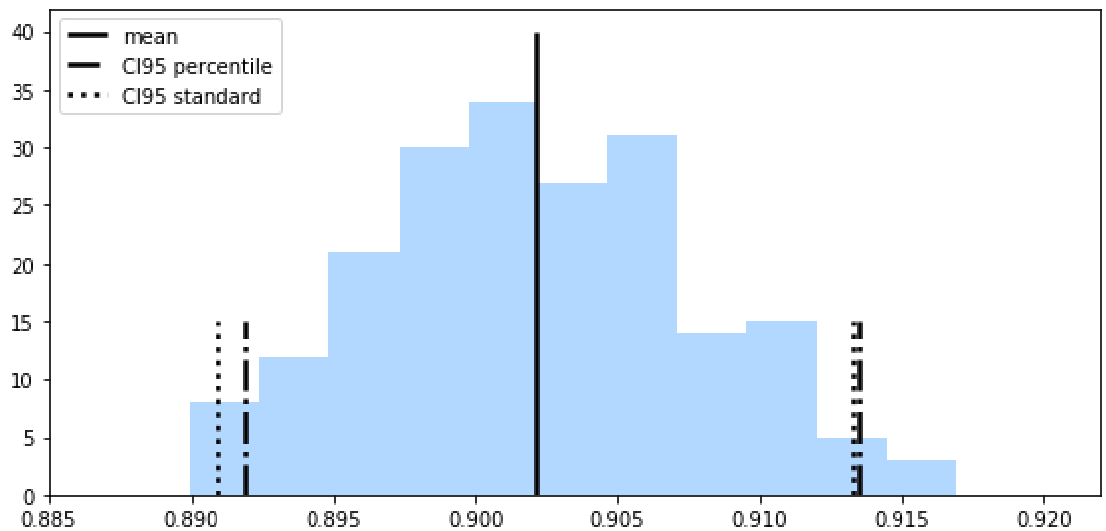
3.2.2 5k MNIST Subset

[18]:
```
from mlxtend.data import mnist_data
from sklearn.linear_model import LogisticRegression


rng = np.random.RandomState(seed=12345)

X, y = mnist_data()

clf = LogisticRegression(penalty='l2',
                         dual=False,
                         tol=0.0001,
                         C=0.000001,
```

```
                        fit_intercept=True,
                        intercept_scaling=1,
                        class_weight=None,
                        random_state=12,
                        solver='lbfgs',
                        max_iter=1000,
                        multi_class='multinomial',
                        verbose=0,
                        warm_start=False,
                        n_jobs=1)


idx = np.arange(y.shape[0])

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_idx], y[train_idx]
    boot_test_X, boot_test_y = X[test_idx], y[test_idx]

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

[19]:
```
mean = np.mean(accuracies)

#se = np.sqrt( (1. / (100-1)) * np.sum([(acc - mean)**2 for acc in␣
↪accuracies]))
#ci = 1.984 * se

se = np.sqrt( (1. / (200-1)) * np.sum([(acc - mean)**2 for acc in accuracies]))
ci = 1.97 * se

lower = np.percentile(accuracies, 2.5)
upper = np.percentile(accuracies, 97.5)

fig, ax = plt.subplots(figsize=(8, 4))
ax.vlines(mean, [0], 40, lw=2.5, linestyle='-', label='mean')
#ax.vlines(med, [0], 60, lw=2.5, linestyle='--', label='median')
ax.vlines(lower, [0], 15, lw=2.5, linestyle='-.', label='CI95 percentile')
ax.vlines(upper, [0], 15, lw=2.5, linestyle='-.')

ax.vlines(mean + ci, [0], 15, lw=2.5, linestyle=':', label='CI95 standard')
```

```
ax.vlines(mean - ci, [0], 15, lw=2.5, linestyle=':')


ax.hist(accuracies, bins=11,
        color='#0080ff', edgecolor="none",
        alpha=0.3)
plt.legend(loc='upper left')

plt.xlim([0.885, 0.922])
plt.tight_layout()

# plt.savefig('figures/bootstrap-histo-2.svg')

plt.show()
```



3.2.3 Out of Bag Bootstrap

[20]:
```
from mlxtend.evaluate import BootstrapOutOfBag
import numpy as np


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

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

[21]:
```python
from mlxtend.data import iris_data
from sklearn.tree import DecisionTreeClassifier
from sklearn.model_selection import cross_val_score

X, y = iris_data()
model = DecisionTreeClassifier()
```

[22]:
```python
cv_scores = cross_val_score(model, X, y, cv=5)
print('CV scores', cv_scores)
print('Mean CV score', np.mean(cv_scores))
print('CV score Std', np.std(cv_scores))
```

```
CV scores [0.96666667 0.96666667 0.9        1.         1.        ]
Mean CV score 0.9666666666666668
CV score Std 0.036514837167011066
```

[23]:
```python
bootstrap_scores = \
    cross_val_score(model, X, y,
                    cv=BootstrapOutOfBag(n_splits=5, random_seed=456))

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

```
Bootstrap scores [0.92727273 0.98113208 0.92592593 0.98305085 0.90909091]
Mean Bootstrap score 0.9452944970437775
Score Std 0.030726208804992074
```

[24]:
```python
bootstrap_scores = \
    cross_val_score(model, X, y,
                    cv=BootstrapOutOfBag(n_splits=200, random_seed=456))

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

```
Mean Bootstrap score 0.9448327329412445
Score Std 0.030836791007487842
```

[25]:
```python
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: [87.27, 100.00]
```

3.2.4 .632 Bootstrap

[26]:
```
from mlxtend.evaluate import bootstrap_point632_score


bootstrap_scores = bootstrap_point632_score(model, X, y, n_splits=200)
print('Mean Bootstrap score', np.mean(bootstrap_scores))
print('Score Std', np.std(bootstrap_scores))
```

```
Mean Bootstrap score 0.9627083103060582
Score Std 0.016892377745312225
```

[27]:
```
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: [92.81, 98.89]
```