

Assignment 3 - Supervised Learning

SOLUTIONS

Learning Objectives:

This assignment will provide structured practice to help enable you to...

1. Understand the primary workflow in machine learning: (1) identifying a hypothesis function set of models, (2) determining a loss/cost/error/objective function to minimize, and (3) minimizing that function through gradient descent
2. Implement batch gradient descent and become familiar with how that technique is used and its dependence on the choice of learning rate
3. Gain practice in implementing machine learning algorithms to understand the math and programming behind them to achieve practical proficiency with the techniques
4. Evaluate supervised learning algorithm performance through ROC curves and using cross validation
5. How to work with imagery data and the basics of computer vision approaches to machine learning
6. Develop and understanding of Bayes rule and the optimal minimum misclassification error classifier (Bayes' Rule)

```
In [1]: # MAC USERS TAKE NOTE:  
# For clearer plots in Jupyter notebooks on macs, run the following line of code:  
# %config InlineBackend.figure_format = 'retina'
```

1

[40 points] From theory to practice: classification through logistic regression

Introduction

For this problem you will derive, implement through gradient descent, and test the performance of a logistic regression classifier for a binary classification problem.

In this case, we'll assume our logistic regression problem will be applied to a two dimensional feature space. Our logistic regression model is:

$$f(\mathbf{x}_i, \mathbf{w}) = \sigma(\mathbf{w}^T \mathbf{x}_i)$$

where the sigmoid function is defined as $\sigma(x) = \frac{e^x}{1 + e^x} = \frac{1}{1 + e^{-x}}$. Also, since this is a two-dimensional problem, we define $\mathbf{w}^T \mathbf{x}_i = w_0 x_{i,0} + w_1 x_{i,1} + w_2 x_{i,2}$ and here, $\mathbf{x}_i = [x_{i,0}, x_{i,1}, x_{i,2}]^T$, and $x_{i,0} \triangleq 1$

As in class, we will interpret the response of the logistic regression classifier to be the likelihood of the data given the model parameters. For one sample, (y_i, \mathbf{x}_i) , this is given as:

$$P(Y = y_i | X = \mathbf{x}_i) = f(\mathbf{x}_i, \mathbf{w}) = \sigma(\mathbf{w}^T \mathbf{x}_i)$$

Aside: the careful reader will recognize this expression looks different from when we talk about the likelihood of our data given the true class label, typically expressed as $P(x|y)$, or the posterior probability of a class label given our data, typically expressed as $P(y|x)$. In the context of training a logistic regression model, we know the training \mathbf{x} values and y values, so the above probability is primarily a function of the logistic regression parameters, \mathbf{w} . It's our goal to use this to choose the parameters to maximize the probability of our data by adjusting our model

Find the cost function that we can use to choose the model parameters, \mathbf{w} , that best fit the training data.

- (a) What is the likelihood function for all the N samples in our training dataset that we will wish to maximize?
- (b) Since a logarithm is a monotonic function, maximizing the $f(x)$ is equivalent to maximizing $\ln[f(x)]$. Express part (a) as a cost function of the model parameters, $C(\mathbf{w})$, that is the negative of the logarithm of (a).
- (c) Calculate the gradient of the cost function with respect to the model parameters $\nabla_{\mathbf{w}}C(\mathbf{w})$. Express this in terms of the partial derivatives of the cost function with respect to each of the parameters, e.g.

$$\nabla_{\mathbf{w}}C(\mathbf{w}) = \left[\frac{\partial C}{\partial w_0}, \frac{\partial C}{\partial w_1}, \frac{\partial C}{\partial w_2} \right].$$

- (d) Write out the gradient descent update equation, assuming η represents the learning rate.

Prepare and plot your data

- (e) Load the data and scatter plot the data by class. In the data folder in the same directory of this notebook, you'll find the data in `A3_Q1_data.csv`. This file contains the binary class labels, y , and the features x_1 and x_2 . Comment on the data: do the data appear separable? Why might logistic regression be a good choice for these data or not?
- (f) Do the data require any preprocessing due to missing values, scale differences, etc? If so, how did you remediate this?

Implement gradient descent and your logistic regression algorithm

- (g) Create a function or class to implement your logistic regression. It should take as inputs the model parameters, $\mathbf{w} = [w_0, w_1, w_2]^T$, and output the class confidence probabilities, $P(Y = y_i | X = \mathbf{x}_i)$.
- (h) Create a function that computes the cost function $C(\mathbf{w})$ for a given dataset and corresponding class labels.
- (i) Create a function or class to run gradient descent on your training data. We'll refer to this as "batch" gradient descent since it takes into account the gradient based on all our data at each iteration (or "epoch") of the algorithm. In doing this we'll need to make some assumptions about and/or experiment with the following:
 1. The initialization of the algorithm - what should you initialize the model parameters to? For this, randomly initialize the weights to a different values between 0 and 1.
 2. The learning rate - how slow/fast should the algorithm proceed in the direction opposite the gradient? This you will experiment with.
 3. Stopping criteria - when should the algorithm be finished searching for the optimum? Set this to be when the cost function changes by no more than 10^{-6} between iterations. Since we have a weight vector, you can compute this by seeing if the L2 norm of the weight vector changes by no more than 10^{-6} between iterations.

Please compute your cost function for a batch as the average cost for the data in your current batch (in this case, a batch is your entire training dataset). In other words, divide your cost by the number of samples in each batch.

(j) Design your approach so that at each step in the gradient descent algorithm it will produce updated parameter estimates. For each set of estimates, calculate the cost function for both the training and the test data (no output is necessary here, but this is used in the following question).

(k) Divide your data into a training and testing set where the test set accounts for 30 percent of the data and the training set the remaining 70 percent. Show the gradient descent process for different learning rates by plotting the resulting cost as a function of each iteration (or "epoch"). What is the impact that each parameter has on the process and the results? What choices did you make in your chosen approach and why? Use the parameter you choose here for the learning rate for the remainder of this question.

Test your model performance through cross validation

(l) Test the performance of your trained classifier using K-folds cross validation (while this can be done manually, the scikit-learn package [StratifiedKFolds](http://scikit-learn.org/stable/modules/generated/sklearn.model_selection.StratifiedKFold.html#sklearn.model_selection.StratifiedKFold) (http://scikit-learn.org/stable/modules/generated/sklearn.model_selection.StratifiedKFold.html#sklearn.model_selection.StratifiedKFold) may be helpful). Produce Receiver Operating Characteristic curves (ROC curves) of your cross validated performance.

(m) Why do we use cross validation?

(n) Make two plots - one of your training data, and one for your test data - with the data scatter-plot and the decision boundary for your classifier. Comment on your decision boundary. Could it be improved?

(o) Compare your trained model to random guessing. Show the ROC curve for your model and plot the chance diagonal. What area under the curve (AUC) does your model achieve? How does your model compare in terms of performance?

ANSWER

(a) What is the likelihood function for all the N samples in our training dataset that we will wish to maximize?

$$l(\mathbf{w}, \mathbf{x}) = \prod_{i=1}^N \sigma(\mathbf{w}^T \mathbf{x})^{y_i} (1 - \sigma(\mathbf{w}^T \mathbf{x}))^{1-y_i}, \text{ where } \sigma(\mathbf{w}^T \mathbf{x}) = \frac{\exp(\mathbf{w}^T \mathbf{x})}{1 + \exp(\mathbf{w}^T \mathbf{x})} = \frac{\exp(w_0 + w_1 x_1 + w_2 x_2)}{1 + \exp(w_0 + w_1 x_1 + w_2 x_2)}$$

(b) Since a logarithm is a monotonic function, maximizing the $f(x)$ is equivalent to maximizing $\ln[f(x)]$. Express part (a) as a cost function of the model parameters, $C(\mathbf{w})$, that is the negative of the logarithm of (a).

$$\begin{aligned} C(\mathbf{w}) &= -\ln(l(\mathbf{w}, \mathbf{x})) \\ &= -\sum_{i=1}^N \ln[\sigma(\mathbf{w}^T \mathbf{x})^{y_i} (1 - \sigma(\mathbf{w}^T \mathbf{x}))^{1-y_i}] \\ &= -\sum_{i=1}^N [y_i \ln \sigma(\mathbf{w}^T \mathbf{x}) + (1 - y_i) \ln(1 - \sigma(\mathbf{w}^T \mathbf{x}))] \\ &= -\sum_{i=1}^N [y_i \mathbf{w}^T \mathbf{x} - \ln(1 + e^{\mathbf{w}^T \mathbf{x}})] \end{aligned}$$

(c) Calculate the gradient of the cost function with respect to the model parameters $\nabla_{\mathbf{w}} C(\mathbf{w})$. Express this in terms of the partial derivatives of the cost function with respect to each of the parameters, e.g.

$$\nabla_{\mathbf{w}} C(\mathbf{w}) = \left[\frac{\partial C}{\partial w_0}, \frac{\partial C}{\partial w_1}, \frac{\partial C}{\partial w_2} \right].$$

$$\begin{aligned}\frac{\partial C}{\partial w_0} &= -\sum_{i=1}^N \left[y_i - \frac{e^{\mathbf{w}^T \mathbf{x}}}{1 + e^{\mathbf{w}^T \mathbf{x}}} \right] x_0 = -\sum_{i=1}^N [y_i - \sigma(\mathbf{w}^T \mathbf{x})] x_0 \\ \frac{\partial C}{\partial w_1} &= -\sum_{i=1}^N \left[y_i - \frac{e^{\mathbf{w}^T \mathbf{x}}}{1 + e^{\mathbf{w}^T \mathbf{x}}} \right] x_1 = -\sum_{i=1}^N [y_i - \sigma(\mathbf{w}^T \mathbf{x})] x_1 \\ \frac{\partial C}{\partial w_2} &= -\sum_{i=1}^N \left[y_i - \frac{e^{\mathbf{w}^T \mathbf{x}}}{1 + e^{\mathbf{w}^T \mathbf{x}}} \right] x_2 = -\sum_{i=1}^N [y_i - \sigma(\mathbf{w}^T \mathbf{x})] x_2\end{aligned}$$

$$\nabla_{\mathbf{w}} C(\mathbf{w}) = \begin{bmatrix} \frac{\partial C}{\partial w_0} \\ \frac{\partial C}{\partial w_1} \\ \frac{\partial C}{\partial w_2} \end{bmatrix} = \begin{bmatrix} -\sum_{i=1}^N [y_i - \sigma(\mathbf{w}^T \mathbf{x})] x_0 \\ -\sum_{i=1}^N [y_i - \sigma(\mathbf{w}^T \mathbf{x})] x_1 \\ -\sum_{i=1}^N [y_i - \sigma(\mathbf{w}^T \mathbf{x})] x_2 \end{bmatrix}$$

(d) Write out the gradient descent update equation, assuming η represents the learning rate.

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \eta \nabla_{\mathbf{w}} C(\mathbf{w}), \text{ where } k \text{ is the step number}$$

...or written out more explicitly:

$$\begin{bmatrix} w_0^{(k+1)} \\ w_1^{(k+1)} \\ w_2^{(k+1)} \end{bmatrix} = \begin{bmatrix} w_0^{(k)} \\ w_1^{(k)} \\ w_2^{(k)} \end{bmatrix} - \eta \begin{bmatrix} -\sum_{i=1}^N [y_i - \sigma(\mathbf{w}^T \mathbf{x})] x_0 \\ -\sum_{i=1}^N [y_i - \sigma(\mathbf{w}^T \mathbf{x})] x_1 \\ -\sum_{i=1}^N [y_i - \sigma(\mathbf{w}^T \mathbf{x})] x_2 \end{bmatrix}$$

(e) Load the data and scatter plot the data by class. In the data folder in the same directory of this notebook, you'll find the data in `A3_Q1_data.csv`. This file contains the binary class labels, y , and the features x_1 and x_2 . Comment on the data: do the data appear separable? Why might logistic regression be a good choice for these data or not?

```
In [7]: # import libraries
import struct
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

# Globally, we'll make the font size larger for increased readability:
%config InlineBackend.figure_format = 'retina' # Optional - best for macs
plt.rcParams.update({'font.size': 15})
```

```

In [8]: df = pd.read_csv('./data/A3_Q1_data.csv') # read data
X = df.values[:, :2]
y = df.values[:, -1]
H0 = X[np.where(y == 0)[0], :] # seperate two classes
H1 = X[np.where(y == 1)[0], :]

# scatter plot the data
plt.figure(figsize=(5, 5))
plt.scatter(H0[:, 0], H0[:, 1], color='b', alpha=0.05, s=2, label='Class 0')
plt.scatter(H1[:, 0], H1[:, 1], color='r', alpha=0.05, s=2, label='Class 1')
plt.xlabel("Feature 1")
plt.ylabel("Feature 2")
plt.title("Scatter Plot of the Data")
lgnd = plt.legend()

# change the marker size manually for both lines
lgnd.legendHandles[0]._sizes = [5]
lgnd.legendHandles[1]._sizes = [5]
plt.axis('equal') # this will be useful for ne
plt.show()

```

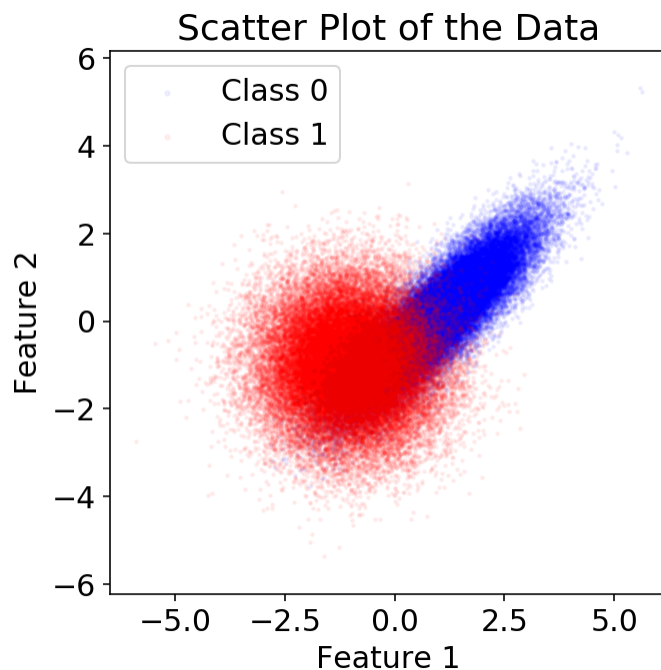


Figure 1: Scatter plot of the two classes of synthetic data

The data do not appear to be separable since almost half of the class 0 values overlap with class 1. However, it does appear that the optimal boundary may be quadratic, but close to linear. Logistic regression may be a good first algorithm to apply to the data, but likely not the optimal model. The data are not separable, so the β

parameters will not go to infinite and thus fail to converge.

(f) Do the data require any preprocessing due to missing values, scale differences, etc? If so, how did you remediate this?

There are no missing values in the data. The feature 1 and feature 2 are in the same scale. Therefore the data does not require any preprocessing.

(g) Create a function or class to implement your logistic regression. It should take as inputs the model parameters, $\mathbf{w} = [w_0, w_1, w_2]$, and output the class confidence probabilities, $P(Y = y_i | X = \mathbf{x}_i)$.

(h) Create a function that computes the cost function $C(\mathbf{w})$ for a given dataset and corresponding class labels.

(i) Create a function or class to run gradient descent on your training data. We'll refer to this as "batch" gradient descent since it takes into account the gradient based on all our data at each iteration (or "epoch") of the algorithm.

```

In [9]: # Logistic regression class
class Logistic_regression(object):
    # Class constructor
    def __init__(self, lr):
        self.learningrate = learningrate    # learning rate
        self.w = None                       # logistic regression weights

    # Method for calculating the sigmoid function
    def sigmoid(self, X):
        sigma = np.exp(X @ self.w)
        return sigma/(1 + sigma)

    # Cost function - calculates the cost/loss/error
    def cost(self, X, y):
        pred = self.sigmoid(X)
        return -(y.T @ np.log(pred) + (1-y).T @ np.log(1 - pred))/X.shape[0]

    # gradient descent
    def gradient_descent(self, X, y):
        delta = self.learningrate * np.sum(X.T @ (self.sigmoid(X) - y))
        self.w -= delta
        return np.linalg.norm(delta)

    # Fit the logistic regression model to the data through gradient descent
    def fit(self, X, y, X_test, y_test, w, thresh, n_iter=500):
        X = np.concatenate([np.ones((X.shape[0], 1)), X], axis=1)
        X_test = np.concatenate([np.ones((X_test.shape[0], 1)), X_test], axis=1)
        self.w = w
        self.loss = [self.cost(X, y)]
        self.loss_test = [self.cost(X_test, y_test)]
        for i in range(n_iter):
            delta = self.gradient_descent(X, y)
            self.loss.append(self.cost(X, y))
            self.loss_test.append(self.cost(X_test, y_test))
            if delta <= thresh:
                break

    # Use the trained model to make predictions
    def pred(self, X):
        X = np.concatenate([np.ones((X.shape[0], 1)), X], axis=1)
        return self.sigmoid(X)

    # Compute the linear decision boundary in the two dimensional case
    def decision_boundary(self, X):
        return -(self.w[0] + self.w[1] * X)/self.w[2]

```

Divide your data into a training and testing set where the test set accounts for 30 percent of the data and the test set the remaining 70 percent. In doing this we'll need to make some assumptions / experiment with the following:

1. The initialization of the algorithm - what should you initialize the model parameters to? For this, randomly initialize the weights to a different values between 0 and 1.
2. The learning rate - how slow/fast should the algorithm proceed in the direction opposite the gradient? This you will experiment with.
3. Stopping criteria - when should the algorithm be finished searching for the optimum? Set this to be when the cost function changes by no more than 10^{-6} between iterations. Since we have a weight vector, you can compute this by seeing if the L2 norm of the weight vector changes by no more than 10^{-6} between iterations.

Please compute your cost function for a batch as the average cost for the data in your current batch (in this case, a batch is your entire training dataset). In other words, divide your cost by the number of samples in each batch.

(j) At each step in the gradient descent algorithm it will produce updated parameter estimates. For each set of estimates, calculate the cost function for both the training and the test data (no output is necessary here, but this is used in the following question).

Answer included following item (k)

(k) Divide your data into a training and testing set where the test set accounts for 30 percent of the data and the training set the remaining 70 percent. Show the gradient descent process for different learning rates by plotting the resulting cost as a function of each iteration (or "epoch"). What is the impact that each parameter has on the process and the results? What choices did you make in your chosen approach and why? Use the parameter you choose here for the learning rate for the remainder of this question.


```
In [10]: # divide the data into training and test datasets
n_sample = X.shape[0]
n_train = int(n_sample * 0.7)
X_train = X[:n_train, :]
y_train = y[:n_train]
X_test = X[n_train:, :]
y_test = y[n_train:]

# Compare the model cost/loss/error for different weight initializations and learning rates
color = ['#ca0020', '#f4a582', '#92c5de', '#0571b0']
plt.figure(figsize=(10, 5))
for (index, i) in enumerate(range(5, 9)):
    learningrate = 1/np.power(10, i)
    w = np.random.rand(X.shape[1]+1) # Initialize the weights randomly
    clf = Logistic_regression(learningrate)
    clf.fit(X_train, y_train, X_test, y_test, w, 1e-6, n_iter=100)
    plt.plot(clf.loss, '-',
             label='LR={ } Cost={:.2f} (train)'.format(learningrate, clf.loss[-1]),
             color=color[index])
    plt.plot(clf.loss_test, 'o',
             label='LR={ } Cost={:.2f} (test)'.format(learningrate, clf.loss_test[-1]),
             color=color[index])
plt.xlabel('Epoch')
plt.ylabel('Cost / Loss / Error')
plt.title('Learn Rate Comparison with Weights Initilized Randomly')
plt.legend(loc='center left', bbox_to_anchor=(1, 0.5))
plt.axis([0, 100, 0, 2.1])
plt.grid('on')
plt.tight_layout()
plt.show()
```

Learn Rate Comparison with Weights Initilized Randomly

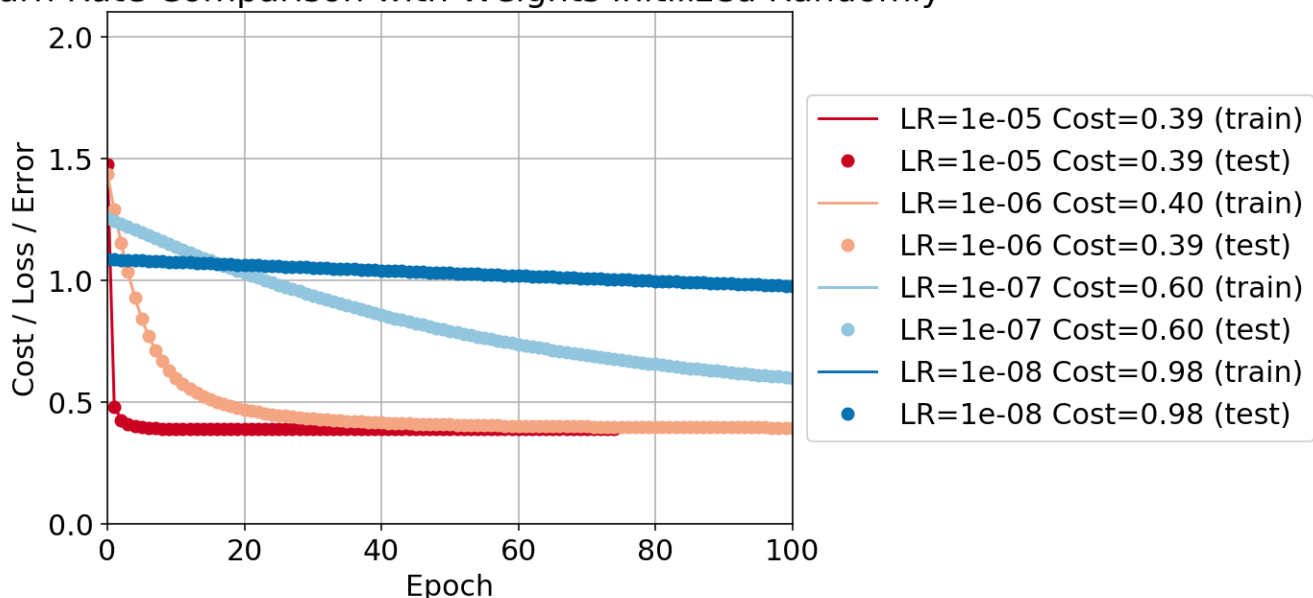


Figure 2: Comparison of the stochastic gradient descent model fitting process using random weight initialization and varying the learning rate. The legend includes the learning rate that resulted in that particular curve and the lowest cost achieved by the algorithm.

As shown in Figure 2, the algorithm was tested using random initialization of \mathbf{w} and plotted the results. In this plot, 4 different learning rates were tested, ranging from 10^{-5} to 10^{-8} . The training cost curves are plotted in solid lines and test cost curves are plotted in dashed lines. The stopping criteria was chosen so that the fitting process (SGD) either reaches the maximum number of epochs (which was set to 100 by default) or converges

such that the norm of weights is smaller than $1e-5$. This stopping criteria is a common choice in many implementations of SGD in the literature. It is reasonable to stop the gradient descent process when there's only minor updates in \mathbf{w} as it's unlikely to change significantly in the future. The final costs are also provided in legend of each plot.

Learning rates: The learning rates affect the convergence speed significantly. When $\eta = 10^{-5}$, the algorithm converges less than 10 epochs, but yields the lowest cost in both the training and testing data with a slower learning rate of $\eta = 10^{-6}$.

(I) Test the performance of your trained classifier using K-folds cross validation (while this can be done manually, the scikit-learn package [StratifiedKFolds](http://scikit-learn.org/stable/modules/generated/sklearn.model_selection.StratifiedKFold.html#sklearn.model_selection.StratifiedKFold) (http://scikit-learn.org/stable/modules/generated/sklearn.model_selection.StratifiedKFold.html#sklearn.model_selection.StratifiedKFold) may be helpful). Produce Receiver Operating Characteristic Curves (ROC curves) of your cross validated performance.

```
In [11]: # do 5 folds cross validation
pred_rf = []

from sklearn.model_selection import KFold
kf = KFold(n_splits=5)
for cnt, (train_idx, test_idx) in enumerate(kf.split(X)):
    print('Training on fold {}'.format(cnt+1))
    X_train, X_test = X[train_idx, :], X[test_idx, :]
    y_train, y_test = y[train_idx], y[test_idx]
    clf = LogisticRegression(1e-6)
    w = np.ones(X.shape[1]+1)
    clf.fit(X_train, y_train, X_test, y_test, w, 1e-6, n_iter=100)
    pred_rf.append(-clf.predict(X_test))
pred_rf = np.concatenate(pred_rf)
```

```
Training on fold 1
Training on fold 2
Training on fold 3
Training on fold 4
Training on fold 5
```

```
In [12]: # plot ROC curve
from sklearn.metrics import roc_curve, auc
plt.figure(figsize=(8, 6))
fpr_rf, tpr_rf, _ = roc_curve(y, pred_rf)
plt.plot(fpr_rf, tpr_rf, label='AUC = {:.2f}'.format(auc(fpr_rf, tpr_rf)))
plt.plot([0, 1], [0, 1], color='grey', lw=2, linestyle='--')
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Comparison')
plt.legend(loc="lower right")
plt.show()
```

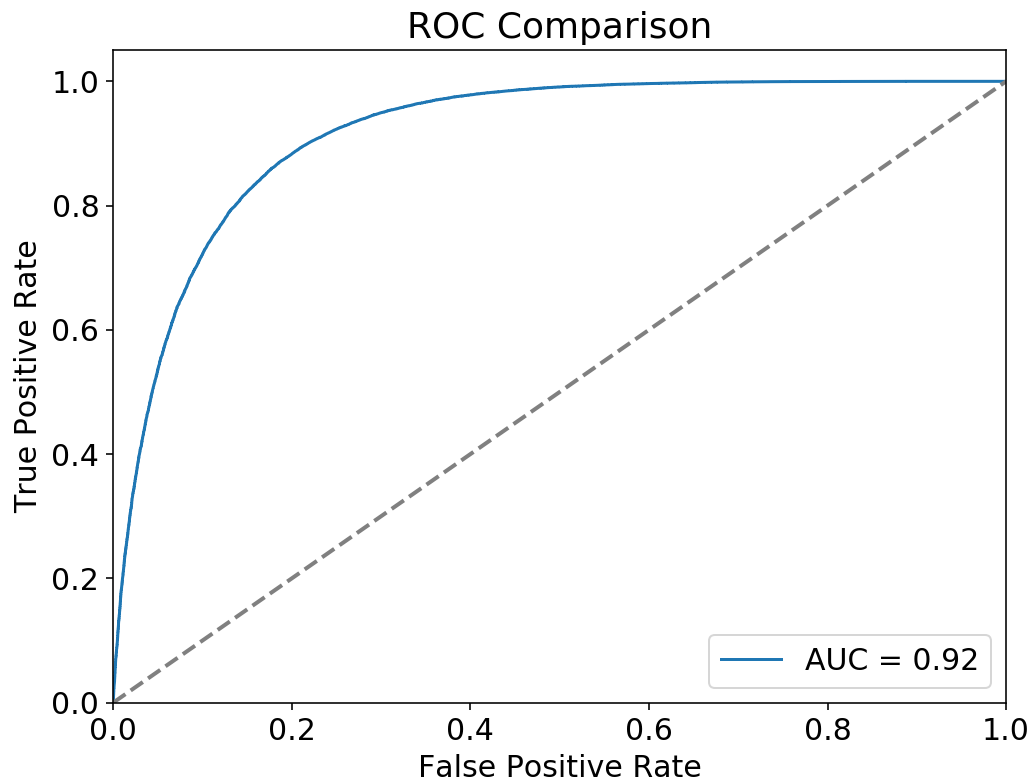


Figure 3: ROC curve demonstrating the logistic regression classifier performance

The result has a high AUC of 0.92 and results in a smooth ROC curve since there are many normally-distributed points in the training sample.

(m) Why do we use cross validation?

Cross validation makes it possible to test the performance of the classifier on unseen data and this enables us to evaluate model generalization performance. Additionally, k-folds cross validation also makes an efficient use of data, which is extremely important when our dataset may be limited.

(n) Make two plots - one of your training data, and one for your test data - with the data scatterplotted and the decision boundary for your classifier. Comment on your decision boundary. Could it be improved?

```

In [13]: # Scatter plot the training data data
x_range = np.array([-6, 6])
plt.figure(figsize=(14, 6))
plt.subplot(121)
plt.scatter(X_train[np.where(y_train==0)], 0], X_train[np.where(y_train==0), 1],
            color='b',
            alpha=0.1,
            s=2,
            label='Class 0')
plt.scatter(X_train[np.where(y_train==1), 0], X_train[np.where(y_train==1), 1],
            color='r',
            alpha=0.1,
            s=2,
            label='Class 1')
plt.plot(x_range, clf.decision_boundary(x_range), 'k-', label='Decision Boundary')
plt.xlabel("Feature 1")
plt.ylabel("Feature 2")
plt.title("Scatter Plot of the Training Data")
lgnd = plt.legend()

# Scatter plot the test data
plt.xlim([-5, 5])
plt.ylim([-5, 5])
plt.subplot(122)
plt.scatter(X_test[np.where(y_test==0)], 0], X_test[np.where(y_test==0), 1],
            color='b',
            alpha=0.1,
            s=2,
            label='Class 0')
plt.scatter(X_test[np.where(y_test==1), 0], X_test[np.where(y_test==1), 1],
            color='r',
            alpha=0.1,
            s=2,
            label='Class 1')
plt.plot(x_range, clf.decision_boundary(x_range), 'k-', label='Decision Boundary')
plt.xlabel("Feature 1")
plt.ylabel("Feature 2")
plt.title("Scatter Plot of the Test Data")
lgnd = plt.legend()
plt.axis([-5, 5, -5, 5])
plt.show()

```

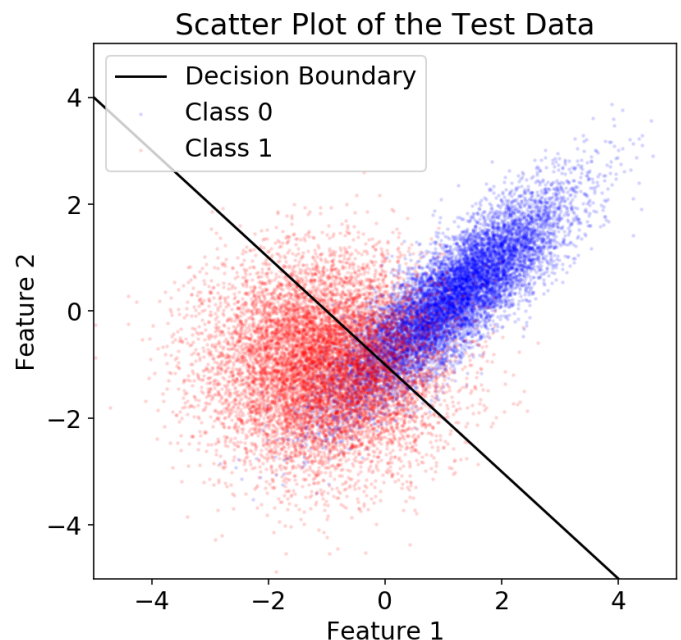
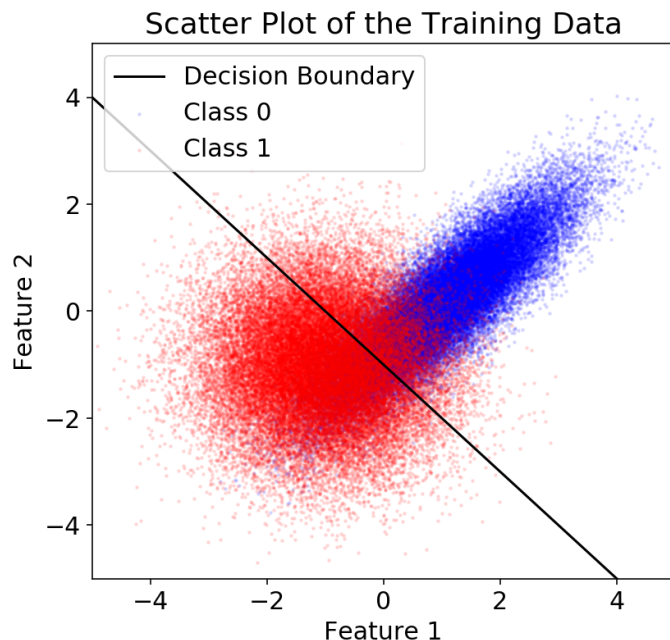


Figure 4: Scatter plots of the training and test datasets along with the logistic regression decision boundary

The decision boundary is almost perpendicular to the direction of greatest variance of class 0. Given the fact that the two classes in this dataset have a large overlapping region, the decision boundary is can be considered reasonable. To improve the the classifier, one simple way is to improve the flexibility of the model to enable the decision boundary to be quadratic or at least have a highly regularized non-linear decision boundary.

(o) Compare your trained model to random guessing. Show the ROC curve for your model and plot the chance diagonal. What area under the curve (AUC) does your model achieve? How does your model compare in terms of performance?

```
In [14]: from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import KFold

# Initialize variable for storing the predictions
pred_lr = [] # Logistic regression
pred_rand = pred_rand = np.random.randint(2, size=n_sample)

# Compute 5 folds cross validated performance comparison for logistic regression,
# linear regression, and random guessing

kf = KFold(n_splits=5)
for cnt, (train_idx, test_idx) in enumerate(kf.split(X)):
    print('Training on fold {}'.format(cnt+1))
    X_train, X_test = X[train_idx, :], X[test_idx, :]
    y_train, y_test = y[train_idx], y[test_idx]

    # Logistic regression (from the function we created)
    clf = Logistic_regression(1e-6)
    w = np.zeros(X.shape[1]+1)
    clf.fit(X_train, y_train, X_test, y_test, w, 1e-5, n_iter=100)
    pred_lr.append(clf.pred(X_test))

# Store the results
pred_lr = np.concatenate(pred_lr)
```

```
Training on fold 1
Training on fold 2
Training on fold 3
Training on fold 4
Training on fold 5
```

```

In [15]: the ROC curves
figure(figsize=(8, 6))

compute the TPR and FPR for each set of predictions
fpr_lr, tpr_lr, _ = roc_curve(y, pred_lr)
fpr_rand, tpr_rand, _ = roc_curve(y, pred_rand)

plot those rates in the form of the ROC curves
plt.plot(fpr_lr, tpr_lr, label='Logistic Regression (AUC = {:.2f})'.format(auc(fpr_lr, tpr_lr)))
plt.plot(fpr_rand, tpr_rand, label='Chance (AUC = {:.2f})'.format(auc(fpr_rand, tpr_rand)))
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Comparison')
plt.legend(loc="lower right")
plt.show()

```

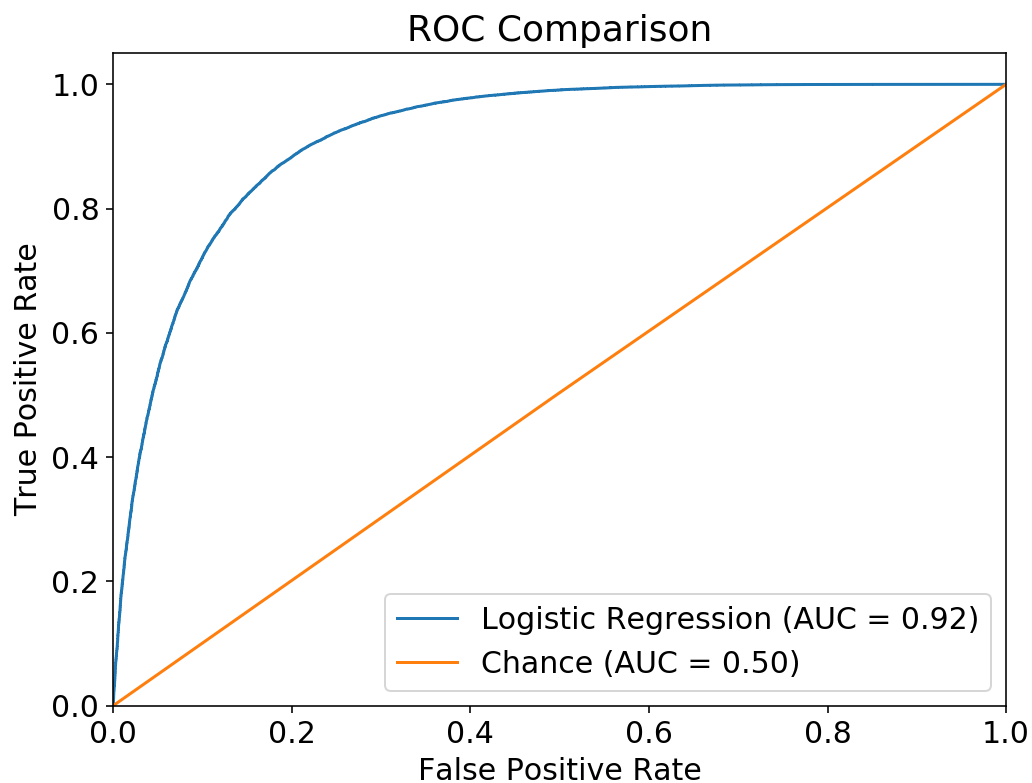


Figure 5: ROC curves for logistic regression, linear regression, and random guessing

From the ROC curves, we can see that random guess has an AUC of 0.5. It is the worst case for a classifier, where you are just flipping a coin. Logistic Regression and Linear Regression has similar performance, but Linear Regression does slightly better for this particular case with normally distributed data.

2

[20 points] Digits classification

(a) Construct your dataset from the [MNIST dataset \(http://yann.lecun.com/exdb/mnist/\)](http://yann.lecun.com/exdb/mnist/) of handwritten digits, which has a training set of 60,000 examples, and a test set of 10,000 examples. The digits have been size-normalized and centered in a fixed-size image.

Your goal is to determine whether or not an example is a 3, therefore your binary classifier will seek to estimate $y = 1$ if the digit is a 3, and $y = 0$ otherwise. Create your dataset by transforming your labels into a binary format.

(b) Plot 10 examples of each class (i.e. class $y = 0$, which are not 3's and class $y = 1$ which are 3's), from the training dataset.

(c) How many examples are present in each class? Show a histogram of samples by class. Are the classes balanced? What issues might this cause?

(d) Using cross-validation, train and test a classifier. Compare your performance against (1) a classifier that randomly guesses the class, and (2) a classifier that guesses that all examples are NOT 3's. Plot corresponding ROC curves and precision-recall curves. Describe the algorithm's performance and explain any discrepancies you find.

(f) Using a logistic regression classifier (a linear classifier), apply lasso regularization and retrain the model and evaluate its performance over a range of values on the regularization coefficient. You can implement this using the [LogisticRegression \(http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html\)](http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html) module (DO NOT use your function from question 1) and activating the 'l1' penalty; the parameter C is the inverse of the regularization strength. As you vary the regularization coefficient, plot (1) the number of model parameters that are estimated to be nonzero; (2) the logistic regression cost function, which you created a function to evaluate in the Question 1; (3) F_1 -score, and (4) area under the curve (AUC). Describe the implications of your findings.

ANSWER

(a) Construct your dataset from the [MNIST dataset \(http://yann.lecun.com/exdb/mnist/\)](http://yann.lecun.com/exdb/mnist/) of handwritten digits, which has a training set of 60,000 examples, and a test set of 10,000 examples. The digits have been size-normalized and centered in a fixed-size image.

Your goal is to determine whether or not an example is a 3, therefore your binary classifier will seek to estimate $y = 1$ if the digit is a 3, and $y = 0$ otherwise. Create your dataset by transforming your labels into a binary format.

In [16]:

o <https://gist.github.com/akesling/5358964> for a great example for reading MNIST data

ou will need to have the MNIST data downloaded to: './data/MNIST/'
r for this section of code to work properly

```
def load_ds(dataset = "training", path = "./data/MNIST/"):
    """
    A helper function for importing the MNIST data set. It returns an iterator
    over 2-tuples with the first element being the label and the second element
    being a numpy.uint8 2D array of pixel data for the given image.
    """
    if dataset is "training":
        fname_img = path + 'train-images.idx3-ubyte'
        fname_lbl = path + 'train-labels.idx1-ubyte'
    elif dataset is "testing":
        fname_img = path + 't10k-images.idx3-ubyte'
        fname_lbl = path + 't10k-labels.idx1-ubyte'
    else:
        raise ValueError("dataset must be 'testing' or 'training'")

    # Load everything in some numpy arrays
    with open(fname_lbl, 'rb') as flbl:
        magic, num = struct.unpack(">II", flbl.read(8))
        lbl = np.fromfile(flbl, dtype=np.int8)

    # Linearize the label array
    [np.where(lbl != 3)] = 0
    lbl = lbl/3

    with open(fname_img, 'rb') as fimg:
        magic, num, rows, cols = struct.unpack(">IIII", fimg.read(16))
        img = np.fromfile(fimg, dtype=np.uint8).reshape(len(lbl), rows, cols)

    return lbl, img
```

(b) Plot 10 examples of each class 0 and 1, from the training dataset.

```
In [17]: # load image and label data
lbl, img = read_ds('training')
h1_idx = np.where(lbl == 1)[0]
h0_idx = np.where(lbl == 0)[0]

# plot 10 samples
n_sample = 10
h1_idx_sample = np.random.choice(h1_idx, n_sample)
h0_idx_sample = np.random.choice(h0_idx, n_sample)
plt.figure(figsize=(14, 3))
for cnt, (h1, h0) in enumerate(zip(h1_idx_sample, h0_idx_sample)):
    plt.subplot(2, 10, 1+cnt)
    plt.imshow(img[h1, :, :], cmap='binary')
    plt.axis('off')
    plt.subplot(2, 10, 11+cnt)
    plt.imshow(img[h0, :, :], cmap='binary')
    plt.axis('off')
plt.show()
```

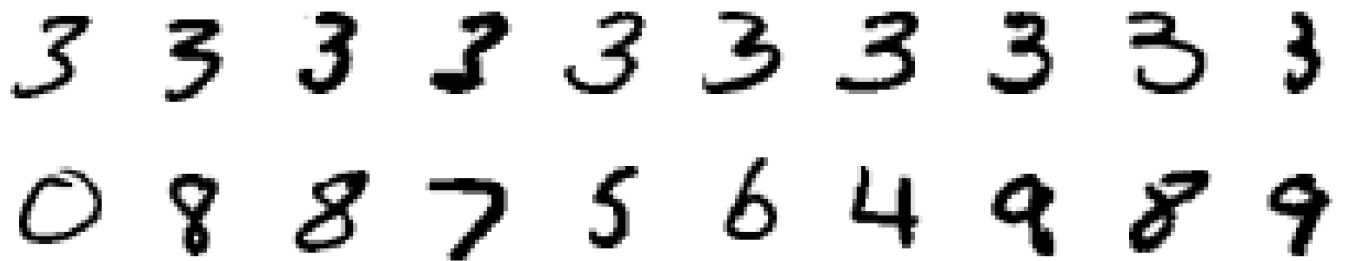


Figure 6: Example digits. The first row represents samples from class 1 (threes) the second row contains examples of class 0 (other digits)

(c) How many examples are present in each class? Show a histogram of samples by class. Are the classes balanced? What issues might this cause?

```
In [18]: plt.figure(figsize=(8, 5))
#plt.hist(lbl, align='mid')
hist = np.histogram(lbl, bins=2)
plt.bar(np.array([0,1]),hist[0])
plt.xlabel('Class')
plt.ylabel('Number of Samples')
plt.xticks([0,1])
plt.show()
```

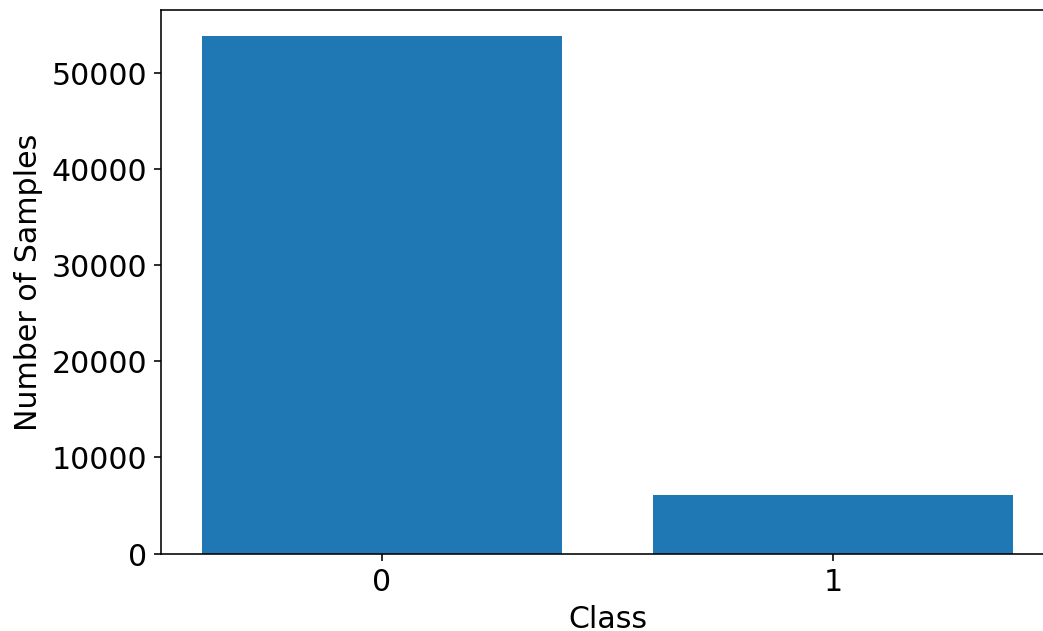


Figure 7: Histogram of the two classes demonstrating the imbalance between the classes

```
In [17]: print('{} examples in H1, {} examples in H0'.format(len(h1_idx), len(h0_idx)))
6131 examples in H1, 53869 examples in H0
```

There are 6131 examples in H1 and 53869 examples in H0 and so the classes are heavily imbalanced. This may cause the overall classification accuracy to be heavily dominated by the performance on one class. For example, a classifier that only predicts class 0 will be accurate 90 percent of the time. The classifier trained from imbalanced dataset will, therefore, tend to have higher missed detection rates for the under represented class.

(d) Using cross-validation, train and test a classifier. Compare your performance against (1) a classifier that randomly guesses the class, and (2) a classifier that guesses that all examples are NOT 3's. Plot corresponding ROC curves and precision-recall curves. Describe the algorithm's performance and explain any discrepancies you find.

```

In [19]: arn.ensemble import RandomForestClassifier
arn.decomposition import PCA
arn.model_selection import KFold

# We'll explore using a random forest classifier in conjunction with PCA
# THIS CODE SEGMENT MAY TAKE SOME TIME TO COMPUTE
m = img.shape[0]
n = []

# folds cross validation
kf = KFold(n_splits=5)

# the image data for processing
img_flat = np.reshape(img, (img.shape[0], -1))

# 1) Perform PCA to reduce the data to a lower dimensional space for improved performance
pca = PCA(n_components=3)
img_flat = pca.fit_transform(img_flat)
# Reduced feature dimension to 3

# cross-validated performance assessment
for (train_idx, test_idx) in enumerate(kf.split(img_flat)):
    print('Training on fold {}'.format(cnt+1))
    X_train, X_test = img_flat[train_idx, :], img_flat[test_idx, :]
    y_train, y_test = lbl[train_idx], lbl[test_idx]
    clf = RandomForestClassifier(n_estimators = 5000)
    clf.fit(X_train, y_train)
    rf.append(clf.predict_proba(X_test))
    pred_rf = np.concatenate(pred_rf)

```

```

Reduced feature dimension to 3
Training on fold 1
Training on fold 2
Training on fold 3
Training on fold 4
Training on fold 5

```

```
In [20]: from sklearn.metrics import roc_curve, auc, precision_recall_curve

pred_rand = np.random.randint(2, size=sample_num) # Randomly guess a class
pred_h0    = np.zeros(sample_num)                # Always predict zeros

# Compute the ROC curve data
fpr_rf, tpr_rf, _ = roc_curve(lbl, pred_rf[:, 1])
fpr_rand, tpr_rand, _ = roc_curve(lbl, pred_rand)
fpr_h0, tpr_h0, th = roc_curve(lbl, pred_h0)

# Plot the ROC curves
plt.figure(figsize=(14, 6))
plt.subplot(121)
plt.plot(fpr_rf, tpr_rf, label='Random Forest (AUC = {:.2f})'.format(auc(fpr_rf, tpr_rf)))
plt.plot(fpr_h0, tpr_h0, label='Always predict 0 (AUC = {:.2f})'.format(auc(fpr_h0, tpr_h0)))
plt.plot(fpr_rand, tpr_rand, 'k--', label='Random (AUC = {:.2f})'.format(auc(fpr_rand, tpr_rand)))
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Comparison')
plt.legend(loc="lower right")

# Compute the precision Recall curve data
p_rf, r_rf, _ = precision_recall_curve(lbl, pred_rf[:, 1])
p_h0, r_h0, th = precision_recall_curve(lbl, pred_h0)
p_rand, r_rand, _ = precision_recall_curve(lbl, pred_rand)

# Plot the PR curves
plt.subplot(122)
plt.plot(r_rf, p_rf, label='Random Forest')
plt.plot(r_h0, p_h0, label='Always predict 0')
plt.plot(r_rand, p_rand, 'k--', label='Random')
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('Recall')
plt.ylabel('Precision')
plt.title('PR Comparison')
plt.legend(loc="upper right")
plt.show()
```

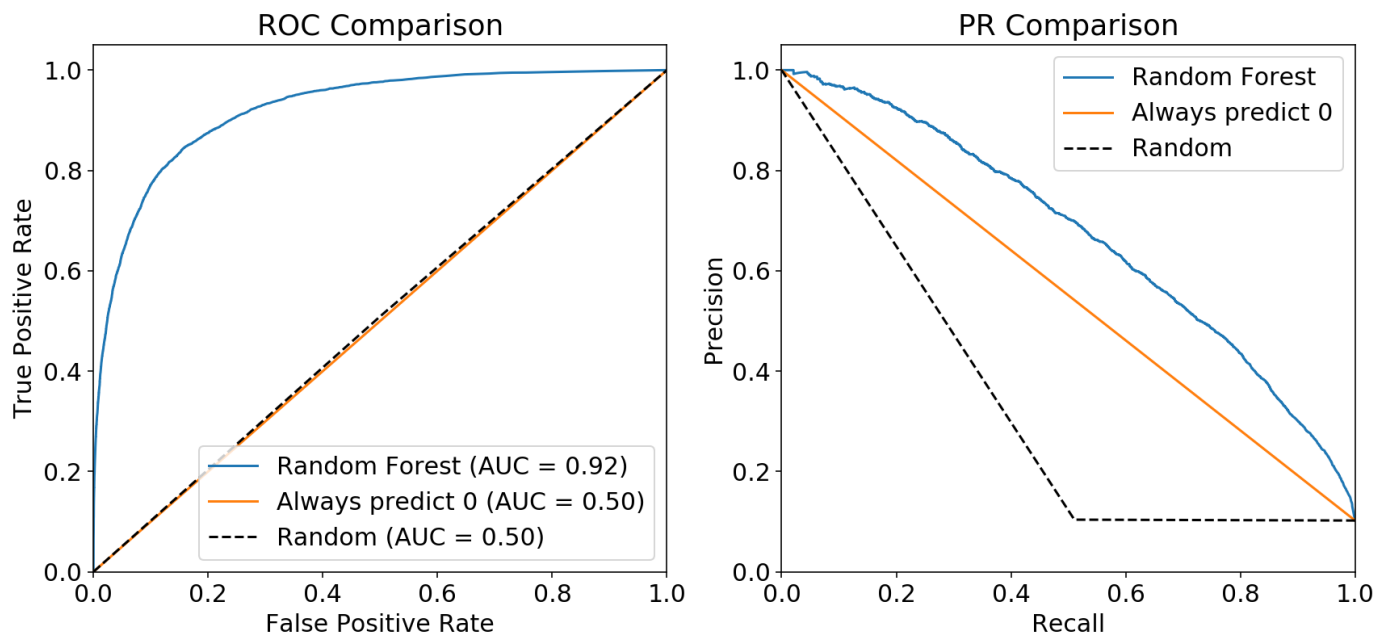


Figure 8: ROC and PR curves for the digits data comparing a random forest classifier to a classifier that always predicts class 0, and to random chance

In the ROC plot shown above, Random Forest yields the best results overall, with an AUC of 0.92 while random guessing or the " H_0 classifier since it always guesses the null hypothesis). Both random guessing and the H_0 classifier have AUCs around 0.5. For the PR curves, it is clear that Random Forest performs better than the H_0 classifier, which is always better than random guessing. Random guessing is the worst case so it has worst performance in both metrics. For the H_0 classifier, due to the imbalance of the data, the Precision-Recall curve is better than random guessing because there are more examples of class zero than class one in the data.

(f) Using a logistic regression classifier (a linear classifier), apply lasso regularization and retrain the model and evaluate its performance over a range of values on the regularization coefficient. You can implement this using the [LogisticRegression \(http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html\)](http://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html) module (DO NOT use your function from question 1) and activating the 'l1' penalty; the parameter C is the inverse of the regularization strength. As you vary the regularization coefficient, plot (1) the number of model parameters that are estimated to be nonzero; (2) the logistic regression cost function, which you created a function to evaluate in the Question 1; (3) F_1 -score, and (4) area under the curve (AUC). Describe the implications of your findings.

```
In [20]: from sklearn.linear_model import LogisticRegression

# Define a helper function for our logistic regression classifier with the $L_1$ per
def lr_clf(c, X_train, y_train, X_test, penalty='l1'):
    lr = LogisticRegression(penalty=penalty, C=c)
    lr.fit(X_train, y_train)
    return lr.predict_proba(X_test)[:, 1], lr.coef_
```

Due to computational constraints we will hold out 30% of data for testing in this problem.

```
In [21]: from sklearn.model_selection import train_test_split
from sklearn.metrics import log_loss, f1_score
from sklearn.metrics import roc_curve, auc

img_flat = np.reshape(img, (img.shape[0], -1))
X_train, X_test, y_train, y_test = train_test_split(img_flat, lbl, test_size=0.3)
np.random.seed(1234)

non_zero = []
lr_cost = []
f1 = []
AUC = []
c_array = np.arange(0.1, 1, 0.1)
c_array = np.logspace(-4, 0, 10)

# Iterate over the regularization coefficient, C
for c in c_array:
    pred, params = lr_clf(c, X_train, y_train, X_test)

    # number of non-zero params
    non_zero.append(np.sum(params != 0))

    # logistic regression cost function
    lr_cost.append(log_loss(y_true=y_test, y_pred=pred))

    # f1 score
    f1.append(f1_score(y_true=y_test, y_pred=pred>0.5))

    # AUC
    fpr, tpr, _ = roc_curve(y_test, pred)
    AUC.append(auc(fpr, tpr))
```

```
In [28]: # Number of nonzero parameters
plt.figure(figsize=(13, 8))
plt.subplot(221)
plt.plot(c_array, non_zero, marker='.')
plt.grid(True)
plt.xticks(c_array, c_array)
plt.xlabel('C')
plt.ylabel('Non-zero Params')
plt.xscale('log')

# Logistic regression cost
plt.subplot(222)
plt.plot(c_array, lr_cost, marker='.')
plt.grid(True)
plt.xticks(c_array, c_array)
plt.xlabel('C')
plt.ylabel('Cost')
plt.xscale('log')

# F1 Score
plt.subplot(223)
plt.plot(c_array, f1, marker='.')
plt.grid(True)
plt.xticks(c_array, c_array)
plt.xlabel('C')
plt.ylabel('F1 Score')
plt.xscale('log')

# Area under the ROC curve (AUC)
plt.subplot(224)
plt.plot(c_array, AUC, marker='.')
plt.grid(True)
plt.xticks(c_array, c_array)
plt.xlabel('C')
plt.ylabel('AUC')
plt.tight_layout()
plt.xscale('log')
plt.show()
```

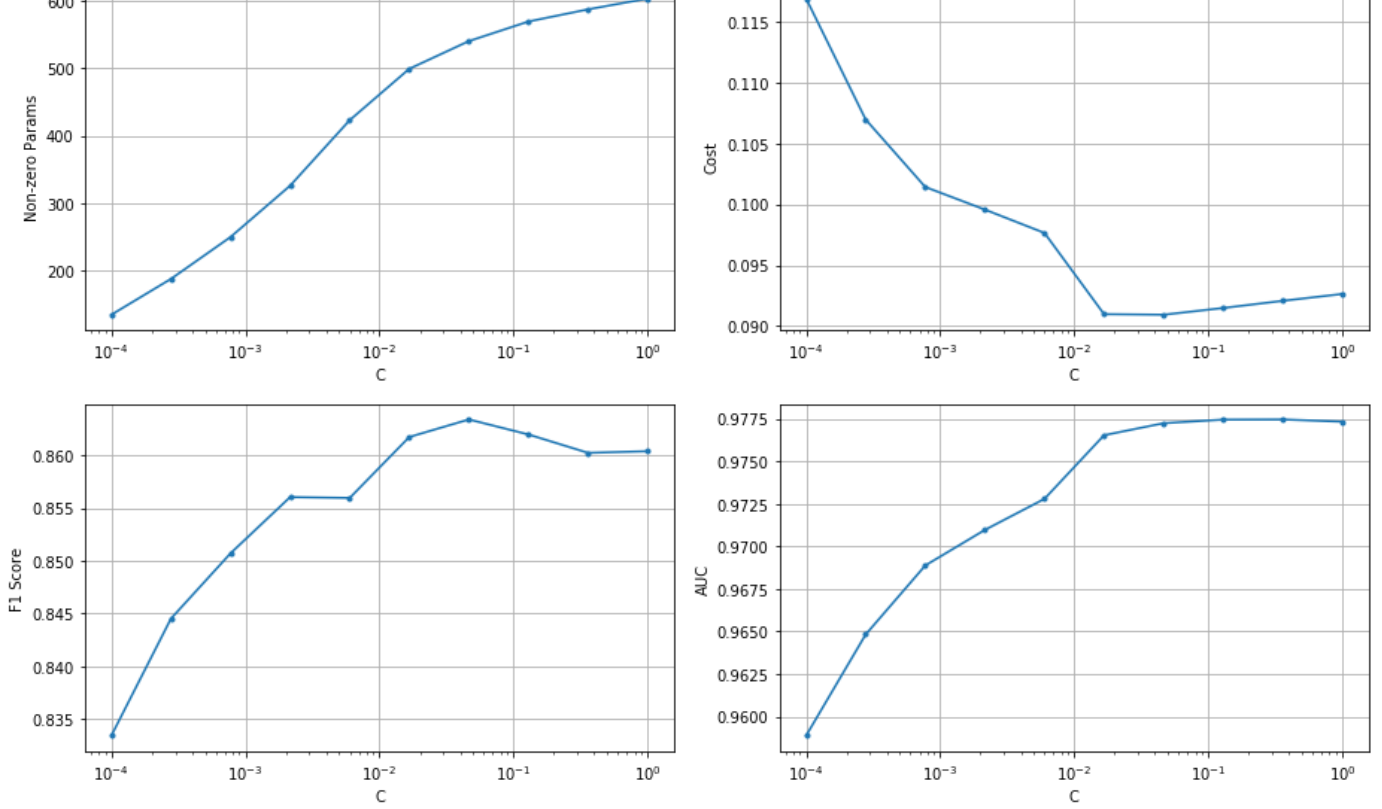



Figure 9: A comparison of the number of nonzero parameters, cost (or loss), F_1 score, and ROC area under the curve (AUC) for the logistic regression classifier on the MNIST data as the inverse of the L_1 regularization parameter, C , varies.

The parameter C (which corresponds to increased model flexibility) is varied from a very small amount (10^{-4}) to 1. We see that the cost begins high when the system is overly regularized, but decreases to a minimum value around $C \simeq 0.02$ after which the cost begins to rise again. We see similar optima for the F_1 score and the area under the ROC curve indicating that $C \simeq 0.02$ corresponds to the best operating point for generalization performance. At the same time, the number of non-zero parameters increase as C is increased, since the penalty on the number of predictors is loosened as C increases.

3

[10 points] Comparing the Bayes' decision rule with logistic regression

The phrase "Bayes' decision rule" is often used to describe a classifier decision rule that minimizes misclassification rate (equally penalizing false positives and false negatives). In this exercise you will first determine the Bayes's decision rule for a binary classification problem where you know the likelihood of data from each class. The binary classification problem has two classes with data distributed as exponential random variables:

$$P(x|C_i) = \lambda_i e^{-\lambda_i x}$$

Where C_i represents the class from which the sample is drawn (0 or 1). We also know that $\lambda_0 = 1$ and $\lambda_1 = 5$.

(a) Plot the probability of each class conditional distribution (e.g. likelihood function), $P(x|C_0)$ and $P(x|C_1)$ on the sample plot in the domain $x \in [0, 2]$. You can use [scipy's expon module](https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.expon.html#scipy.stats.expon) (<https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.expon.html#scipy.stats.expon>) for this. Note that the `scale` parameter for this module is defined as $1/\lambda$.

(b) Assuming the prior class distributions are $P(C_0) = P(C_1) = 0.5$, determine the Bayes' decision rule using the information above including the posterior distributions and the prior distributions. You will assign the most probable class to the data based on the value of x . The decision rule will be of the form:

If $x > x^*$, then predict Class 0, otherwise predict Class 1

Determine the value x^* that minimizes misclassification (equally penalizing false positives and false negatives, and no penalty/reward for correct detections). Show your work in deriving this value.

(c) How does your answer in (b) relate to the the plot you made in (a)? Why?

(d) Load the test data in the file `A3_Q3_test.csv`. Apply your decision rule to the data. What is the misclassification rate (error rate, or fraction of misclassified samples) of this decision rule?

(e) Load the training data in the file `A3_Q3_train.csv` and train a logistic regression classifier on the data (using default parameters). What is your misclassification error for your test dataset? How does this compare with the Bayes' classifier?

(f) What is your decision rule for your logistic regression model? To compute this, extract the parameters from your fit model (look for the `coef_` and `intercept_` attributes) and since the classes are balanced, the decision rule will be to classify a sample x as Class 1 when your logistic regression sigmoid is greater than 0.5 (the halfway point from the two extremes of 0 and 1). How does this compare with the Bayes' classifier?

(g) If the prior probabilities were not $P(C_0) = P(C_1) = 0.5$, but instead if $P(C_1) > P(C_0)$. How would this impact the optimal decision rule? Would it change, if so, would x^* be larger or smaller?

ANSWER

(a) Plot the probability of each class conditional distribution (e.g. likelihood function), $P(x|C_0)$ and $P(x|C_1)$ on the sample plot in the domain $x \in [0, 2]$. You can use [scipy's `expon` module](https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.expon.html#scipy.stats.expon) (<https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.expon.html#scipy.stats.expon>) for this. Note that the `scale` parameter for this module is defined as $1/\lambda$.

```

In [5]: import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import expon

x = np.linspace(0,2,1001)

lambda0 = 1
lambda1 = 5

scale0 = 1/lambda0
scale1 = 1/lambda1

distribution0 = expon.pdf(x, scale=scale0)
distribution1 = expon.pdf(x, scale=scale1)

plt.plot(x,distribution0,'r', label='Class 0')
plt.plot(x,distribution1,'b', label='Class 1')
plt.legend()
plt.xlabel('$x$')
plt.ylabel('$P(x|C_i)$')

```

Out[5]: Text(0, 0.5, '\$P(x|C_i)\$')

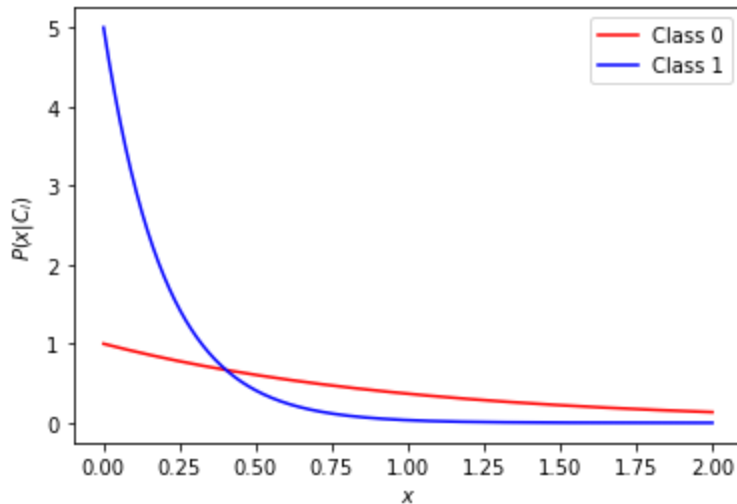


Figure 10: A comparison of the class conditional probability density functions for Class 0 and Class 1

(b) Assuming the prior class distributions are $P(C_0) = P(C_1) = 0.5$, determine the Bayes' decision rule using the information above including the posterior distributions and the prior distributions. You will assign the most probable class to the data based on the value of x . The decision rule will be of the form:

If $x > x^*$, then predict Class 1, otherwise predict Class 0

Determine the value x^* that minimizes misclassification (equally penalizing false positives and false negatives, and no penalty/reward for correct detections). Show your work in deriving this value.

We start with the decision rule: if $P(C_1|x) > P(C_0|x)$, then predict Class 1. Otherwise, predict Class 0. Another way of stating that inequality is:

$$\frac{P(C_1|x)}{P(C_0|x)} > 1$$

Using Bayes' rule, we know that:

$$P(C_i|x) = \frac{P(x|C_i)P(C_i)}{P(x)}$$

Plugging this in for each class yields:

$$\frac{P(C_1|x)}{P(C_0|x)} = \frac{\frac{P(x|C_1)P(C_1)}{P(x)}}{\frac{P(x|C_0)P(C_0)}{P(x)}} = \frac{P(x|C_1)}{P(x|C_0)}$$

The above simplifies since $P(C_0) = P(C_1) = 0.5$. Now we can plug in the probability density functions and solve for x :

$$\begin{aligned} \frac{P(x|C_1)}{P(x|C_0)} &> 1 \\ \frac{\lambda_1 \exp(-\lambda_1 x)}{\lambda_0 \exp(-\lambda_0 x)} &> 1 \\ \exp(-\lambda_1 x + \lambda_0 x) &> \frac{\lambda_0}{\lambda_1} \\ -\lambda_1 x + \lambda_0 x &> \ln\left(\frac{\lambda_0}{\lambda_1}\right) \\ (\lambda_0 - \lambda_1)x &> \ln\left(\frac{\lambda_0}{\lambda_1}\right) \\ x &< \frac{\ln\left(\frac{\lambda_0}{\lambda_1}\right)}{\lambda_0 - \lambda_1} \\ x &< \frac{\ln(\lambda_0) - \ln(\lambda_1)}{\lambda_0 - \lambda_1} \end{aligned}$$

Note that we had to flip the direction of the greater than sign when we divided by $\lambda_0 - \lambda_1$ since that value is negative. Using $\lambda_0 = 1$ and $\lambda_1 = 5$, we arrive at our answer:

$$x^* = \frac{\ln(1) - \ln(5)}{1 - 5} = \frac{0 - \ln(5)}{-4} = \frac{\ln(5)}{4} = \frac{1.609}{4} = 0.402$$

Our decision rule is: If $x < 0.402$, then predict Class 1, otherwise predict Class 0

(c) How does your answer in (b) relate to the the plot you made in (a)? Why?

The answer in (b) is the point at which the likelihood of classes 0 and 1 are equal. For values smaller than $x = 0.402$ the likelihood of Class 1 is greater than Class 0, and opposite otherwise. This agrees with the decision rule. Since the prior distribution is uniform, the ratio of the likelihoods provides the same decision boundary as the ratio of the posteriors in this case.

(d) Load the test data in the file `A3_Q3_test.csv`. Apply your decision rule to the data. What is the misclassification rate of this decision rule?

```
In [10]: import numpy as np
import pandas as pd
import os.path

directory = './data'
test_data = pd.read_csv(os.path.join(directory, 'A3_Q3_test.csv'))
x_test = test_data.x.values
y_test = test_data.y.values

y_pred = x_test < 0.402
y_pred = y_pred.astype(int)
misclassification_rate = sum(abs(y_test-y_pred))/y_test.shape[0]
print('Misclassification rate = {}'.format(misclassification_rate))
```

Misclassification rate = 0.234

(e) Load the training data in the file `A3_Q3_train.csv` and train a logistic regression classifier on the data (using default parameters). What is your misclassification error for your test dataset? How does this compare with the Bayes' classifier?

```
In [22]: from sklearn.linear_model import LogisticRegression

train_data = pd.read_csv(os.path.join(directory, 'A3_Q3_train.csv'))
x_train = train_data.x.values
y_train = train_data.y.values

lr = LogisticRegression()
lr.fit(x_train.reshape(-1,1), y_train.reshape(-1,1))
y_pred_lr = lr.predict(x_test.reshape(-1, 1))

misclassification_rate_lr = sum(abs(y_test-y_pred_lr))/y_test.shape[0]
print('Misclassification rate = {}'.format(misclassification_rate_lr))
```

C:\Users\kjb17\AppData\Local\Continuum\anaconda3\lib\site-packages\sklearn\utils\validation.py:744: 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)
```

Misclassification rate = 0.234

The misclassification rate for the logistic regression classifier is equivalent to that of the Bayes decision rule misclassification rate, and therefore the best we could achieve in this scenario for minimizing misclassification error.

(f) What is your decision rule for your logistic regression model? To compute this, extract the parameters from your fit model (look for the `coef_` and `intercept_` attributes) and since the classes are balanced, the decision rule will be to classify a sample x as Class 1 when your logistic regression sigmoid is greater than 0.5 (the halfway point from the two extremes of 0 and 1). How does this compare with the Bayes' classifier?

The decision rule will be to classify as Class 1 if: $\sigma(w_0 + w_1 x) > 0.5$, where $\sigma(z) = \frac{1}{1+\exp(-z)}$. Solving this inequality for x yields: $x > -\frac{w_0}{w_1}$. We can get those values directly:

```
In [31]: w_0 = lr.intercept_[0]
w_1 = lr.coef_[0][0]

print('w0 = {}'.format(w_0))
print('w1 = {}'.format(w_1))
print('x > {}'.format(-w_0/w_1))

w0 = 1.6034817841465452
w1 = -3.9755216480974047
x > 0.4033387127734383
```

As we can see, the decision rule is if $x > 0.403$, predict Class 1, otherwise predict Class 0. This is the same as the Bayes decision rule above, and therefore the best we could achieve in this scenario for minimizing misclassification error.

(g) If the prior probabilities were not $P(C_0) = P(C_1) = 0.5$, but instead if $P(C_1) > P(C_0)$. How would this impact the optimal decision rule? Would it change, if so, would x^* be larger or smaller?

The decision rule would change. The described change in prior probabilities would make Class 1 more likely for a larger array of values thereby moving the decision boundary further in the direction of positive x-values.

4

[30 points] Supervised learning exploration

For this exercise, you will construct and implement a supervised learning problem solution/experiment. Describe your process and answer these questions clearly and thoroughly. Part of the grade in this assignment is devoted to the quality and professionalism of your work.

(a) Identify a question or problem that's of interest to you and that could be addressed using classification or regression. Explain why it's interesting and what you'd like to accomplish. You're encouraged to be creative.

(b) Download the data and plot the data to describe it. You can use any dataset of interest to you with the exception of the Iris dataset, the Kaggle Titanic dataset, or the Kaggle chocolate dataset. Possible sources of dataset include (but are not limited to):

- [UCI Machine Learning Repository \(https://archive.ics.uci.edu/ml/index.php\)](https://archive.ics.uci.edu/ml/index.php)
- [Kaggle Datasets \(https://www.kaggle.com/datasets\)](https://www.kaggle.com/datasets)
- [Amazon Open Datasets \(https://registry.opendata.aws/\)](https://registry.opendata.aws/)
- [Microsoft's Open Data \(https://msrpendata.com/\)](https://msrpendata.com/)
- [Google's Dataset Search \(https://datasetsearch.research.google.com/\)](https://datasetsearch.research.google.com/)
- [Awesomedata's list of datasets \(https://github.com/awesomedata/awesome-public-datasets\)](https://github.com/awesomedata/awesome-public-datasets)

(c) Formulate your supervised learning question: (a) What is your target variable (what are you trying to predict) and what predictors do you have available? Does your dataset require any preprocessing: is it clean (no missing values or erroneous data) and normalized (are each of the predictors of the same magnitude)?

(d) What supervised learning technique will you use and why?

(e) How will you evaluate performance and know whether you succeeded (e.g. ROC curves for binary classification, mean square error or R^2 for regression)?

(f) Divide your dataset into training and testing datasets OR implement cross validation. Explain your approach and why you adopted it.

(g) Run your analysis and show your performance. Include plots of your data and of performance.

(h) Describe how your system performed, where your supervised learning algorithm performed well, where it did not, and how you could improve it. Summarize the conclusions from your work (this should involve a degree of interpretation more so than "my classifier achieved an AUC of 0.8").

This grade for this question is based on (a) the completeness of the answer in addressing each of the above components, (b) the quality of the work and accuracy of the interpretation of the results of the analysis, (c) the presentation and professionalism of the work, and (d) the amount of creativity demonstrated by the work.

ANSWER