Assignments 5

December 1, 2019

1 MScBMI 33200 – Machine Learning for Biomedical Informatics

2 Assignment V

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2.0.1 Directions:

1. Fill out below information (tables and methods)

2. Submit this document along with your code in an HTML/PDF format

2.0.2 Gusto study

Using the training datasets, create the following models:
1. GLM model: This model utilizes all features to predict 30-day mortality in a logistic regression framework.
2. Ridge Regression model: This model utilizes all features to predict 30-day mortality in a logistic regression framework with regularization.
3. ANN model: This model utilizes all features to predict 30-day mortality using an artificial neural network. Feature engineering steps should use normalization/standardization of continuous variables.
4. Random Forest model: This model utilizes all features to predict 30-day mortality using a random forest.
5. GBM model: This model utilizes all features to predict 30-day mortality using a gradient boosted machine.
6. SVM model: This model utilizes all features to predict 30-day mortality using a support vector machine.

3 Gusto

[1]:
```
import pandas as pd
import numpy as np
from random import seed
from sklearn.model_selection import GridSearchCV, StratifiedKFold,␣
↪train_test_split
```

[2]:
```
gusto = pd.read_csv("gusto_data.csv")
gusto['GROUP'] = gusto['GROUP'].replace('west',0)
gusto['GROUP'] = gusto['GROUP'].replace('sample2',1)
gusto['GROUP'] = gusto['GROUP'].replace('sample4',2)
gusto['GROUP'] = gusto['GROUP'].replace('sample5',3)
gusto['GROUP'] = gusto['GROUP'].astype('category').cat.codes
```

[3]:
```
gu_train = gusto.loc[(gusto['GROUP'] == 1
                     ) | (gusto['GROUP'] == 2
                         ) | (gusto['GROUP'] == 3)]
gu_test = gusto[gusto['GROUP']==0]

gu_Xtrain = gu_train.drop("DAY30",axis=1)
gu_ytrain = gu_train[['DAY30']]
gu_Xtest = gu_test.drop("DAY30",axis=1)
gu_ytest = gu_test[['DAY30']]
```

4 GLM Model

[4]:
```
from sklearn.linear_model import LogisticRegression
seed(0)

params6 = {'tol' : [1e-6,1e-5,1e-4,1e-3,1e-2],
           'C': [0.5,1.0,1.5,2.0,2.5]}
lg2 = LogisticRegression(random_state=0, solver='warn',multi_class='warn')
lg2 = GridSearchCV(lg2, cv=5, param_grid=params6, scoring = 'roc_auc',refit =␣
↪True,
                   n_jobs=-1, verbose = 5, return_train_score=True)

lg2.fit(gu_Xtrain, gu_ytrain)
lg2.cv_results_
```

```
Fitting 5 folds for each of 25 candidates, totalling 125 fits
```

```
[Parallel(n_jobs=-1)]: Using backend LokyBackend with 12 concurrent workers.
[Parallel(n_jobs=-1)]: Done  48 tasks      | elapsed:    2.3s
[Parallel(n_jobs=-1)]: Done 102 out of 125 | elapsed:    2.4s remaining:    0.5s
[Parallel(n_jobs=-1)]: Done 125 out of 125 | elapsed:    2.4s finished
```

```
/usr/local/lib/python3.7/site-packages/sklearn/linear_model/logistic.py:432:
FutureWarning: Default solver will be changed to 'lbfgs' in 0.22. Specify a
solver to silence this warning.
  FutureWarning)
/usr/local/lib/python3.7/site-packages/sklearn/utils/validation.py:724:
DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples, ), for example using
ravel().
  y = column_or_1d(y, warn=True)
```

[4]:

```
{'mean_fit_time': array([0.01549258, 0.01680298, 0.0150424 , 0.01326494,
0.01069741,
        0.01661963, 0.01575599, 0.01225686, 0.01076236, 0.00720906,
        0.01093097, 0.00964594, 0.00972013, 0.00796862, 0.00657158,
        0.01530442, 0.01240044, 0.01265583, 0.01129794, 0.00876784,
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 'std_fit_time': array([0.00115231, 0.00119659, 0.00132425, 0.00050567,
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        0.0009199 , 0.0006528 , 0.00173847, 0.00090499, 0.00108703,
        0.00330497, 0.0005184 , 0.00250276, 0.00089983, 0.00115839,
        0.00041526, 0.00091637, 0.00040188, 0.00088579, 0.00106507]),
 'mean_score_time': array([0.00408983, 0.00572977, 0.00534897, 0.00464754,
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        0.00443459, 0.00421901, 0.00333691, 0.00309634, 0.00283136,
        0.0026135 , 0.00253634, 0.00232868, 0.0024735 , 0.00302091,
        0.00366516, 0.00370235, 0.00417194, 0.00349503, 0.00354609,
        0.00336518, 0.00322495, 0.00360041, 0.00309124, 0.00269351]),
 'std_score_time': array([2.71781452e-04, 1.62394445e-03, 9.39529853e-04,
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        5.69342688e-04, 2.35531522e-04, 3.67651233e-04, 5.24449201e-04,
        6.43647860e-05, 2.39373897e-04, 6.55439440e-04, 1.60827313e-04,
        9.63255997e-04, 1.02442156e-03, 1.60160537e-04, 1.50101915e-04,
        3.84713998e-04, 4.38880428e-04, 1.79079774e-04, 6.23171376e-04,
        6.67047475e-04]),
 'param_C': masked_array(data=[0.5, 0.5, 0.5, 0.5, 0.5, 1.0, 1.0, 1.0, 1.0, 1.0,
1.5,
                   1.5, 1.5, 1.5, 1.5, 2.0, 2.0, 2.0, 2.0, 2.0, 2.5, 2.5,
                   2.5, 2.5, 2.5],
             mask=[False, False, False, False, False, False, False, False,
                   False, False, False, False, False, False, False, False,
                   False, False, False, False, False, False, False, False,
                   False],
        fill_value='?',
             dtype=object),
 'param_tol': masked_array(data=[1e-06, 1e-05, 0.0001, 0.001, 0.01, 1e-06,
```

```
1e-05,
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                   1e-06, 1e-05, 0.0001, 0.001, 0.01, 1e-06, 1e-05,
                   0.0001, 0.001, 0.01],
             mask=[False, False, False, False, False, False, False, False,
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                   False],
       fill_value='?',
            dtype=object),
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  {'C': 0.5, 'tol': 0.0001},
  {'C': 0.5, 'tol': 0.001},
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  {'C': 1.0, 'tol': 1e-06},
  {'C': 1.0, 'tol': 1e-05},
  {'C': 1.0, 'tol': 0.0001},
  {'C': 1.0, 'tol': 0.001},
  {'C': 1.0, 'tol': 0.01},
  {'C': 1.5, 'tol': 1e-06},
  {'C': 1.5, 'tol': 1e-05},
  {'C': 1.5, 'tol': 0.0001},
  {'C': 1.5, 'tol': 0.001},
  {'C': 1.5, 'tol': 0.01},
  {'C': 2.0, 'tol': 1e-06},
  {'C': 2.0, 'tol': 1e-05},
  {'C': 2.0, 'tol': 0.0001},
  {'C': 2.0, 'tol': 0.001},
  {'C': 2.0, 'tol': 0.01},
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       0.77572464, 0.77572464, 0.77572464, 0.77192029, 0.77518116,
       0.77463768, 0.77463768, 0.77518116, 0.77264493, 0.77518116,
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```

```
 'split2_test_score': array([0.80076555, 0.80038278, 0.80114833, 0.79425837,
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        0.79885167, 0.79885167, 0.7984689 , 0.79980861, 0.80937799,
        0.79827751, 0.79866029, 0.79866029, 0.79885167, 0.80861244,
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        0.77263158, 0.77263158, 0.77358852, 0.77186603, 0.78717703,
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        0.7932431 , 0.7932431 , 0.79312852, 0.79278427, 0.76559259,
        0.7926427 , 0.79264272, 0.79298111, 0.79212776, 0.76578356,
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 'std_test_score': array([0.02036348, 0.02022411, 0.02018156, 0.01897866,
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        0.02178892, 0.02178892, 0.02176089, 0.02289312, 0.04279299,
        0.02182471, 0.02187083, 0.02151123, 0.02318506, 0.04277193,
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 'split0_train_score': array([0.84454324, 0.84453129, 0.84451934, 0.84407715,
0.82021129,
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        0.84521249, 0.84527224, 0.84520054, 0.84371863, 0.82013959,
        0.8454037 , 0.8454037 , 0.84516468, 0.84345571, 0.82015154,
        0.84579808, 0.84578613, 0.84563077, 0.84551126, 0.82016349]),
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```

```
        0.83461004, 0.83461004, 0.83451576, 0.83458647, 0.82507601,
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        0.83567068, 0.83569425, 0.83575318, 0.83485752, 0.82484031,
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        0.84069107, 0.84070285, 0.84089141, 0.84017253, 0.82950715,
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        0.8228958 , 0.82288401, 0.82288401, 0.82143446, 0.7459283 ,
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 'mean_train_score': array([0.83511748, 0.83509858, 0.83513861, 0.83439485,
0.80640881,
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        0.83641362, 0.8364067 , 0.83634993, 0.83590034, 0.80996534,
        0.83671824, 0.83672531, 0.83675059, 0.83581478, 0.80996536,
        0.8369928 , 0.83699748, 0.83698528, 0.83608678, 0.80998426]),
 'std_train_score': array([0.00734174, 0.00734357, 0.00735001, 0.00762646,
0.03078262,
        0.00749531, 0.0074906 , 0.00744432, 0.0076292 , 0.03218524,
        0.0074864 , 0.00749525, 0.00752915, 0.00733498, 0.0322052 ,
        0.00739245, 0.00739305, 0.0073576 , 0.00729514, 0.03220352,
        0.00750743, 0.00749425, 0.00743481, 0.0076214 , 0.03221531])}
```

[5]:
```
lg2.best_estimator_
```

[5]:
```
LogisticRegression(C=0.5, class_weight=None, dual=False, fit_intercept=True,
                   intercept_scaling=1, l1_ratio=None, max_iter=100,
                   multi_class='warn', n_jobs=None, penalty='l2',
                   random_state=0, solver='warn', tol=0.0001, verbose=0,
                   warm_start=False)
```

[6]:
```
lg_pred2 = lg2.best_estimator_.predict(gu_Xtest)
lg_pred2
```

[6]:
```
array([0, 0, 0, …, 0, 0, 0])
```

[7]:
```
prob6 = lg2.best_estimator_.predict_proba(gu_Xtest)
prob6
```

[7]:
```
array([[0.91372545, 0.08627455],
       [0.96230571, 0.03769429],
```

```
        [0.96092094, 0.03907906],
        …,
        [0.96151863, 0.03848137],
        [0.89257942, 0.10742058],
        [0.97582683, 0.02417317]])
```

[8]:
```python
from sklearn import metrics
lg_matrix2 = metrics.confusion_matrix(gu_ytest, lg_pred2)
lg_matrix2
```

[8]:
```
array([[2038,   15],
       [ 116,   19]])
```

[9]:
```python
from sklearn.metrics import classification_report
target_names2 = ['Still alive at 30 day', 'Died in 30 days']
print("", classification_report(gu_ytest, lg_pred2, target_names=target_names2))
```

```
                        precision    recall  f1-score   support

Still alive at 30 day        0.95      0.99      0.97      2053
      Died in 30 days        0.56      0.14      0.22       135

             accuracy                            0.94      2188
            macro avg        0.75      0.57      0.60      2188
         weighted avg        0.92      0.94      0.92      2188
```

[10]:
```python
from sklearn.metrics import roc_auc_score
lg_probs2 = lg2.best_estimator_.predict_proba(gu_Xtest)[:,1]
print(roc_auc_score(gu_ytest, lg_probs2))
```

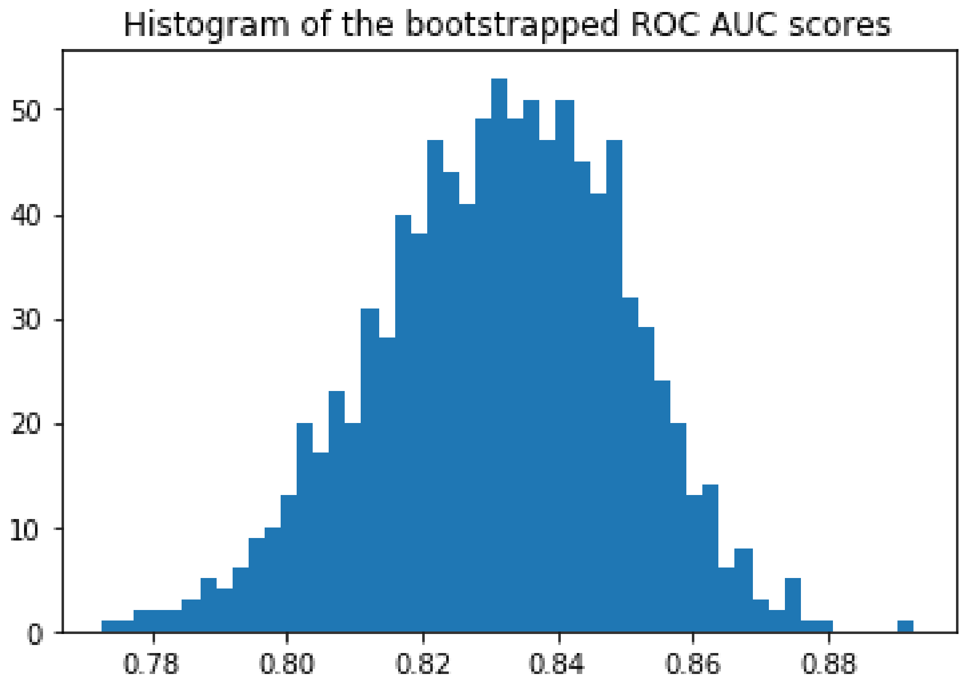
```
0.8302033158341001
```

[11]:
```python
gu_ytest = gu_ytest.values
```

[13]:
```python
#Boostrapping calculated 95% CI
y_pred = lg_probs2
y_true = gu_ytest

print("Original ROC area: {:0.4f}".format(roc_auc_score(y_true, y_pred)))

n_bootstraps = 1000
rng_seed = 42  # control reproducibility
bootstrapped_scores = []

rng = np.random.RandomState(rng_seed)
for i in range(n_bootstraps):
```

```
    # bootstrap by sampling with replacement on the prediction indices
    indices = rng.randint(0, len(y_pred), len(y_pred))
    if len(np.unique(y_true[indices])) < 2:
        # We need at least one positive and one negative sample for ROC AUC
        # to be defined: reject the sample
        continue

    score = roc_auc_score(y_true[indices], y_pred[indices])
    bootstrapped_scores.append(score)
    #print("Bootstrap #{} ROC area: {:0.3f}".format(i + 1, score))

import matplotlib.pyplot as plt
plt.hist(bootstrapped_scores, bins=50)
plt.title('Histogram of the bootstrapped ROC AUC scores')
plt.show()

sorted_scores = np.array(bootstrapped_scores)
sorted_scores.sort()

# Computing the lower and upper bound of the 90% confidence interval
# You can change the bounds percentiles to 0.025 and 0.975 to get
# a 95% confidence interval instead.
confidence_lower = sorted_scores[int(0.05 * len(sorted_scores))]
confidence_upper = sorted_scores[int(0.95 * len(sorted_scores))]
print("Confidence interval for the score: [{:0.4f} - {:0.4}]".format(
    confidence_lower, confidence_upper))
```

```
Original ROC area: 0.8302
```




```
Confidence interval for the score: [0.8000 - 0.8594]
```

[14]:
```
gu_ytest = gu_ytest.reshape((2188,))
```

[15]:
```
#pROC calculated 95% CI without bootstrapping
import numpy as np
import scipy.stats
from scipy import stats

# AUC comparison adapted from
# https://github.com/Netflix/vmaf/
def compute_midrank(x):
    """Computes midranks.
    Args:
       x - a 1D numpy array
    Returns:
       array of midranks
    """
    J = np.argsort(x)
    Z = x[J]
    N = len(x)
    T = np.zeros(N, dtype=np.float)
    i = 0
    while i < N:
        j = i
```

```
        while j < N and Z[j] == Z[i]:
            j += 1
        T[i:j] = 0.5*(i + j - 1)
        i = j
    T2 = np.empty(N, dtype=np.float)
    # Note(kazeevn) +1 is due to Python using 0-based indexing
    # instead of 1-based in the AUC formula in the paper
    T2[J] = T + 1
    return T2


def compute_midrank_weight(x, sample_weight):
    """Computes midranks.
    Args:
       x - a 1D numpy array
    Returns:
       array of midranks
    """
    J = np.argsort(x)
    Z = x[J]
    cumulative_weight = np.cumsum(sample_weight[J])
    N = len(x)
    T = np.zeros(N, dtype=np.float)
    i = 0
    while i < N:
        j = i
        while j < N and Z[j] == Z[i]:
            j += 1
        T[i:j] = cumulative_weight[i:j].mean()
        i = j
    T2 = np.empty(N, dtype=np.float)
    T2[J] = T
    return T2


def fastDeLong(predictions_sorted_transposed, label_1_count, sample_weight):
    if sample_weight is None:
        return fastDeLong_no_weights(predictions_sorted_transposed,␣
 ↪label_1_count)
    else:
        return fastDeLong_weights(predictions_sorted_transposed, label_1_count,␣
 ↪sample_weight)


def fastDeLong_weights(predictions_sorted_transposed, label_1_count,␣
 ↪sample_weight):
    """
```

```
    The fast version of DeLong's method for computing the covariance of
    unadjusted AUC.
    Args:
       predictions_sorted_transposed: a 2D numpy.array[n_classifiers,␣
↪n_examples]
          sorted such as the examples with label "1" are first
    Returns:
       (AUC value, DeLong covariance)
    Reference:
     @article{sun2014fast,
       title={Fast Implementation of DeLong's Algorithm for
              Comparing the Areas Under Correlated Receiver Oerating␣
↪Characteristic Curves},
       author={Xu Sun and Weichao Xu},
       journal={IEEE Signal Processing Letters},
       volume={21},
       number={11},
       pages={1389--1393},
       year={2014},
       publisher={IEEE}
     }
    """
    # Short variables are named as they are in the paper
    m = label_1_count
    n = predictions_sorted_transposed.shape[1] - m
    positive_examples = predictions_sorted_transposed[:, :m]
    negative_examples = predictions_sorted_transposed[:, m:]
    k = predictions_sorted_transposed.shape[0]

    tx = np.empty([k, m], dtype=np.float)
    ty = np.empty([k, n], dtype=np.float)
    tz = np.empty([k, m + n], dtype=np.float)
    for r in range(k):
        tx[r, :] = compute_midrank_weight(positive_examples[r, :],␣
↪sample_weight[:m])
        ty[r, :] = compute_midrank_weight(negative_examples[r, :],␣
↪sample_weight[m:])
        tz[r, :] = compute_midrank_weight(predictions_sorted_transposed[r, :],␣
↪sample_weight)
    total_positive_weights = sample_weight[:m].sum()
    total_negative_weights = sample_weight[m:].sum()
    pair_weights = np.dot(sample_weight[:m, np.newaxis], sample_weight[np.
↪newaxis, m:])
    total_pair_weights = pair_weights.sum()
    aucs = (sample_weight[:m]*(tz[:, :m] - tx)).sum(axis=1) / total_pair_weights
    v01 = (tz[:, :m] - tx[:, :]) / total_negative_weights
```

```python
    v10 = 1. - (tz[:, m:] - ty[:, :]) / total_positive_weights
    sx = np.cov(v01)
    sy = np.cov(v10)
    delongcov = sx / m + sy / n
    return aucs, delongcov


def fastDeLong_no_weights(predictions_sorted_transposed, label_1_count):
    """
    The fast version of DeLong's method for computing the covariance of
    unadjusted AUC.
    Args:
       predictions_sorted_transposed: a 2D numpy.array[n_classifiers,␣
 ↪n_examples]
          sorted such as the examples with label "1" are first
    Returns:
       (AUC value, DeLong covariance)
    Reference:
     @article{sun2014fast,
       title={Fast Implementation of DeLong's Algorithm for
              Comparing the Areas Under Correlated Receiver Oerating
              Characteristic Curves},
       author={Xu Sun and Weichao Xu},
       journal={IEEE Signal Processing Letters},
       volume={21},
       number={11},
       pages={1389--1393},
       year={2014},
       publisher={IEEE}
     }
    """
    # Short variables are named as they are in the paper
    m = label_1_count
    n = predictions_sorted_transposed.shape[1] - m
    positive_examples = predictions_sorted_transposed[:, :m]
    negative_examples = predictions_sorted_transposed[:, m:]
    k = predictions_sorted_transposed.shape[0]

    tx = np.empty([k, m], dtype=np.float)
    ty = np.empty([k, n], dtype=np.float)
    tz = np.empty([k, m + n], dtype=np.float)
    for r in range(k):
        tx[r, :] = compute_midrank(positive_examples[r, :])
        ty[r, :] = compute_midrank(negative_examples[r, :])
        tz[r, :] = compute_midrank(predictions_sorted_transposed[r, :])
    aucs = tz[:, :m].sum(axis=1) / m / n - float(m + 1.0) / 2.0 / n
    v01 = (tz[:, :m] - tx[:, :]) / n
```

```
    v10 = 1.0 - (tz[:, m:] - ty[:, :]) / m
    sx = np.cov(v01)
    sy = np.cov(v10)
    delongcov = sx / m + sy / n
    return aucs, delongcov


def calc_pvalue(aucs, sigma):
    """Computes log(10) of p-values.
    Args:
       aucs: 1D array of AUCs
       sigma: AUC DeLong covariances
    Returns:
       log10(pvalue)
    """
    l = np.array([[1, -1]])
    z = np.abs(np.diff(aucs)) / np.sqrt(np.dot(np.dot(l, sigma), l.T))
    return np.log10(2) + scipy.stats.norm.logsf(z, loc=0, scale=1) / np.log(10)


def compute_ground_truth_statistics(ground_truth, sample_weight):
    assert np.array_equal(np.unique(ground_truth), [0, 1])
    order = (-ground_truth).argsort()
    label_1_count = int(ground_truth.sum())
    if sample_weight is None:
        ordered_sample_weight = None
    else:
        ordered_sample_weight = sample_weight[order]

    return order, label_1_count, ordered_sample_weight


def delong_roc_variance(ground_truth, predictions, sample_weight=None):
    """
    Computes ROC AUC variance for a single set of predictions
    Args:
       ground_truth: np.array of 0 and 1
       predictions: np.array of floats of the probability of being class 1
    """
    order, label_1_count, ordered_sample_weight =␣
↪compute_ground_truth_statistics(
        ground_truth, sample_weight)
    predictions_sorted_transposed = predictions[np.newaxis, order]
    aucs, delongcov = fastDeLong(predictions_sorted_transposed, label_1_count,␣
↪ordered_sample_weight)
    assert len(aucs) == 1, "There is a bug in the code, please forward this to␣
↪the developers"
```

```
    return aucs[0], delongcov


alpha = .95
y_pred = lg_probs2
y_true = gu_ytest

auc, auc_cov = delong_roc_variance(
    y_true,
    y_pred)

auc_std = np.sqrt(auc_cov)
lower_upper_q = np.abs(np.array([0, 1]) - (1 - alpha) / 2)

ci = stats.norm.ppf(
    lower_upper_q,
    loc=auc,
    scale=auc_std)

ci[ci > 1] = 1

print('AUC:', auc)
print('AUC COV:', auc_cov)
print('95% AUC CI:', ci)
```

```
AUC: 0.8302033158341
AUC COV: 0.00034444118566511161
95% AUC CI: [0.7938281  0.86657854]
```

[ ]:

```
```

5 Ridge Regression Model

[16]:

```
from sklearn.linear_model import RidgeCV
ridgecv = RidgeCV(alphas=[1e-3, 1e-2, 1e-1, 1, 10], cv=5, fit_intercept=True,␣
↪scoring=None, normalize=False)
ridgecv=ridgecv.fit(gu_Xtrain,gu_ytrain)
gu_ridgecv = ridgecv.predict(gu_Xtest)
roc_auc_score(gu_ytest, gu_ridgecv)
```

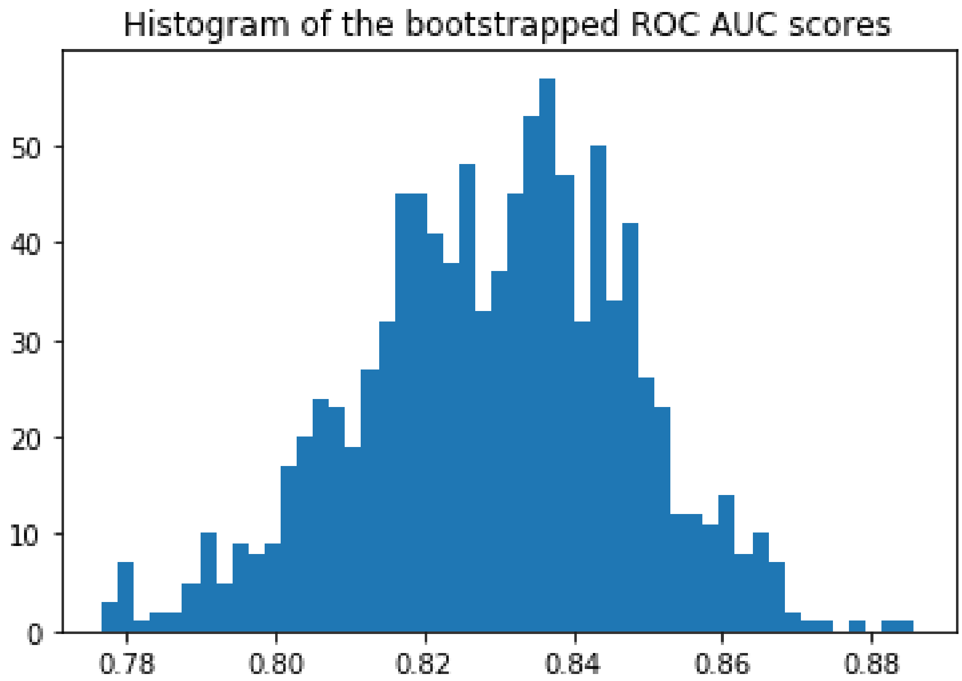
[16]: 0.8279590842669263

[17]:

```
#Boostrapping calculated 95% CI
y_pred = gu_ridgecv
y_true = gu_ytest
```

```python
print("Original ROC area: {:0.4f}".format(roc_auc_score(y_true, y_pred)))

n_bootstraps = 1000
rng_seed = 42  # control reproducibility
bootstrapped_scores = []

rng = np.random.RandomState(rng_seed)
for i in range(n_bootstraps):
    # bootstrap by sampling with replacement on the prediction indices
    indices = rng.randint(0, len(y_pred), len(y_pred))
    if len(np.unique(y_true[indices])) < 2:
        # We need at least one positive and one negative sample for ROC AUC
        # to be defined: reject the sample
        continue

    score = roc_auc_score(y_true[indices], y_pred[indices])
    bootstrapped_scores.append(score)
    #print("Bootstrap #{} ROC area: {:0.3f}".format(i + 1, score))

import matplotlib.pyplot as plt
plt.hist(bootstrapped_scores, bins=50)
plt.title('Histogram of the bootstrapped ROC AUC scores')
plt.show()

sorted_scores = np.array(bootstrapped_scores)
sorted_scores.sort()

# Computing the lower and upper bound of the 90% confidence interval
# You can change the bounds percentiles to 0.025 and 0.975 to get
# a 95% confidence interval instead.
confidence_lower = sorted_scores[int(0.05 * len(sorted_scores))]
confidence_upper = sorted_scores[int(0.95 * len(sorted_scores))]
print("Confidence interval for the score: [{:0.4f} - {:0.4}]".format(
    confidence_lower, confidence_upper))
```

```
Original ROC area: 0.8280
```




```
Confidence interval for the score: [0.7982 - 0.8586]
```

[18]:
```
#pROC calculated 95% CI without bootstrapping
alpha = .95
gu_ridgecv = gu_ridgecv.reshape((2188,))
y_pred = gu_ridgecv
y_true = gu_ytest

auc, auc_cov = delong_roc_variance(
    y_true,
    y_pred)

auc_std = np.sqrt(auc_cov)
lower_upper_q = np.abs(np.array([0, 1]) - (1 - alpha) / 2)

ci = stats.norm.ppf(
    lower_upper_q,
    loc=auc,
    scale=auc_std)

ci[ci > 1] = 1

print('AUC:', auc)
print('AUC COV:', auc_cov)
print('95% AUC CI:', ci)
```

```
AUC: 0.8279590842669264
AUC COV: 0.0003523557006508896
95% AUC CI: [0.79116833 0.86474984]
```

[ ]:

6 Artificial Neural Network

[19]:
```python
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
# Fit only to the training data
scaler = scaler.fit(gu_Xtrain)
gu_Xtrains = scaler.transform(gu_Xtrain)
gu_Xtests = scaler.transform(gu_Xtest)
```

[20]:
```python
from sklearn.neural_network import MLPClassifier
seed(1)
# skf = StratifiedKFold(n_splits=5)
params7 = {'alpha' : [0.0001,0.01],
           'power_t': [0.5,0.75],
           'max_iter': [200,250]}
mlp2 = MLPClassifier(solver='lbfgs', random_state=1)
mlp2 = GridSearchCV(mlp2, cv=5, param_grid=params7, scoring = 'roc_auc',refit =␣
↪True,
                    n_jobs=-1, verbose = 5, return_train_score=True)

mlp2.fit(gu_Xtrains, gu_ytrain)
mlp2.cv_results_
```

```
Fitting 5 folds for each of 8 candidates, totalling 40 fits

[Parallel(n_jobs=-1)]: Using backend LokyBackend with 12 concurrent workers.
[Parallel(n_jobs=-1)]: Done  26 out of  40 | elapsed:    3.0s remaining:    1.6s
[Parallel(n_jobs=-1)]: Done  35 out of  40 | elapsed:    3.2s remaining:    0.5s
[Parallel(n_jobs=-1)]: Done  40 out of  40 | elapsed:    3.3s finished
/usr/local/lib/python3.7/site-
packages/sklearn/neural_network/multilayer_perceptron.py:921:
DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples, ), for example using
ravel().
  y = column_or_1d(y, warn=True)
```

[20]:
```
{'mean_fit_time': array([0.27808437, 0.30123062, 0.30036077, 0.32006493,
0.43673463,
        0.40928383, 0.35798874, 0.26584067]),
 'std_fit_time': array([0.03082211, 0.02415256, 0.02532153, 0.02310814,
```

```
0.04237356,
        0.02055945, 0.01295359, 0.02486431]),
 'mean_score_time': array([0.00549297, 0.00573235, 0.00630546, 0.00546994,
0.00648966,
        0.00515413, 0.00361214, 0.00244021]),
 'std_score_time': array([0.00012062, 0.00074194, 0.0011323 , 0.00083989,
0.00120899,
        0.00105471, 0.00112323, 0.0004813 ]),
 'param_alpha': masked_array(data=[0.0001, 0.0001, 0.0001, 0.0001, 0.01, 0.01,
0.01, 0.01],
              mask=[False, False, False, False, False, False, False, False],
        fill_value='?',
             dtype=object),
 'param_max_iter': masked_array(data=[200, 200, 250, 250, 200, 200, 250, 250],
              mask=[False, False, False, False, False, False, False, False],
        fill_value='?',
             dtype=object),
 'param_power_t': masked_array(data=[0.5, 0.75, 0.5, 0.75, 0.5, 0.75, 0.5,
0.75],
              mask=[False, False, False, False, False, False, False, False],
        fill_value='?',
             dtype=object),
 'params': [{'alpha': 0.0001, 'max_iter': 200, 'power_t': 0.5},
  {'alpha': 0.0001, 'max_iter': 200, 'power_t': 0.75},
  {'alpha': 0.0001, 'max_iter': 250, 'power_t': 0.5},
  {'alpha': 0.0001, 'max_iter': 250, 'power_t': 0.75},
  {'alpha': 0.01, 'max_iter': 200, 'power_t': 0.5},
  {'alpha': 0.01, 'max_iter': 200, 'power_t': 0.75},
  {'alpha': 0.01, 'max_iter': 250, 'power_t': 0.5},
  {'alpha': 0.01, 'max_iter': 250, 'power_t': 0.75}],
 'split0_test_score': array([0.75896739, 0.75896739, 0.75896739, 0.75896739,
0.75126812,
        0.75126812, 0.75126812, 0.75126812]),
 'split1_test_score': array([0.5891495 , 0.5891495 , 0.5891495 , 0.5891495 ,
0.57360793,
        0.57360793, 0.57360793, 0.57360793]),
 'split2_test_score': array([0.74717703, 0.74717703, 0.74717703, 0.74717703,
0.73741627,
        0.73741627, 0.73741627, 0.73741627]),
 'split3_test_score': array([0.6415311 , 0.6415311 , 0.6415311 , 0.6415311 ,
0.66660287,
        0.66660287, 0.66660287, 0.66660287]),
 'split4_test_score': array([0.74220096, 0.74220096, 0.74220096, 0.74220096,
0.74411483,
        0.74411483, 0.74411483, 0.74411483]),
 'mean_test_score': array([0.69581855, 0.69581855, 0.69581855, 0.69581855,
0.6945968 ,
```

```
        0.6945968 , 0.6945968 , 0.6945968 ]),
 'std_test_score': array([0.06800126, 0.06800126, 0.06800126, 0.06800126,
0.06774062,
        0.06774062, 0.06774062, 0.06774062]),
 'rank_test_score': array([1, 1, 1, 1, 5, 5, 5, 5], dtype=int32),
 'split0_train_score': array([1., 1., 1., 1., 1., 1., 1., 1.]),
 'split1_train_score': array([1., 1., 1., 1., 1., 1., 1., 1.]),
 'split2_train_score': array([1., 1., 1., 1., 1., 1., 1., 1.]),
 'split3_train_score': array([1., 1., 1., 1., 1., 1., 1., 1.]),
 'split4_train_score': array([1., 1., 1., 1., 1., 1., 1., 1.]),
 'mean_train_score': array([1., 1., 1., 1., 1., 1., 1., 1.]),
 'std_train_score': array([0., 0., 0., 0., 0., 0., 0., 0.])}
```

[21]:
```
mlp2.best_estimator_
```

[21]:
```
MLPClassifier(activation='relu', alpha=0.0001, batch_size='auto', beta_1=0.9,
              beta_2=0.999, early_stopping=False, epsilon=1e-08,
              hidden_layer_sizes=(100,), learning_rate='constant',
              learning_rate_init=0.001, max_iter=200, momentum=0.9,
              n_iter_no_change=10, nesterovs_momentum=True, power_t=0.5,
              random_state=1, shuffle=True, solver='lbfgs', tol=0.0001,
              validation_fraction=0.1, verbose=False, warm_start=False)
```

[22]:
```
ann_pred2 = mlp2.best_estimator_.predict(gu_Xtests)
ann_pred2
```

[22]:
```
array([0, 0, 0, …, 0, 0, 0])
```

[23]:
```
prob7 = mlp2.best_estimator_.predict_proba(gu_Xtests)
prob7
```

[23]:
```
array([[1.00000000e+00, 4.92987998e-92],
       [1.00000000e+00, 3.30660487e-78],
       [1.00000000e+00, 5.34809233e-83],
       …,
       [1.00000000e+00, 1.21594736e-30],
       [1.00000000e+00, 8.23828743e-48],
       [1.00000000e+00, 8.12154336e-39]])
```

[24]:
```
ann_matrix2 = metrics.confusion_matrix(gu_ytest, ann_pred2)
ann_matrix2
```

[24]:
```
array([[1947,  106],
       [  93,   42]])
```

[25]:
```
target_names2 = ['Still alive at 30 day', 'Died in 30 days']
print("", classification_report(gu_ytest, ann_pred2,
```

```
                                 target_names=target_names2))
```

```
                        precision    recall  f1-score   support

Still alive at 30 day       0.95      0.95      0.95      2053
      Died in 30 days       0.28      0.31      0.30       135

             accuracy                           0.91      2188
            macro avg       0.62      0.63      0.62      2188
         weighted avg       0.91      0.91      0.91      2188
```

[26]:
```
ann_probs2 = mlp2.best_estimator_.predict_proba(gu_Xtests)[:,1]
print(roc_auc_score(gu_ytest, ann_probs2))
```

```
0.759576771120853
```

[27]:
```
#Boostrapping calculated 95% CI
y_pred = ann_probs2
y_true = gu_ytest

print("Original ROC area: {:0.4f}".format(roc_auc_score(y_true, y_pred)))

n_bootstraps = 1000
rng_seed = 42  # control reproducibility
bootstrapped_scores = []

rng = np.random.RandomState(rng_seed)
for i in range(n_bootstraps):
    # bootstrap by sampling with replacement on the prediction indices
    indices = rng.randint(0, len(y_pred), len(y_pred))
    if len(np.unique(y_true[indices])) < 2:
        # We need at least one positive and one negative sample for ROC AUC
        # to be defined: reject the sample
        continue

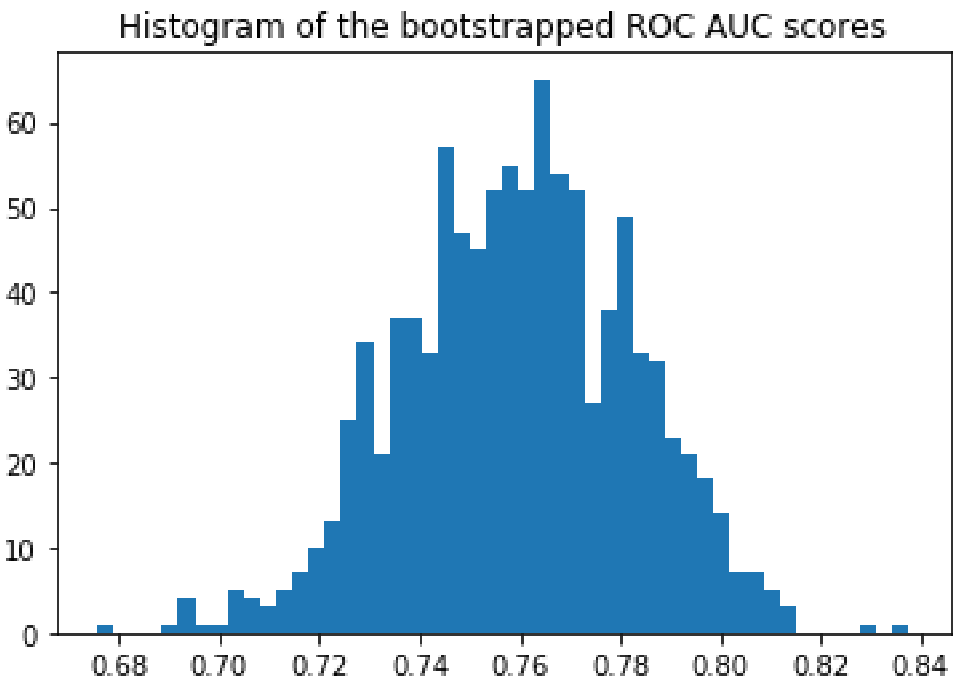
    score = roc_auc_score(y_true[indices], y_pred[indices])
    bootstrapped_scores.append(score)
    #print("Bootstrap #{} ROC area: {:0.3f}".format(i + 1, score))

import matplotlib.pyplot as plt
plt.hist(bootstrapped_scores, bins=50)
plt.title('Histogram of the bootstrapped ROC AUC scores')
plt.show()

sorted_scores = np.array(bootstrapped_scores)
sorted_scores.sort()
```

```
# Computing the lower and upper bound of the 90% confidence interval
# You can change the bounds percentiles to 0.025 and 0.975 to get
# a 95% confidence interval instead.
confidence_lower = sorted_scores[int(0.05 * len(sorted_scores))]
confidence_upper = sorted_scores[int(0.95 * len(sorted_scores))]
print("Confidence interval for the score: [{:0.4f} - {:0.4}]".format(
    confidence_lower, confidence_upper))
```

```
Original ROC area: 0.7596
```




```
Confidence interval for the score: [0.7232 - 0.7963]
```

[28]:
```
#pROC calculated 95% CI without bootstrapping
alpha = .95
y_pred = ann_probs2
y_true = gu_ytest

auc, auc_cov = delong_roc_variance(
    y_true,
    y_pred)

auc_std = np.sqrt(auc_cov)
lower_upper_q = np.abs(np.array([0, 1]) - (1 - alpha) / 2)
```

```
ci = stats.norm.ppf(
    lower_upper_q,
    loc=auc,
    scale=auc_std)

ci[ci > 1] = 1

print('AUC:', auc)
print('AUC COV:', auc_cov)
print('95% AUC CI:', ci)
```

```
AUC: 0.759576771120853
AUC COV: 0.0005295762772071846
95% AUC CI: [0.71447305 0.80468049]
```

[ ]:

7 Random Forest

[29]:

```
from sklearn.ensemble import RandomForestClassifier
seed(42)

params8 = {'n_estimators' : [10,100,150],
           'min_samples_leaf': [1,2,3]}
rf2 = RandomForestClassifier(random_state=42)
rf2 = GridSearchCV(rf2, cv=5, param_grid=params8, scoring = 'roc_auc',refit =␣
 ↪True,
                   n_jobs=-1, verbose = 5, return_train_score=True)

rf2.fit(gu_Xtrain,gu_ytrain)
rf2.cv_results_
```

```
Fitting 5 folds for each of 9 candidates, totalling 45 fits

[Parallel(n_jobs=-1)]: Using backend LokyBackend with 12 concurrent workers.
[Parallel(n_jobs=-1)]: Done  32 out of  45 | elapsed:    2.9s remaining:    1.2s
[Parallel(n_jobs=-1)]: Done  42 out of  45 | elapsed:    3.1s remaining:    0.2s
[Parallel(n_jobs=-1)]: Done  45 out of  45 | elapsed:    3.2s finished
/usr/local/lib/python3.7/site-packages/sklearn/model_selection/_search.py:715:
DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples,), for example using
ravel().
  self.best_estimator_.fit(X, y, **fit_params)
```

[29]:

```
{'mean_fit_time': array([0.03426881, 0.27883363, 0.41557159, 0.03126526,
0.26815095,
```

```
       0.39476094, 0.03139949, 0.25758681, 0.27651353]),
 'std_fit_time': array([0.00141601, 0.00441368, 0.00469748, 0.00190913,
0.00351207,
       0.00498689, 0.0020941 , 0.00279042, 0.03816554]),
 'mean_score_time': array([0.00626278, 0.01958594, 0.02709827, 0.00515699,
0.01952624,
       0.02721171, 0.00534773, 0.01840653, 0.01495228]),
 'std_score_time': array([9.31513526e-04, 3.06682837e-04, 1.34821106e-03,
8.77498277e-05,
       6.76603885e-04, 5.90346595e-04, 1.60732816e-04, 1.65642035e-03,
       9.19618958e-04]),
 'param_min_samples_leaf': masked_array(data=[1, 1, 1, 2, 2, 2, 3, 3, 3],
             mask=[False, False, False, False, False, False, False, False,
                   False],
       fill_value='?',
            dtype=object),
 'param_n_estimators': masked_array(data=[10, 100, 150, 10, 100, 150, 10, 100,
150],
             mask=[False, False, False, False, False, False, False, False,
                   False],
       fill_value='?',
            dtype=object),
 'params': [{'min_samples_leaf': 1, 'n_estimators': 10},
  {'min_samples_leaf': 1, 'n_estimators': 100},
  {'min_samples_leaf': 1, 'n_estimators': 150},
  {'min_samples_leaf': 2, 'n_estimators': 10},
  {'min_samples_leaf': 2, 'n_estimators': 100},
  {'min_samples_leaf': 2, 'n_estimators': 150},
  {'min_samples_leaf': 3, 'n_estimators': 10},
  {'min_samples_leaf': 3, 'n_estimators': 100},
  {'min_samples_leaf': 3, 'n_estimators': 150}],
 'split0_test_score': array([0.73632246, 0.81757246, 0.81666667, 0.69248188,
0.79981884,
       0.81322464, 0.77753623, 0.83115942, 0.83822464]),
 'split1_test_score': array([0.72053776, 0.73951182, 0.74094203, 0.63567887,
0.75629291,
       0.74980931, 0.70061022, 0.76735317, 0.76372998]),
 'split2_test_score': array([0.71406699, 0.79282297, 0.79110048, 0.78593301,
0.77358852,
       0.77339713, 0.73645933, 0.78832536, 0.79406699]),
 'split3_test_score': array([0.69253589, 0.76870813, 0.7569378 , 0.7508134 ,
0.77521531,
       0.76669856, 0.69416268, 0.76669856, 0.75923445]),
 'split4_test_score': array([0.85339713, 0.8476555 , 0.85090909, 0.74277512,
0.82593301,
       0.8430622 , 0.83732057, 0.84976077, 0.85550239]),
 'mean_test_score': array([0.74334697, 0.79325071, 0.79131144, 0.72143872,
```

```
0.78616797,
        0.78924417, 0.74922326, 0.80067826, 0.80217458]),
 'std_test_score': array([0.05672565, 0.03752678, 0.03977511, 0.05229473,
0.02423484,
        0.03400995, 0.05311361, 0.0339244 , 0.03880603]),
 'rank_test_score': array([8, 3, 4, 9, 6, 5, 7, 2, 1], dtype=int32),
 'split0_train_score': array([0.99986257, 1.        , 1.        , 0.99442492,
0.99960562,
        0.99955782, 0.98568287, 0.99600841, 0.99709594]),
 'split1_train_score': array([0.99840169, 1.        , 1.        , 0.9910471 ,
0.99961074,
        0.9997169 , 0.9869658 , 0.99639053, 0.99689774]),
 'split2_train_score': array([0.99987037, 1.        , 1.        , 0.9958517 ,
0.99892757,
        0.99923398, 0.98869823, 0.99629953, 0.99648809]),
 'split3_train_score': array([0.99989983, 1.        , 1.        , 0.99582224,
0.99926933,
        0.9992929 , 0.98688925, 0.99560421, 0.99604026]),
 'split4_train_score': array([0.99975252, 1.        , 1.        , 0.99544512,
0.99951682,
        0.99963467, 0.98635303, 0.99675914, 0.99698305]),
 'mean_train_score': array([0.99955739, 1.        , 1.        , 0.99451822,
0.99938602,
        0.99948725, 0.98691784, 0.99621236, 0.99670102]),
 'std_train_score': array([5.80011721e-04, 4.96506831e-17, 0.00000000e+00,
1.81080856e-03,
        2.60624598e-04, 1.90457287e-04, 1.00170650e-03, 3.87232642e-04,
        3.88884105e-04])}
```

[30]:
```
rf2.best_estimator_
```

[30]:
```
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
                       max_depth=None, max_features='auto', max_leaf_nodes=None,
                       min_impurity_decrease=0.0, min_impurity_split=None,
                       min_samples_leaf=3, min_samples_split=2,
                       min_weight_fraction_leaf=0.0, n_estimators=150,
                       n_jobs=None, oob_score=False, random_state=42, verbose=0,
                       warm_start=False)
```

[31]:
```
rf_pred2 = rf2.best_estimator_.predict(gu_Xtest)
rf_pred2
```

[31]:
```
array([0, 0, 0, …, 0, 0, 0])
```

[32]:
```
prob8 = rf2.best_estimator_.predict_proba(gu_Xtest)
prob8
```

[32]:
```
array([[0.96881419, 0.03118581],
       [0.94229728, 0.05770272],
       [0.99634343, 0.00365657],
       …,
       [0.97513973, 0.02486027],
       [0.83568952, 0.16431048],
       [0.97687497, 0.02312503]])
```

[33]:
```
rf_matrix2 = metrics.confusion_matrix(gu_ytest, rf_pred2)
rf_matrix2
```

[33]:
```
array([[2051,    2],
       [ 128,    7]])
```

[34]:
```
print("", classification_report(gu_ytest, rf_pred2,
                                target_names=target_names2))
```

```
                        precision    recall  f1-score   support

Still alive at 30 day       0.94      1.00      0.97      2053
      Died in 30 days       0.78      0.05      0.10       135

             accuracy                           0.94      2188
            macro avg       0.86      0.53      0.53      2188
         weighted avg       0.93      0.94      0.92      2188
```

[35]:
```
rf_probs2 = rf2.best_estimator_.predict_proba(gu_Xtest)[:,1]
print(roc_auc_score(gu_ytest, rf_probs2))
```

```
0.885331312803305
```

[36]:
```
#Boostrapping calculated 95% CI
y_pred = rf_probs2
y_true = gu_ytest

print("Original ROC area: {:0.4f}".format(roc_auc_score(y_true, y_pred)))

n_bootstraps = 1000
rng_seed = 42  # control reproducibility
bootstrapped_scores = []

rng = np.random.RandomState(rng_seed)
for i in range(n_bootstraps):
    # bootstrap by sampling with replacement on the prediction indices
    indices = rng.randint(0, len(y_pred), len(y_pred))
    if len(np.unique(y_true[indices])) < 2:
```

```
            # We need at least one positive and one negative sample for ROC AUC
            # to be defined: reject the sample
            continue

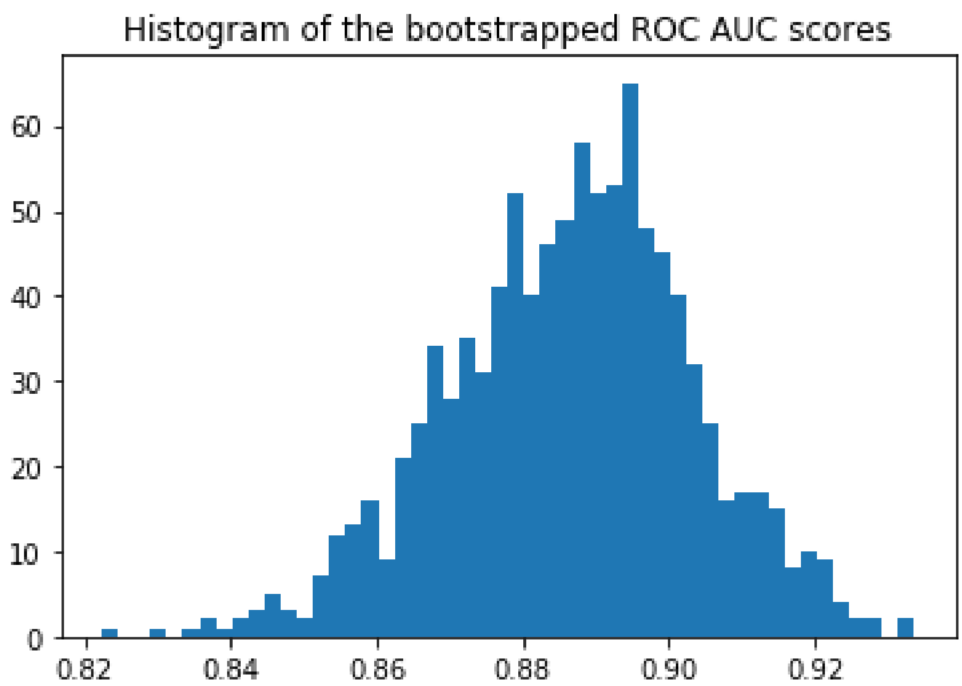
        score = roc_auc_score(y_true[indices], y_pred[indices])
        bootstrapped_scores.append(score)
        #print("Bootstrap #{} ROC area: {:0.3f}".format(i + 1, score))

import matplotlib.pyplot as plt
plt.hist(bootstrapped_scores, bins=50)
plt.title('Histogram of the bootstrapped ROC AUC scores')
plt.show()

sorted_scores = np.array(bootstrapped_scores)
sorted_scores.sort()

# Computing the lower and upper bound of the 90% confidence interval
# You can change the bounds percentiles to 0.025 and 0.975 to get
# a 95% confidence interval instead.
confidence_lower = sorted_scores[int(0.05 * len(sorted_scores))]
confidence_upper = sorted_scores[int(0.95 * len(sorted_scores))]
print("Confidence interval for the score: [{:0.4f} - {:0.4}]".format(
    confidence_lower, confidence_upper))
```

```
Original ROC area: 0.8853
```



```
Confidence interval for the score: [0.8575 - 0.9138]
```

[37]:
```
#pROC calculated 95% CI without bootstrapping
alpha = .95
y_pred = rf_probs2
y_true = gu_ytest

auc, auc_cov = delong_roc_variance(
    y_true,
    y_pred)

auc_std = np.sqrt(auc_cov)
lower_upper_q = np.abs(np.array([0, 1]) - (1 - alpha) / 2)

ci = stats.norm.ppf(
    lower_upper_q,
    loc=auc,
    scale=auc_std)

ci[ci > 1] = 1

print('AUC:', auc)
print('AUC COV:', auc_cov)
print('95% AUC CI:', ci)
```

```
AUC: 0.885331312803305
AUC COV: 0.0002835084573262921
95% AUC CI: [0.85233001 0.91833262]
```

[ ]:

8 Gradient Boosting Machines

[38]:
```
from sklearn.ensemble import GradientBoostingClassifier
seed(10)

params9 = {'learning_rate' : [0.05,0.1,0.2],
           'n_estimators': [100,150],
           'min_samples_split': [2,3,4]}
gbm2 = GradientBoostingClassifier(random_state=10)
gbm2 = GridSearchCV(gbm2, cv=5, param_grid=params9, scoring = 'roc_auc',refit =␣
 ↪True,
                    n_jobs=-1, verbose = 5, return_train_score=True)
```

```
gbm2.fit(gu_Xtrain,gu_ytrain)
gbm2.cv_results_
```

```
Fitting 5 folds for each of 18 candidates, totalling 90 fits
```

```
[Parallel(n_jobs=-1)]: Using backend LokyBackend with 12 concurrent workers.
[Parallel(n_jobs=-1)]: Done  48 tasks      | elapsed:    3.3s
[Parallel(n_jobs=-1)]: Done  86 out of  90 | elapsed:    4.1s remaining:    0.2s
[Parallel(n_jobs=-1)]: Done  90 out of  90 | elapsed:    4.2s finished
/usr/local/lib/python3.7/site-
packages/sklearn/ensemble/gradient_boosting.py:1450: DataConversionWarning: A
column-vector y was passed when a 1d array was expected. Please change the shape
of y to (n_samples, ), for example using ravel().
  y = column_or_1d(y, warn=True)
```

[38]:
```
{'mean_fit_time': array([0.21591759, 0.31171274, 0.21119657, 0.30165682,
0.20505085,
        0.31778083, 0.21604004, 0.31748967, 0.21064258, 0.30856447,
        0.19796476, 0.29425311, 0.20156455, 0.31398468, 0.2083787 ,
        0.30039825, 0.19774466, 0.20412064]),
 'std_fit_time': array([0.0056044 , 0.00702359, 0.01232283, 0.00609257,
0.00772605,
        0.01428885, 0.01009541, 0.00883545, 0.00734894, 0.0096207 ,
        0.00407808, 0.00844164, 0.00828902, 0.00990215, 0.00551054,
        0.01645469, 0.00495295, 0.02872154]),
 'mean_score_time': array([0.00563526, 0.00516491, 0.00454321, 0.00547996,
0.00660977,
        0.00500064, 0.00556917, 0.0047678 , 0.00544276, 0.00471015,
        0.00444007, 0.0050961 , 0.00572243, 0.00481868, 0.00482841,
        0.00471101, 0.00447583, 0.00257258]),
 'std_score_time': array([8.69524816e-04, 2.34852026e-04, 3.57920292e-04,
8.49180947e-04,
        1.95817910e-03, 4.04191528e-04, 1.16676813e-03, 2.35012840e-04,
        1.81804900e-03, 1.43596595e-04, 1.15136279e-04, 6.36400680e-04,
        1.36987998e-03, 5.35703957e-04, 5.79642088e-04, 1.33745581e-03,
        4.81773102e-05, 1.36307002e-04]),
 'param_learning_rate': masked_array(data=[0.05, 0.05, 0.05, 0.05, 0.05, 0.05,
0.1, 0.1, 0.1, 0.1,
                    0.1, 0.1, 0.2, 0.2, 0.2, 0.2, 0.2, 0.2],
              mask=[False, False, False, False, False, False, False, False,
                    False, False, False, False, False, False, False, False,
                    False, False],
        fill_value='?',
             dtype=object),
 'param_min_samples_split': masked_array(data=[2, 2, 3, 3, 4, 4, 2, 2, 3, 3, 4,
4, 2, 2, 3, 3, 4, 4],
              mask=[False, False, False, False, False, False, False, False,
                    False, False, False, False, False, False, False, False,
```

```
                    False, False],
        fill_value='?',
             dtype=object),
 'param_n_estimators': masked_array(data=[100, 150, 100, 150, 100, 150, 100,
150, 100, 150, 100,
                    150, 100, 150, 100, 150, 100, 150],
              mask=[False, False, False, False, False, False, False, False,
                    False, False, False, False, False, False, False, False,
                    False, False],
        fill_value='?',
             dtype=object),
 'params': [{'learning_rate': 0.05,
   'min_samples_split': 2,
   'n_estimators': 100},
  {'learning_rate': 0.05, 'min_samples_split': 2, 'n_estimators': 150},
  {'learning_rate': 0.05, 'min_samples_split': 3, 'n_estimators': 100},
  {'learning_rate': 0.05, 'min_samples_split': 3, 'n_estimators': 150},
  {'learning_rate': 0.05, 'min_samples_split': 4, 'n_estimators': 100},
  {'learning_rate': 0.05, 'min_samples_split': 4, 'n_estimators': 150},
  {'learning_rate': 0.1, 'min_samples_split': 2, 'n_estimators': 100},
  {'learning_rate': 0.1, 'min_samples_split': 2, 'n_estimators': 150},
  {'learning_rate': 0.1, 'min_samples_split': 3, 'n_estimators': 100},
  {'learning_rate': 0.1, 'min_samples_split': 3, 'n_estimators': 150},
  {'learning_rate': 0.1, 'min_samples_split': 4, 'n_estimators': 100},
  {'learning_rate': 0.1, 'min_samples_split': 4, 'n_estimators': 150},
  {'learning_rate': 0.2, 'min_samples_split': 2, 'n_estimators': 100},
  {'learning_rate': 0.2, 'min_samples_split': 2, 'n_estimators': 150},
  {'learning_rate': 0.2, 'min_samples_split': 3, 'n_estimators': 100},
  {'learning_rate': 0.2, 'min_samples_split': 3, 'n_estimators': 150},
  {'learning_rate': 0.2, 'min_samples_split': 4, 'n_estimators': 100},
  {'learning_rate': 0.2, 'min_samples_split': 4, 'n_estimators': 150}],
 'split0_test_score': array([0.77382246, 0.74565217, 0.78623188, 0.77028986,
0.76449275,
        0.75199275, 0.76539855, 0.75742754, 0.76105072, 0.7509058 ,
        0.74873188, 0.74764493, 0.75797101, 0.75181159, 0.77952899,
        0.77663043, 0.7365942 , 0.71050725]),
 'split1_test_score': array([0.73455378, 0.74523265, 0.74780702, 0.74599542,
0.74885584,
        0.75076278, 0.74084668, 0.73455378, 0.73741419, 0.70747521,
        0.73779558, 0.7305492 , 0.73512586, 0.71720061, 0.70175439,
        0.67982456, 0.71929825, 0.69012204]),
 'split2_test_score': array([0.77205742, 0.77301435, 0.77148325, 0.77799043,
0.77186603,
        0.77875598, 0.78373206, 0.78411483, 0.77952153, 0.78009569,
        0.78296651, 0.79043062, 0.78047847, 0.78028708, 0.78392344,
        0.78354067, 0.76574163, 0.74392344]),
 'split3_test_score': array([0.71100478, 0.68956938, 0.70258373, 0.6815311 ,
```

```
0.72114833,
       0.68660287, 0.64210526, 0.65129187, 0.63751196, 0.6845933 ,
       0.62411483, 0.63559809, 0.6076555 , 0.5691866 , 0.58660287,
       0.5984689 , 0.62602871, 0.58947368]),
 'split4_test_score': array([0.82755981, 0.81818182, 0.82526316, 0.82315789,
0.82870813,
       0.81952153, 0.81913876, 0.8061244 , 0.82411483, 0.83062201,
       0.81741627, 0.81033493, 0.82277512, 0.79177033, 0.82507177,
       0.8292823 , 0.8262201 , 0.81722488]),
 'mean_test_score': array([0.7637934 , 0.75431212, 0.76668756, 0.75979783,
0.76699846,
       0.75751508, 0.75025846, 0.7467088 , 0.74793334, 0.75070926,
       0.74221088, 0.74290959, 0.74082065, 0.72208836, 0.73541342,
       0.73357139, 0.73476854, 0.71023694]),
 'std_test_score': array([0.03965896, 0.04185947, 0.04071548, 0.04637067,
0.0353775 ,
       0.04331702, 0.05974167, 0.05342025, 0.06203115, 0.05190187,
       0.06524184, 0.06075918, 0.07252206, 0.08058388, 0.08433274,
       0.08319232, 0.06534065, 0.07418203]),
 'rank_test_score': array([ 3,  6,  2,  4,  1,  5,  8, 10,  9,  7, 12, 11, 13,
17, 14, 16, 15,
       18], dtype=int32),
 'split0_train_score': array([0.96441632, 0.97920551, 0.96136288, 0.98126105,
0.96078923,
       0.98096228, 0.98704527, 0.99378555, 0.98962666, 0.99580525,
       0.98771452, 0.99539892, 0.99916344, 1.        , 0.99998805,
       1.        , 0.99939051, 1.        ]),
 'split1_train_score': array([0.96179978, 0.9758425 , 0.9625606 , 0.9752999 ,
0.95852059,
       0.97386083, 0.99284004, 0.99933944, 0.98685964, 0.99902096,
       0.99203793, 0.99542329, 0.99911533, 1.        , 1.        ,
       1.        , 1.        , 1.        ]),
 'split2_train_score': array([0.94661418, 0.97316567, 0.94852335, 0.9745563 ,
0.94762769,
       0.97388455, 0.98368963, 0.99614632, 0.98559879, 0.99629953,
       0.98736064, 0.99589884, 0.99985858, 1.        , 0.99981144,
       1.        , 0.99941075, 1.        ]),
 'split3_train_score': array([0.95035001, 0.97647135, 0.94496429, 0.97045513,
0.95118085,
       0.97113866, 0.9809732 , 0.99402503, 0.98148585, 0.99641738,
       0.98154477, 0.99252834, 1.        , 1.        , 0.99868009,
       1.        , 0.9985151 , 1.        ]),
 'split4_train_score': array([0.94395668, 0.96426804, 0.94526481, 0.96371414,
0.94537087,
       0.96552903, 0.97766752, 0.99895114, 0.98188653, 0.99645273,
       0.98304146, 0.99435501, 0.99545101, 1.        , 0.99949325,
       1.        , 0.99996465, 1.        ]),
```

```
 'mean_train_score': array([0.9534274 , 0.97379061, 0.95253518, 0.97305731,
0.95269785,
        0.97307507, 0.98444313, 0.9964495 , 0.98509149, 0.99679917,
        0.98633987, 0.99472088, 0.99871767, 1.        , 0.99959456,
        1.        , 0.9994562 , 1.        ]),
 'std_train_score': array([0.0082029 , 0.00513396, 0.00780652, 0.00580764,
0.00601776,
        0.00498344, 0.00521145, 0.00235272, 0.00307323, 0.00113487,
        0.00372215, 0.0012068 , 0.00167176, 0.        , 0.0004925 ,
        0.        , 0.00053783, 0.        ])}
```

[39]:
```
gbm2.best_estimator_
```

[39]:
```
GradientBoostingClassifier(criterion='friedman_mse', init=None,
                           learning_rate=0.05, loss='deviance', max_depth=3,
                           max_features=None, max_leaf_nodes=None,
                           min_impurity_decrease=0.0, min_impurity_split=None,
                           min_samples_leaf=1, min_samples_split=4,
                           min_weight_fraction_leaf=0.0, n_estimators=100,
                           n_iter_no_change=None, presort='auto',
                           random_state=10, subsample=1.0, tol=0.0001,
                           validation_fraction=0.1, verbose=0,
                           warm_start=False)
```

[40]:
```
gbm_pred2 = gbm2.best_estimator_.predict(gu_Xtest)
gbm_pred2
```

[40]:
```
array([0, 0, 0, …, 0, 0, 0])
```

[41]:
```
prob9 = gbm2.best_estimator_.predict_proba(gu_Xtest)
prob9
```

[41]:
```
array([[0.947186  , 0.052814  ],
       [0.97310495, 0.02689505],
       [0.97898104, 0.02101896],
       …,
       [0.9711283 , 0.0288717 ],
       [0.87880754, 0.12119246],
       [0.98384301, 0.01615699]])
```

[42]:
```
gbm_matrix2 = metrics.confusion_matrix(gu_ytest, gbm_pred2)
gbm_matrix2
```

[42]:
```
array([[2044,    9],
       [ 113,   22]])
```

[43]:
```
print("", classification_report(gu_ytest, gbm_pred2,
                                target_names=target_names2))
```

```
                    precision    recall  f1-score   support

Still alive at 30 day       0.95      1.00      0.97      2053
      Died in 30 days       0.71      0.16      0.27       135

             accuracy                           0.94      2188
            macro avg       0.83      0.58      0.62      2188
         weighted avg       0.93      0.94      0.93      2188
```

[44]:
```
gbm_probs2 = gbm2.best_estimator_.predict_proba(gu_Xtest)[:,1]
print(roc_auc_score(gu_ytest, gbm_probs2))
```

0.8720806047157728

[45]:
```
#Boostrapping calculated 95% CI
y_pred = gbm_probs2
y_true = gu_ytest

print("Original ROC area: {:0.4f}".format(roc_auc_score(y_true, y_pred)))

n_bootstraps = 1000
rng_seed = 42  # control reproducibility
bootstrapped_scores = []

rng = np.random.RandomState(rng_seed)
for i in range(n_bootstraps):
    # bootstrap by sampling with replacement on the prediction indices
    indices = rng.randint(0, len(y_pred), len(y_pred))
    if len(np.unique(y_true[indices])) < 2:
        # We need at least one positive and one negative sample for ROC AUC
        # to be defined: reject the sample
        continue

    score = roc_auc_score(y_true[indices], y_pred[indices])
    bootstrapped_scores.append(score)
    #print("Bootstrap #{} ROC area: {:0.3f}".format(i + 1, score))

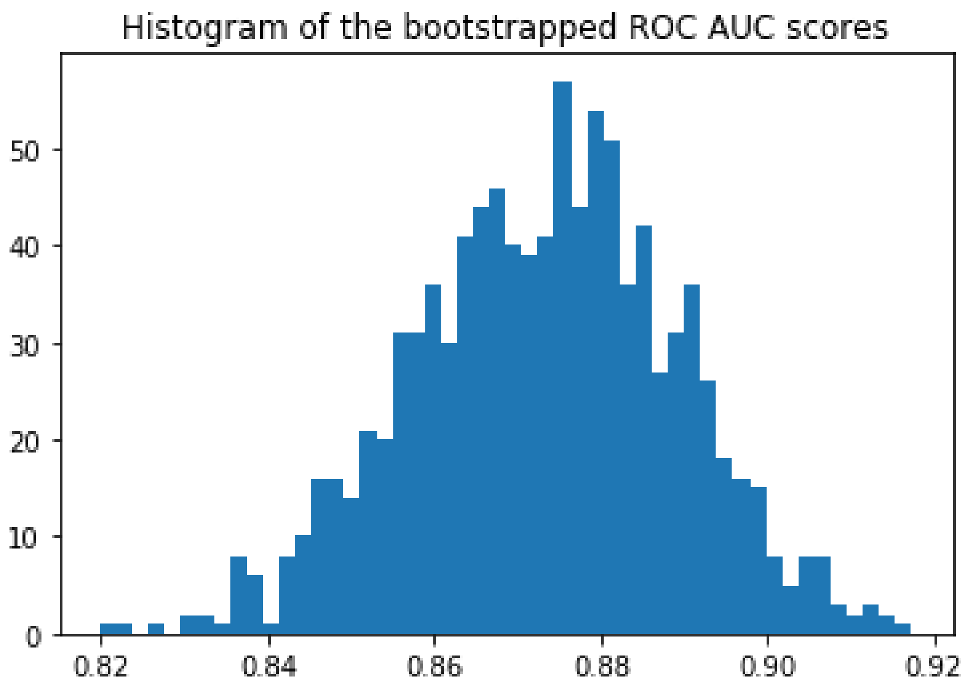
import matplotlib.pyplot as plt
plt.hist(bootstrapped_scores, bins=50)
plt.title('Histogram of the bootstrapped ROC AUC scores')
plt.show()

sorted_scores = np.array(bootstrapped_scores)
```

```
sorted_scores.sort()

# Computing the lower and upper bound of the 90% confidence interval
# You can change the bounds percentiles to 0.025 and 0.975 to get
# a 95% confidence interval instead.
confidence_lower = sorted_scores[int(0.05 * len(sorted_scores))]
confidence_upper = sorted_scores[int(0.95 * len(sorted_scores))]
print("Confidence interval for the score: [{:0.4f} - {:0.4}]".format(
    confidence_lower, confidence_upper))
```

```
Original ROC area: 0.8721
```




```
Confidence interval for the score: [0.8468 - 0.8985]
```

[46]:
```
#pROC calculated 95% CI without bootstrapping
alpha = .95
y_pred = gbm_probs2
y_true = gu_ytest

auc, auc_cov = delong_roc_variance(
    y_true,
    y_pred)

auc_std = np.sqrt(auc_cov)
lower_upper_q = np.abs(np.array([0, 1]) - (1 - alpha) / 2)
```

```
ci = stats.norm.ppf(
    lower_upper_q,
    loc=auc,
    scale=auc_std)

ci[ci > 1] = 1

print('AUC:', auc)
print('AUC COV:', auc_cov)
print('95% AUC CI:', ci)
```

```
AUC: 0.8720806047157728
AUC COV: 0.000262844614256567
95% AUC CI: [0.84030472 0.90385649]
```

[ ]:

9 Support Vector Machine

[47]:

```
# mlp2 = MLPClassifier(solver='lbfgs', random_state=1)
# mlp2 = GridSearchCV(mlp2, cv=5, param_grid=params7, scoring = 'roc_auc',refit␣
 ↪= True,
#                      n_jobs=-1, verbose = 5, return_train_score=True)

# mlp2.fit(gu_Xtrains, gu_ytrain)
# mlp2.cv_results_
```

[48]:

```
from sklearn.svm import SVC
seed(0)
params0 = {'degree' : [2,3,4],
           'C': [0.5,1.0,1.5,2.0,2.5],
           'tol':[1e-5,1e-3,1e-1],
           'max_iter':[-1,-2,-3]}
svc = SVC(random_state=0,probability=True)
svc = GridSearchCV(svc, cv=5, param_grid=params0, scoring = 'roc_auc',refit =␣
 ↪True,
                   n_jobs=-1, verbose = 5, return_train_score=True)

svc.fit(gu_Xtrains, gu_ytrain)
svc.cv_results_
```

```
Fitting 5 folds for each of 135 candidates, totalling 675 fits
```

```
[Parallel(n_jobs=-1)]: Using backend LokyBackend with 12 concurrent workers.
[Parallel(n_jobs=-1)]: Done  48 tasks      | elapsed:    2.5s
```

```
[Parallel(n_jobs=-1)]: Done 360 tasks      | elapsed:    4.3s
[Parallel(n_jobs=-1)]: Done 675 out of 675 | elapsed:    6.5s finished
/usr/local/lib/python3.7/site-packages/sklearn/utils/validation.py:724:
DataConversionWarning: A column-vector y was passed when a 1d array was
expected. Please change the shape of y to (n_samples, ), for example using
ravel().
  y = column_or_1d(y, warn=True)
```

[48]:

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       0.5       , 0.5       , 0.70332359, 0.7030926 , 0.697668  ,
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       0.        , 0.        , 0.        , 0.04645699, 0.04664472,
       0.05268863, 0.        , 0.        , 0.        , 0.        ,
```

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       0.04620279, 0.04253053, 0.        , 0.        , 0.        ,
       0.        , 0.        , 0.        , 0.04618664, 0.04620279,
       0.04253053, 0.        , 0.        , 0.        , 0.        ,
       0.        , 0.        , 0.04618664, 0.04620279, 0.04253053,
       0.        , 0.        , 0.        , 0.        , 0.        ,
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       0.        , 0.        , 0.        , 0.        , 0.        ,
       0.0466069 , 0.04666253, 0.04779264, 0.        , 0.        ,
       0.        , 0.        , 0.        , 0.        , 0.0466069 ,
       0.04666253, 0.04779264, 0.        , 0.        , 0.        ,
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       0.04682372, 0.        , 0.        , 0.        , 0.        ,
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       0.        , 0.        , 0.        , 0.        , 0.        ,
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       46, 46,  1, 10, 34, 46, 46, 46, 46, 46, 46,  1, 10, 34, 46, 46, 46,
       46, 46, 46, 13, 16, 43, 46, 46, 46, 46, 46, 46, 13, 16, 43, 46, 46,
       46, 46, 46, 46, 13, 16, 43, 46, 46, 46, 46, 46, 46, 19, 22, 25, 46,
       46, 46, 46, 46, 46, 19, 22, 25, 46, 46, 46, 46, 46, 46, 19, 22, 25,
       46, 46, 46, 46, 46, 46, 28, 31, 40, 46, 46, 46, 46, 46, 46, 28, 31,
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      dtype=int32),
 'split0_train_score': array([0.99435919, 0.99433529, 0.97523782, 0.5       ,
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       0.5       , 0.5       , 0.5       , 0.5       , 0.5       ,
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       0.5       , 0.5       , 0.5       , 0.5       , 0.5       ,
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       0.5       , 0.5       , 0.5       , 0.9944787 , 0.99446675,
       0.99396482, 0.5       , 0.5       , 0.5       , 0.5       ,
```

```
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       0.5       , 0.5       , 0.5       , 0.5       , 0.5       ,
       0.99498064, 0.99498064, 0.99514795, 0.5       , 0.5       ,
       0.5       , 0.5       , 0.5       , 0.5       , 0.99498064,
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       0.5       , 0.5       , 0.5       , 0.98992651, 0.98993831,
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       0.5       , 0.98992651, 0.98992651, 0.99313493, 0.5       ,
       0.5       , 0.5       , 0.5       , 0.5       , 0.5       ,
       0.98992651, 0.98992651, 0.99313493, 0.5       , 0.5       ,
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       0.5       , 0.5       , 0.5       , 0.99045732, 0.99075221,
       0.99279286, 0.5       , 0.5       , 0.5       , 0.5       ,
       0.5       , 0.5       , 0.99045732, 0.99075221, 0.99279286,
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       0.5       , 0.5       , 0.5       , 0.5       , 0.99470375,
       0.99469196, 0.99442066, 0.5       , 0.5       , 0.5       ,
       0.5       , 0.5       , 0.5       , 0.99525815, 0.99525815,
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       0.5       , 0.5       , 0.99525815, 0.99525815, 0.99529353,
       0.5       , 0.5       , 0.5       , 0.5       , 0.5       ,
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       0.5       , 0.5       , 0.5       , 0.5       , 0.5       ]),
 'split2_train_score': array([0.99226907, 0.99225729, 0.98568129, 0.5       ,
0.5       ,
       0.5       , 0.5       , 0.5       , 0.5       , 0.99226907,
       0.99225729, 0.98568129, 0.5       , 0.5       , 0.5       ,
       0.5       , 0.5       , 0.5       , 0.99226907, 0.99225729,
       0.98568129, 0.5       , 0.5       , 0.5       , 0.5       ,
```

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 'split3_train_score': array([0.99305867, 0.99305867, 0.97720791, 0.5       ,
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       0.5       , 0.99305867, 0.99304688, 0.98767294, 0.5       ,
       0.5       , 0.5       , 0.5       , 0.5       , 0.5       ,
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       0.5       , 0.5       , 0.99345935, 0.99345935, 0.99098451,
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       0.99358899, 0.5       , 0.5       , 0.5       , 0.5       ,
       0.5       , 0.5       , 0.99472034, 0.99472034, 0.99358899,
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       0.5       , 0.5       , 0.5       , 0.5       , 0.5       ]),
 'split4_train_score': array([0.98874537, 0.98850968, 0.97104438, 0.5       ,
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       0.5       , 0.5       , 0.5       , 0.98874537, 0.98850968,
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       0.5       , 0.98874537, 0.98701299, 0.98657694, 0.5       ,
       0.5       , 0.5       , 0.5       , 0.5       , 0.5       ,
       0.98874537, 0.98701299, 0.98657694, 0.5       , 0.5       ,
       0.5       , 0.5       , 0.5       , 0.5       , 0.98913428,
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       0.5       , 0.5       , 0.5       , 0.5       , 0.5       ,
       0.5       , 0.99014778, 0.99017135, 0.99266976, 0.5       ,
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       0.99067811, 0.5       , 0.5       , 0.5       , 0.5       ,
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 'mean_train_score': array([0.99167176, 0.99161985, 0.97890424, 0.5       , 0.5
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       0.5       , 0.5       , 0.99170712, 0.99135822, 0.99016723,
       0.5       , 0.5       , 0.5       , 0.5       , 0.5       ,
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       0.5       , 0.5       , 0.5       , 0.99273048, 0.99278471,
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         0.5       , 0.5       , 0.99518086, 0.99518086, 0.99470024,
         0.5       , 0.5       , 0.5       , 0.5       , 0.5       ,
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 'std_train_score': array([0.00205486, 0.00211428, 0.0057545 , 0.        , 0.
,
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         0.        , 0.        , 0.        , 0.        , 0.        ,
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         0.0025199 , 0.        , 0.        , 0.        , 0.        ,
         0.        , 0.        , 0.00281492, 0.00281492, 0.0025199 ,
         0.        , 0.        , 0.        , 0.        , 0.        ,
         0.        , 0.00281492, 0.00281492, 0.0025199 , 0.        ,
         0.        , 0.        , 0.        , 0.        , 0.        ])}
```

[49]:
```
svc.best_estimator_
```

[49]:
```
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovr', degree=2, gamma='auto_deprecated',
    kernel='rbf', max_iter=-1, probability=True, random_state=0, shrinking=True,
    tol=1e-05, verbose=False)
```

[50]:
```
svc_pred = svc.best_estimator_.predict(gu_Xtests)
svc_pred
```

[50]:
```
array([0, 0, 0, …, 0, 0, 0])
```

[51]:
```
prob_svc = svc.best_estimator_.predict_proba(gu_Xtests)
prob_svc
```

[51]:
```
array([[0.95247783, 0.04752217],
       [0.91819468, 0.08180532],
       [0.93822348, 0.06177652],
       …,
       [0.92257555, 0.07742445],
       [0.93326204, 0.06673796],
       [0.9271016 , 0.0728984 ]])
```

[52]:
```
svc_matrix = metrics.confusion_matrix(gu_ytest, svc_pred)
svc_matrix
```

[52]:
```
array([[2052,    1],
       [ 131,    4]])
```

[53]:
```
target_names2 = ['Still alive at 30 day', 'Died in 30 days']
print("", classification_report(gu_ytest, svc_pred,
                                target_names=target_names2))
```

```
                        precision    recall  f1-score   support

Still alive at 30 day       0.94      1.00      0.97      2053
      Died in 30 days       0.80      0.03      0.06       135

             accuracy                           0.94      2188
            macro avg       0.87      0.51      0.51      2188
         weighted avg       0.93      0.94      0.91      2188
```

[54]:
```
svc_probs = svc.best_estimator_.predict_proba(gu_Xtests)[:,1]
print(roc_auc_score(gu_ytest, svc_probs))
```

```
0.7897854990889575
```

[55]:
```
#Boostrapping calculated 95% CI
y_pred = svc_probs
y_true = gu_ytest

print("Original ROC area: {:0.4f}".format(roc_auc_score(y_true, y_pred)))
```

```
n_bootstraps = 1000
rng_seed = 42  # control reproducibility
bootstrapped_scores = []

rng = np.random.RandomState(rng_seed)
for i in range(n_bootstraps):
    # bootstrap by sampling with replacement on the prediction indices
    indices = rng.randint(0, len(y_pred), len(y_pred))
    if len(np.unique(y_true[indices])) < 2:
        # We need at least one positive and one negative sample for ROC AUC
        # to be defined: reject the sample
        continue

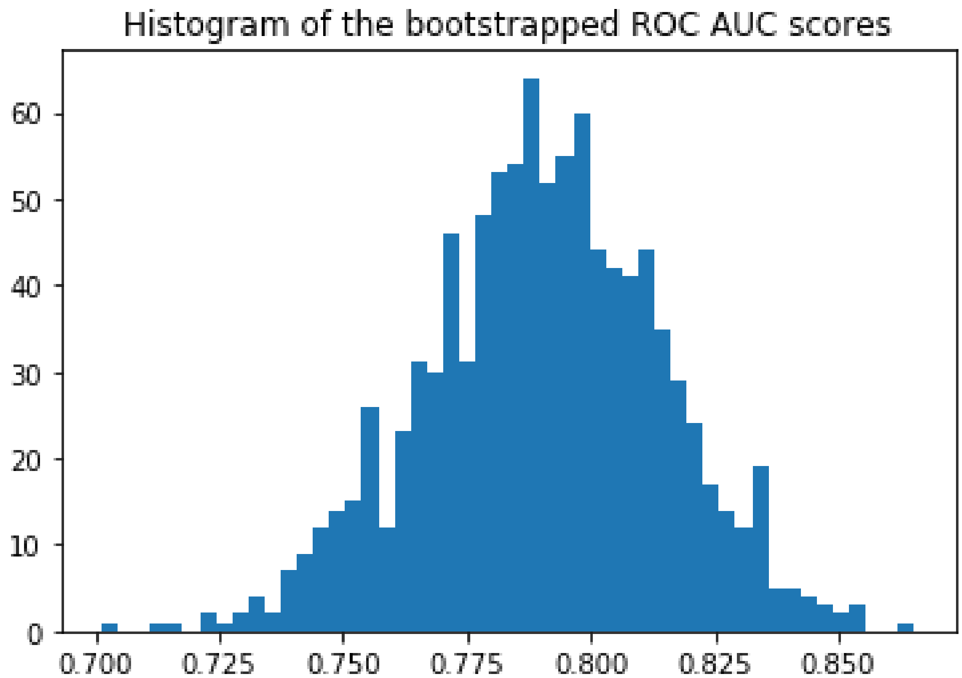
    score = roc_auc_score(y_true[indices], y_pred[indices])
    bootstrapped_scores.append(score)
    #print("Bootstrap #{} ROC area: {:0.3f}".format(i + 1, score))

import matplotlib.pyplot as plt
plt.hist(bootstrapped_scores, bins=50)
plt.title('Histogram of the bootstrapped ROC AUC scores')
plt.show()

sorted_scores = np.array(bootstrapped_scores)
sorted_scores.sort()

# Computing the lower and upper bound of the 90% confidence interval
# You can change the bounds percentiles to 0.025 and 0.975 to get
# a 95% confidence interval instead.
confidence_lower = sorted_scores[int(0.05 * len(sorted_scores))]
confidence_upper = sorted_scores[int(0.95 * len(sorted_scores))]
print("Confidence interval for the score: [{:0.4f} - {:0.4}]".format(
    confidence_lower, confidence_upper))
```

```
Original ROC area: 0.7898
```



Confidence interval for the score: [0.7489 - 0.8302]

[56]:
```
#pROC calculated 95% CI without bootstrapping
alpha = .95
y_pred = svc_probs
y_true = gu_ytest

auc, auc_cov = delong_roc_variance(
    y_true,
    y_pred)

auc_std = np.sqrt(auc_cov)
lower_upper_q = np.abs(np.array([0, 1]) - (1 - alpha) / 2)

ci = stats.norm.ppf(
    lower_upper_q,
    loc=auc,
    scale=auc_std)

ci[ci > 1] = 1

print('AUC:', auc)
print('AUC COV:', auc_cov)
print('95% AUC CI:', ci)
```

```
AUC: 0.7897854990889575
AUC COV: 0.0005276809118318064
95% AUC CI: [0.74476257 0.83480843]
```

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