COMP9417 - Machine Learning and Data Mining
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Homework 2: Logistic Regression & Optimization

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Q1

a) we first shall rewrite $L(\beta, \beta_0)$ in a form we can further analyse.

$$L(\beta,\beta_0) = \sum_{i=1}^{n} y_i \ln\left(\frac{1}{s(\beta_0+\beta^T x_i)}\right) + (1-y_i)\ln\left(\frac{1}{1-s(\beta_0+\beta^T x_i)}\right)$$

$$= \sum_{i=1}^{n} y_i \ln\left(\frac{1}{s(\beta_0+\beta^T x_i)}\right) + \ln\left(\frac{1}{1-s(\beta_0+\beta^T x_i)}\right) - y_i \ln\left(\frac{1}{1-s(\beta_0+\beta^T x_i)}\right)$$

$$= \sum_{i=1}^{n} \ln\left(\frac{1}{1-s(\beta_0+\beta^T x_i)}\right) + y_i \ln\left(\frac{1-s(\beta_0+\beta^T x_i)}{s(\beta_0+\beta^T x_i)}\right)$$

→ But we know $s(z) = (1+e^{-z})^{-1}$

$$e^{-z} = \frac{1-s(z)}{s(z)} \Rightarrow -z = \ln\left(\frac{1-s(z)}{s(z)}\right)$$

Hence:

$$= \sum_{i=1}^{n} -\ln(1-s(\beta_0+\beta^T x_i)) - y_i \ln\left(\frac{s(\beta_0+\beta^T x_i)}{1-s(\beta_0+\beta^T x_i)}\right)$$

$$= -1 \sum_{i=1}^{n} \ln\left(1 - \frac{e^{\beta_0+\beta^T x_i}\cdot 1}{1+e^{(\beta_0+\beta^T x_i)}}\right) + y_i(\beta_0+\beta^T x_i)$$

→ as $s(z) = \frac{1}{1+e^{-z}} = \frac{e^z}{e^z+e^{-z}e^z} = \frac{e^z}{1+e^z}$

$$\Leftrightarrow z = \ln\left(\frac{s(z)}{1-s(z)}\right)$$

We have:

$$= -\sum_{i=1}^{n} -\ln(1+e^{\beta_0+\beta^T x_i}) + y_i(\beta_0+\beta^T x_i)$$

$$L(\beta_0,\beta_0) = \sum_{i=1}^{n} \ln(1+e^{\beta_0+\beta^T x_i}) - y_i(\beta_0+\beta^T x_i) \quad (*)$$

(see (γ))

(γ)

$$\ln\left(1-\frac{1}{1+e^{-(\beta_0+\beta^T x_i)}}\right)$$

$$= \ln\left(\frac{e^{-(\beta_0+\beta^T x_i)}}{1+e^{-(\beta_0+\beta^T x_i)}}\right)$$

$$= \ln\left(\left(\frac{1+e^{-(\beta_0+\beta^T x_i)}}{e^{-(\beta_0+\beta^T x_i)}}\right)^{-1}\right)$$

$$= -\ln\left(e^{-(\beta_0+\beta^T x_i)}+1\right)$$

→ now consider what happens to each minimization criterion when $y=0, \tilde{y}=-1$, & $y=1, \tilde{y}=1$.

→ When $y=1, \tilde{y}=1$

① if $y=1$ the loss for each observation can be written as:

→ $\ln(1+e^{\beta_0+\beta^T x_i}) - y_i(\beta_0+\beta^T x_i)$

nxt pg. →

$\rightarrow \ln\left(1 + e^{\beta_0 + \beta^T x_i}\right) - (1)\left(\beta^T x_i + \beta_0\right)$

$\rightarrow \ln\left(1 + e^{\beta_0 + \beta^T x_i}\right) - \left(\beta^T x_i + \beta_0\right)$.

② for sklearn minimization criterion, when $\tilde{y} = -1$ then the loss for each observation can be written as.

$\rightarrow \ln\left(1 + e^{\left(-\tilde{y}_i (w^T x_i + c)\right)}\right)$ ignoring $\|w\|$ & c

$\rightarrow \ln\left(1 + \frac{1}{\exp(w^T x_i + c)}\right) = \ln\left(\frac{\exp(w^T x_i + c) + 1}{\exp(w^T x_i + c)}\right)$

$\rightarrow \ln(\exp(w^T x_i + c) + 1) - \ln(\exp(w^T x_i + c))$

$\rightarrow \ln\left(1 + e^{w^T x_i + c}\right) - (w^T x_i + c)$

→ Note that the form of the loss is the same for each obs of the form $(x_i, y = 1)$ between the two criterions.

when $y = 0$, $\tilde{y} = -1$.

③ if $y = 0$ the loss for each obs can be written as:

$\rightarrow \ln\left(1 + e^{\beta_0 + \beta^T x_i}\right) + 0$ // using $L(\beta, \beta_0)$ (*) from prev pg.

$\rightarrow \ln\left(1 + e^{\beta_0 + \beta^T x_i}\right)$

④ if $\tilde{y} = -1$ the loss for each obs in the sklearn minimization case can be written as: $\ln\left(1 + \exp(-(-1)(w^T x_i + c))\right)$

$\rightarrow \ln\left(1 + \exp(w^T x_i + c)\right)$

$\rightarrow \ln\left(1 + e^{c + w^T x_i}\right)$

→ Note the form of the loss for each criterion is the same.

⇒ As the form of loss is the same between the minimization criterions for each respective observation set:

$(x_i \ \$ \ y = 0 \cup \tilde{y} = -1)$.

$(x_i \ \$ \ y = 1 \cup \tilde{y} = 1)$.

they will produce the same coefficients during the minimization procedures as your effectively minimizing the same criterion. Hence $(\hat{\beta}_0 = c \ \$ \ \hat{\beta} = \hat{w})$

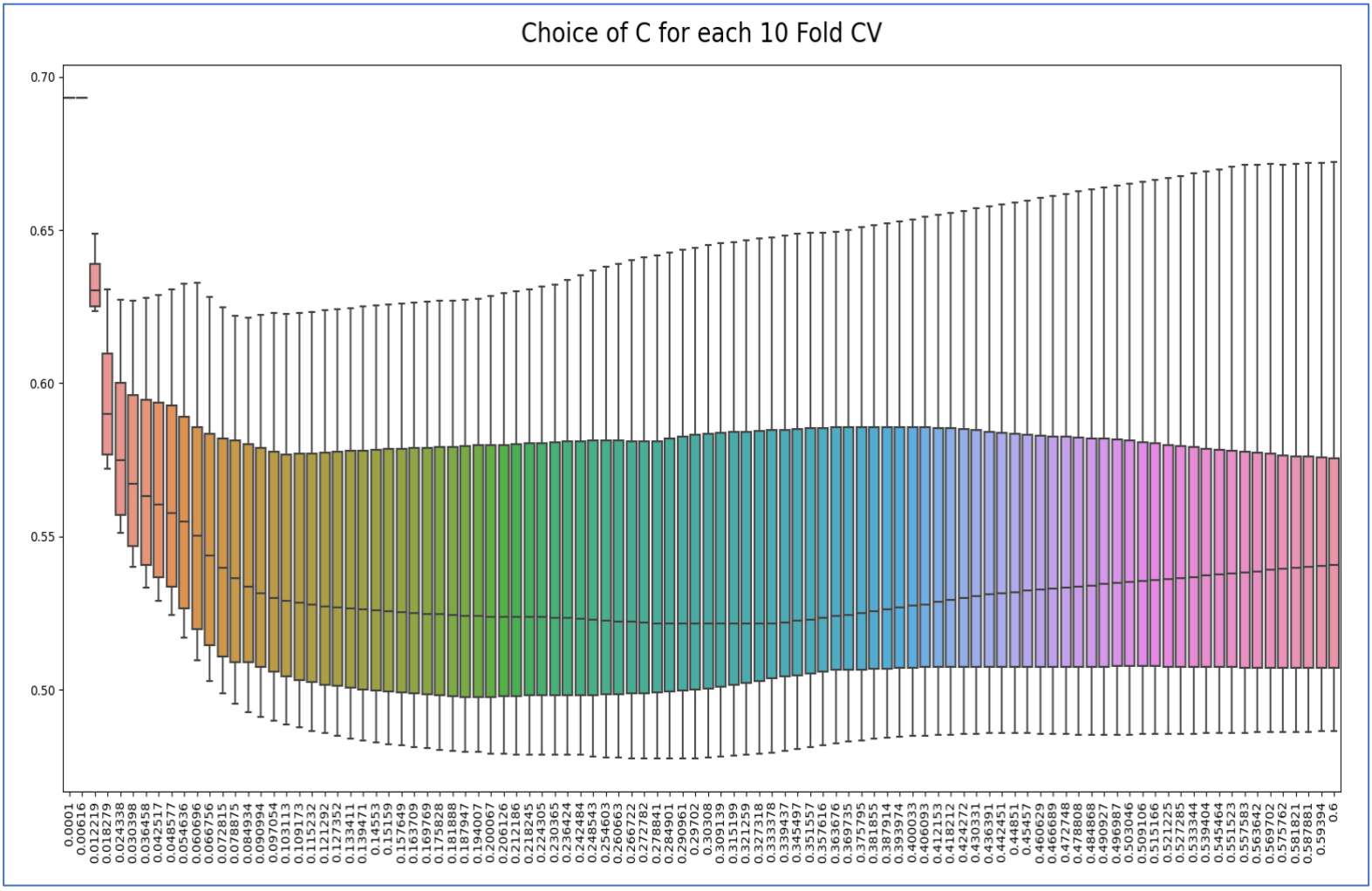
Question 1. Regularized Logistic Regression & the Bootstrap

Q1 a) continued:

A vector (w in this case) is said to be sparse when most of its cells (wi's in this case) are zero. This is the advantage of L1 regularization which minimizes a function that penalizes large values of the parameters and takes some weights to zero. Most often the function is $\lambda\Sigma\Theta_j^2$, which is some constant λ times the sum of the squared parameter values Θ_j^2. The larger λ is the less likely it is that the parameters will be increased in magnitude simply to adjust for small perturbations in the data. Here the parameter C is simply the inverse of regularization strength in Logistic Regression i.e., $C=1/\lambda$.

We can see that large values of C give more freedom to the model. Conversely, smaller values of C constrain the model more. In the L1 penalty case, this leads to sparser solutions. (scikit-learn.org)

Q1 b) Graph indicating the cross-validation scores for each C value in the form of a box plot.




```
MIN avg =  0.5397000191672515 --------------------------
best C =  0.18794747474747472 --------------------------
train accuracy  =  0.752 -------------------------
test accuracy  =  0.74 -------------------------
best para grd search {'C': 0.18188787878787877}
```

The value of C that gives the best CV performance is 0.18794. The training accuracy is 0.752 and Test accuracy is 0.74. Also depicted to is the minimum average cross validation score out of all the C choices and the best C value found through sklearn grid search.

Code used for this section:

```
data = pd.read_csv("Q1.csv")
X = data.iloc[:,:-1]
Y = data.iloc[:,-1]

X_train, X_test, Y_train, Y_test = train_test_split(X,Y, test_size=0.23, train_size=0.77,  shuffle=False, stratify=None)
data_train = pd.concat([X_train, Y_train], axis=1)

#cross validation on training set ...
def cross_validation_split(dataset, folds):
        dataset_split = [] # construct an array of arrays
        df_copy = dataset
        fold_size = int(df_copy.shape[0] / folds)

        j = 0 # counter for jth row
        for i in range(folds):
            fold = []
            # while loop to add elements to the folds
            while len(fold) < fold_size:
                # save the selected line
                fold.append(df_copy.loc[j].values.tolist())
                # delete the selected line from dataframe not to select again
                df_copy = df_copy.drop(j)
                #print(df_copy)
                j = j+1
            # save the fold
            dataset_split.append(np.asarray(fold))
        return dataset_split

def cross_validation_split_Y(dataset, folds):
        dataset_split = []
        df_copy = dataset
        fold_size = int(df_copy.shape[0] / folds)
        j = 0
        for i in range(folds):
            fold = []
            while len(fold) < fold_size:
                fold.append(df_copy.loc[j].tolist())
                df_copy = df_copy.drop(j)
                j = j+1
            dataset_split.append(np.asarray(fold))
        return dataset_split

data_k_X=cross_validation_split(X_train,10)
data_k_Y=cross_validation_split_Y(Y_train,10)

# CV to find best C parameter
C_s = np.linspace(start=0.0001, stop=0.6, num=100, endpoint=True)
print(C_s)

logreg = LogisticRegression(penalty='l1', solver='liblinear', random_state=0)
avg_error_C = []
log_errors_all = []
```

Code continued:

```
# CV to find best C parameter
C_s = np.linspace(start=0.0001, stop=0.6, num=100, endpoint=True)
print(C_s)

logreg = LogisticRegression(penalty='l1', solver='liblinear', random_state=0)
avg_error_C = []
log_errors_all = []

i = 0
for a in C_s:
    log_errors = []
    while i < 10:
        # get x and y for the ith fold
        fold_X=data_k_X[i]
        fold_Y=data_k_Y[i]
        # create a 'ith removed' fold
        ith_removed_X = np.delete(data_k_X, i, axis=0)# dataset without i-th observation
        ith_removed_Y = np.delete(data_k_Y, i, axis=0)
        #shaping
        new_arr_X = ith_removed_X.reshape(-1, ith_removed_X.shape[-1])
        ith_removed_X_df = pd.DataFrame(new_arr_X)
        ith_removed_Y = ith_removed_Y.reshape(-1)
        #fit model to df with out the ith fold
        logreg.set_params(C = a) # set to current C
        logreg.fit(ith_removed_X_df, ith_removed_Y)

        # error based on the dropped fold i.e predict using the dropped fold
        y_pred_probs_t = logreg.predict_proba(fold_X)
        loss_test = log_loss(fold_Y, y_pred_probs_t)

        log_errors.append(loss_test)
        i = i+1
    i = 0
    avg = (sum(log_errors))/10 # find the Leave one out error average for lambda = a
    avg_error_C.append(avg)
    log_errors_all.append(log_errors)

df = pd.DataFrame(log_errors_all)

#box plot creation
df_new = df.T
round_C_s = [round(num, 6) for num in C_s]
df_new.columns = round_C_s
print(df_new)

fig, ax = plt.subplots(figsize=(20,10))
sns.boxplot(data=df_new)
plt.title('Choice of C for each 10 Fold CV', fontsize=20, y=1.02)
plt.xticks(rotation='vertical')
plt.tight_layout
plt.show()
```

```
# find best C
minavg = min(avg_error_C)
minavg_index = avg_error_C.index(min(avg_error_C))
best_C = C_s[minavg_index]
print(f"MIN avg =  {minavg} ")
print(f"best C =  {best_C} ")
# Re-fit the model with this chosen C, and report both train and test accuracy
logreg.set_params(C = best_C)
logreg.fit(X_train, Y_train)
#traning error
score_train = accuracy_score(Y_train, logreg.predict(X_train))
# test error
score_test = accuracy_score(Y_test, logreg.predict(X_test))
print(f"train accuracy  =  {score_train} ")
print(f"test accuracy  =  {score_test} ")
```

Q1 c)

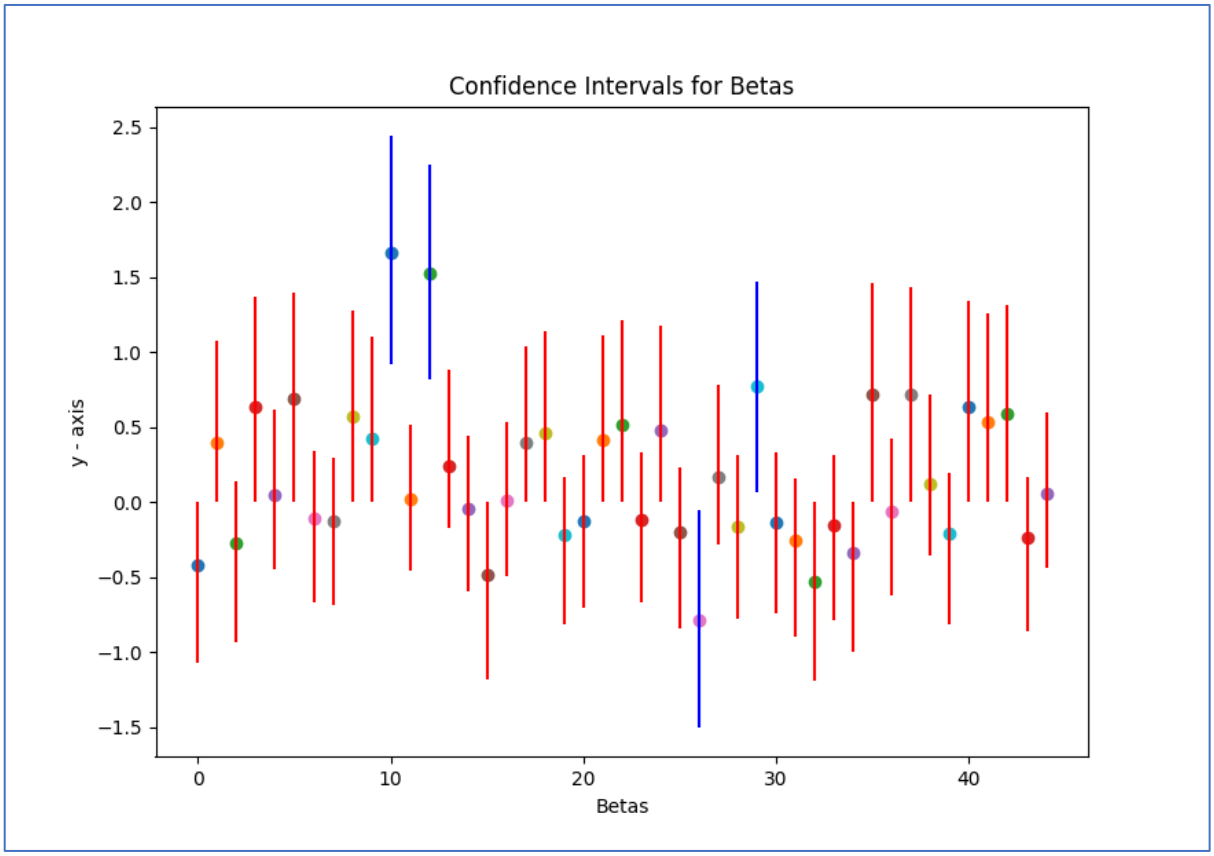
Code used to produce approximately consistent results compared to Q1 b)

```
#Q1 c)
parameter_candidates = [
  {'C': C_s},
]
grid_lr = GridSearchCV(estimator= LogisticRegression(penalty='l1' , solver='liblinear',random_state=0),
                                        cv=10,scoring='neg_log_loss' ,param_grid=parameter_candidates)
grid_lr.fit(X_train, Y_train)
best_parameters = grid_lr.best_params_
print(f"best para grd search {best_parameters}")

```

The modified code above produces the best C value of 0.181887 which is very similar to the result obtained in Q1b of 0.18794. The first reason the modified code obtains closer results to cross validation procedure made from scratch is due specifying the scoring function to be the neg_log_loss which was not specified in the original code. However, although it produces approximate results it doesn't produce the exact same result due to grid search using randomized folds in its cross-validation procedure whereas the from scratch procedure used a fixed fold selection procedure.

Q1 d)

Plot produced for this section



Code used to produce the above plot:

```
#Q1 d)
np.random.seed(12)
i = 0
coeffs = list()
coeffs_avg = list()
logreg = LogisticRegression(penalty='l1', C=1, solver='liblinear', random_state=0)

while i < 10000:
    choices_X = list()
    choices_Y = list()
    features = X_train.columns
    response = ['Y']
    choice_indices = np.random.choice(len(data_train), 500, replace=True)
    print(f"-{i}-")

    for j in choice_indices:
        choices_X.append(X_train.loc[j].values.tolist())
        choices_Y.append(Y_train.loc[j].tolist())
    choices_X_df = pd.DataFrame(choices_X, columns=features)
    logreg.fit(choices_X_df, choices_Y)
    # dont need intercept
    temp = logreg.coef_
    coeffs.append(temp[0]) # use .tolist if need be
    #print(coeffs)
    i = i+1

coeff_np = np.array(coeffs)
print("================= mean for each beta")
mean_for_each_beta = np.mean(coeff_np, axis = 0)
print(np.mean(coeff_np, axis = 0))
print("================= lower quantiles for each beta ")
L_for_each_beta = np.quantile(coeff_np, .05, axis =0)
print(L_for_each_beta)
print("================= upper quantiles for each beta")
U_for_each_beta = np.quantile(coeff_np, .95, axis =0)
print(U_for_each_beta)


#plotting
plt.figure(figsize=(10,10))
i = 0
while i < 45:
    if L_for_each_beta[i] <= 0 <= U_for_each_beta[i]:
        plt.vlines(i, L_for_each_beta[i],  U_for_each_beta[i], colors='r', linestyles='solid')
        plt.scatter(i, mean_for_each_beta[i])
    else:
        plt.vlines(i, L_for_each_beta[i],  U_for_each_beta[i], colors='b', linestyles='solid')
        plt.scatter(i, mean_for_each_beta[i])
    i = i+1
plt.xlabel(r"Betas")
plt.ylabel("y - axis")
plt.title("Confidence Intervals for Betas")
plt.show()
```

Q1 e)

What do the confidence intervals tell you about the underlying data generating distribution?

The data generating distribution refers to the relationship between the response Y and the covariates X and this ultimately captured in the Beta Coefficients. From the confidence intervals we can be 95% confident that the true coefficient parameter falls between a certain specified range. If the range contains zero, then we hypothesise that there is no relationship between that covariate attached to the beta and y variable. Hence, we can narrow down all the covariates that do matter by looking at the blue lines on the plot given in Q1 e)

How does this relate to the choice of C when running regularized logistic regression on this data? This relates to the choice of C as the greater the C the more freedom a model is given i.e., more Beta coefficients remain significant while if the C is very low more coefficients turn to zero which is exactly what's happening in our case with C=1.

Is regularization necessary? In our case yes. The exception is if you know the data generating process and can model it exactly. Then you merely estimate the model parameters. In general, you will not know the process, so you will have to approximate with a flexible enough model. **We also don't want the model to memorize the training dataset, we want a model that generalizes well to new, unseen data.** Regularization methods introduce bias into the regression solution that can reduce variance considerably. The lower variance solutions produced by regularization techniques provide superior MSE performance which is better for out of sample prediction and avoids overfitting.

Q2) a) deriving an equation for the explicit gradient update.

→ The general framework : $x^{k+1} = x^k - \alpha_k \nabla f(x_k)$ $k = 0, 1, 2 \cdots$

where $\alpha_k > 0$.

→ $f(x) = \frac{1}{2} \| Ax - b \|_2^2 = \frac{1}{2} (Ax-b)^T (Ax-b)$.

$= \frac{1}{2} (x^T A^T - b^T)(Ax - b)$

$= \frac{1}{2} (x^T A^T A x - x^T A^T b - b^T A x + b^T b)$

→ But $x^T A^T b$ is a scalar, we know the transpose of a scalar is itself. $\therefore (x^T A^T b)^T = x^T A^T b$

$b^T A x = x^T A^T b$.

→ $f(x) = \frac{1}{2} (x^T A^T A x - 2 b^T A x + b^T b)$

$\nabla f(x) = \frac{\partial}{\partial x} \left[x^T A^T x - 2 (A^T B)^T x + b^T b \right] \times \frac{1}{2}$.

$= (A^T A x + (A^T A)^T x - 2 A^T b) \times \frac{1}{2}$.

$= (A^T A x + A^T A x - 2 A^T b) \times \frac{1}{2}$.

$= (2 A^T A x - 2 A^T b) \frac{1}{2}$

$\nabla f(x) = A^T A x - A^T b$.

Hence our GD equation is:

$$x^{k+1} = x^k - \alpha_k \left[A^T A x^k - A^T b \right]$$

We can also derive an explicit solution for the minimum vector by setting $\nabla f(x) = 0$.

→ $\nabla f(x) = 0 \Rightarrow A^T A x = A^T b$

$x = (A^T A)^{-1} A^T b$.

Question 2. Gradient Based Optimization

Q2 a) continued

Results:

```
====first 5========
k = 0 --- x(k) = [1 1 1 1]
k = 1 --- x(k) = [1.  0.5 0.  1.5]
k = 2 --- x(k) = [ 1.2   0.25 -0.25  1.45]
k = 3 --- x(k) = [ 1.345  0.125 -0.36   1.44 ]
k = 4 --- x(k) = [ 1.4565  0.0625 -0.4075  1.459 ]
====last 5========
k = 218 --- x(k) = [ 3.99699850e+00 -6.82054860e-17 -5.61531549e-04  2.99812156e+00]
k = 219 --- x(k) = [ 3.99709142e+00 -6.82054860e-17 -5.44147417e-04  2.99817971e+00]
k = 220 --- x(k) = [ 3.99718146e+00 -1.12614407e-16 -5.27301471e-04  2.99823607e+00]
k = 221 --- x(k) = [ 3.99726872e+00 -6.82054860e-17 -5.10977048e-04  2.99829068e+00]
k = 222 --- x(k) = [ 3.99735328e+00 -1.12614407e-16 -4.95158004e-04  2.99834359e+00]
```

Code used to produce the results:

```python
# Q2 a
def get_gradient(x):
    A = np.array([[1 , 0 , 1 , -1],[-1, 1 ,0, 2],[0, -1, -2, 1]])
    b = np.array([1,2,3])
    # print(A)
    # print(b)
    AtA = np.matmul(np.transpose(A),A)
    AtAx = np.matmul(AtA,x)
    gradient = -np.matmul(np.transpose(A),b) + AtAx
    return gradient

def get_condition(x_curr):
    grad = get_gradient(x_curr)
    return la.norm(grad)

def gradient_descent(start_x, step):
    x_s = []
    condition = get_condition(start_x)
    x_s.append([0,start_x])

    k = 1
    xk = start_x

    while (condition >= 0.001):
        grad = get_gradient(xk)
        x_new = xk - step * grad
        x_s.append([k,x_new])

        condition = get_condition(x_new)
        xk = x_new # setting to new values
        k = k+1
        print(k)
    return x_s

start_x = np.array([1,1,1,1])
results = gradient_descent(start_x , 0.1)
print("====first 5========")
for num in results[:5]:
     print(f"k = {num[0]} --- x(k) = {num[1]}")

print("====last 5========")
for num in results[-5:]:
     print(f"k = {num[0]} --- x(k) = {num[1]}")
```

Q2 b) deriving an explicit solution for α_k.

→ Method of steepest descen / Exact line search.

→ we have to evaluate $f(x^k - \alpha \nabla f(x^k))$

by taking the derivative wrt to α & solve for α.

$f(x^k - \alpha \nabla f(x^k)) =$

Note from 2a): $f(x) = \frac{1}{2}(Ax-B)^T(Ax-B)$

$= \frac{1}{2}(x^T A^T A x - 2(A^T B)^T x + B^T B).$

$= \frac{1}{2}\Big[(x^k - \alpha \nabla f(x^k))^T A^T A (x^k - \alpha \nabla f(x^k)) - 2(A^T B)^T (x^k - \alpha \nabla f(x^k)) + B^T B \Big].$

$= \frac{1}{2}\Big[(x^{kT} - \alpha \nabla f(x^k)^T) A^T A (x^k - \alpha \nabla f(x^k)) - 2(B^T A)(x^k - \alpha \nabla f(x^k)) + B^T B \Big]$

$= \frac{1}{2}\Big[(x^{kT} A^T A - \alpha \nabla f(x^k)^T A^T A)(x^k - \alpha \nabla f(x^k)) - 2\big[B^T A x^k - \alpha B^T A \nabla f(x^k)\big] + B^T B \Big]$

$= \frac{1}{2}\Big[x^{kT} A^T A x^k - \alpha x^{kT} A^T A \nabla f(x^k) - \alpha \nabla f(x^k)^T A^T A x^k + \alpha^2 \nabla f(x^k)^T A^T A \nabla f(x^k) - 2B^T A x^k + 2\alpha B^T A \nabla f(x^k) + B^T B \Big].$

$= \frac{1}{2}\Big[\alpha^2 \nabla f(x^k)^T A^T A \nabla f(x^k) + \alpha\big[-x^{kT} A^T A \nabla f(x^k) - \nabla f(x^k)^T A^T A x^k + 2\alpha B^T A \nabla f(x^k)\big] + x^{kT} A^T A x^k - 2B^T A x^k + B^T B \Big]$

But this can be written as a quadratic.

$= \frac{1}{2}\big[a\alpha^2 + d\alpha + c\big]$

hence $\arg\min f(x^k - \alpha \nabla f(x^k)) = \frac{-d}{2a}.$

Note: • $a = \nabla f(x^k)^T A^T A \nabla f(x^k)$ is just some constant

→

- $d = -(x^k)^T A^T A \nabla f(x^k) - \nabla f(x^k)^T A^T A x^k + 2 B^T A \nabla f(x^k)$

  which is some constant

- $c = x^{kT} A^T A x^k - 2B^T A x^k + B^T A$ which is a constant.

$$\therefore \alpha_k = \frac{-d}{2a} = \frac{+\left[- x^{kT} A^T A \nabla f(x^k) - \nabla f(x^k)^T A^T A x^k + 2B^T A \nabla f(x^k) \right]}{2 \nabla f(x^k)^T A^T A \nabla f(x^k)}$$

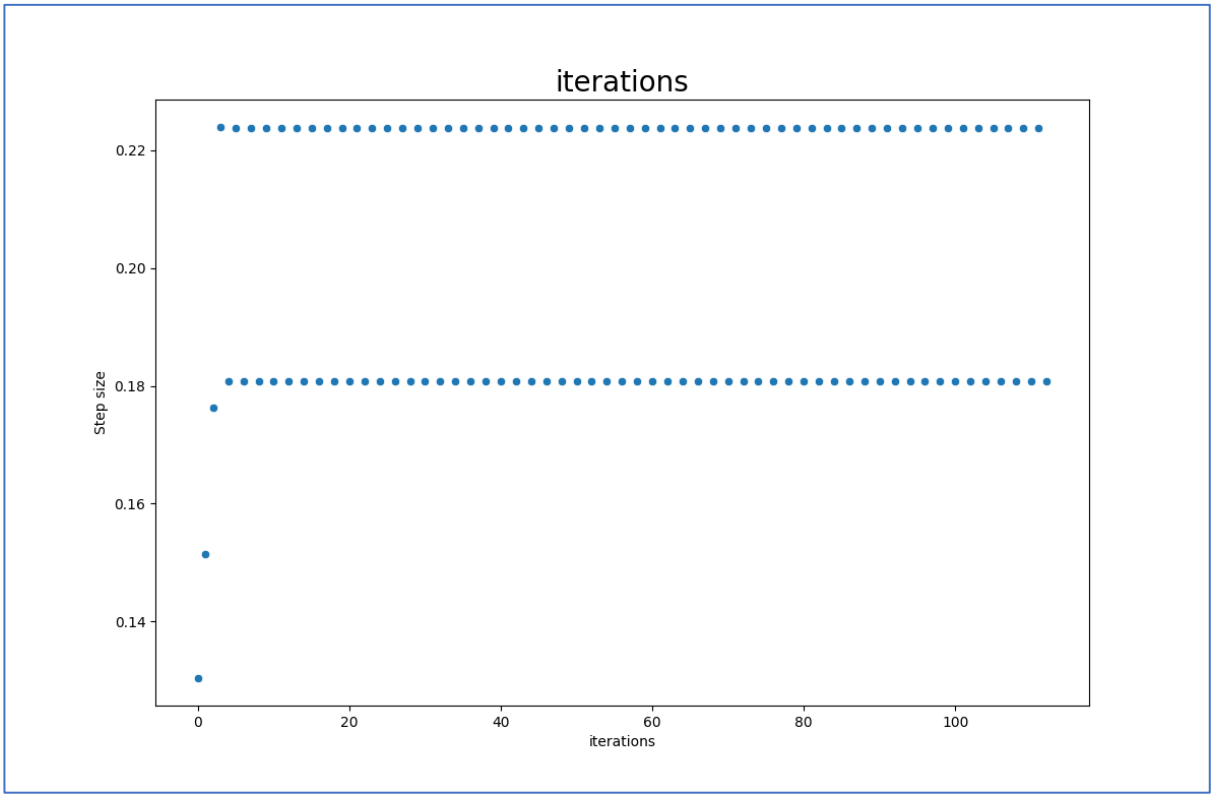
$$\alpha_k := \frac{x^{kT} A^T A \nabla f(x^k) + \nabla f(x^k)^T A^T A x^k + 2B^T A \nabla f(x^k)}{2 \nabla f(x^k)^T A^T A \nabla f(x^k).}$$

Q2 b) continued

Results

```
====first 5========
k = 0 --- x(k) = [1 1 1 1]
k = 1 --- x(k) = [ 1.          0.34782609 -0.30434783  1.65217391]
k = 2 --- x(k) = [ 1.39494706  0.08452804 -0.33726008  1.32305136]
k = 3 --- x(k) = [ 1.50092477  0.01000748 -0.49745676  1.52586073]
k = 4 --- x(k) = [ 1.74348592e+00 -1.19743517e-03 -3.75654918e-01  1.49120345e+00]
====last 5========
k = 109 --- x(k) = [ 3.99737876e+00  7.65011837e-18 -5.33380212e-04  2.99844552e+00]
k = 110 --- x(k) = [ 3.99762774e+00 -9.17438206e-17 -3.93561204e-04  2.99841486e+00]
k = 111 --- x(k) = [ 3.99769691e+00 -9.17438206e-17 -4.68641603e-04  2.99863420e+00]
k = 112 --- x(k) = [ 3.99791567e+00 -1.91137760e-16 -3.45793018e-04  2.99860726e+00]
k = 113 --- x(k) = [ 3.99797645e+00 -1.91137760e-16 -4.11760592e-04  2.99879997e+00]
```

Plot of αk over all iterations



Code used to plot:

```python
start_x = np.array([1,1,1,1])
results = gradient_descent(start_x , 0.1)
print("====first 5========")
for num in results[:5]:
    print(f"k = {num[0]} --- x(k) = {num[1]}")

print("====last 5========")
for num in results[-5:]:
    print(f"k = {num[0]} --- x(k) = {num[1]}")

sns.scatterplot(data = steps)
plt.title('iterations', fontsize=20)
plt.xlabel('iterations')
plt.ylabel('Step size')
plt.show()
```

Code used for GD algorithm:

```python
# Q2 b
def get_gradient(x):
    A = np.array([[1 , 0 , 1 , -1],[-1, 1 ,0, 2],[0, -1, -2, 1]])
    b = np.array([1,2,3])
    # print(A)
    # print(b)
    AtA = np.matmul(np.transpose(A),A)
    AtAx = np.matmul(AtA,x)
    gradient = -np.matmul(np.transpose(A),b) + AtAx
    return gradient

steps = []
def get_step(grad_at_x, x_curr):
    A = np.array([[1 , 0 , 1 , -1],[-1, 1 ,0, 2],[0, -1, -2, 1]])
    b = np.array([1,2,3])

    term1 = -2*np.matmul(np.transpose(b),A)
    term2 = np.matmul(term1,grad_at_x)

    term3 = np.matmul(np.transpose(x_curr),np.transpose(A))
    term4 = np.matmul(term3, A)
    term5 = np.matmul(term4, grad_at_x)

    term6 = np.matmul(np.transpose(grad_at_x), np.transpose(A))
    term7 = np.matmul(term6, A)
    term8 = np.matmul(term7 , x_curr)

    numerator = term2 + term5 + term8

    term9 = 2*np.matmul(np.transpose(grad_at_x),np.transpose(A))
    term10 = np.matmul(term9,A)
    term11 = np.matmul(term10,grad_at_x)

    demoninator = term11

    step = numerator/demoninator
    steps.append(step)
    return step

def get_condition(x_curr):
    grad = get_gradient(x_curr)
    return la.norm(grad)

def gradient_descent(start_x, step):
    x_s = []
    condition = get_condition(start_x)
    x_s.append([0,start_x])

    k = 1
    xk = start_x

    while (condition >= 0.001):
        grad = get_gradient(xk)
        step = get_step(grad, xk)
        x_new = xk - step * grad
        x_s.append([k,x_new])

        condition = get_condition(x_new)
        xk = x_new # setting to new values

        print(k)
        k = k+1
    return x_s
```

Q2 c)

Comment on the differences you observed.

The key differences observed was the number of steps it took to reach a convergence and the size of the step, which aligns with our definitions gradient descent will point in the direction of steepest descent while steepest descent (exact line search) takes a step

Why would we prefer steepest descent over gradient descent?

Fig 1

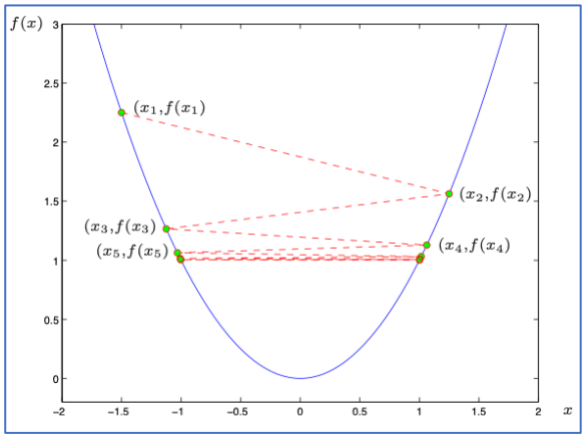
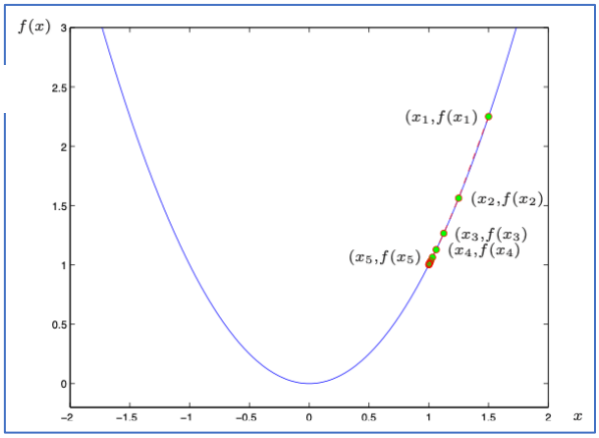


Fig 2



In steepest descent were finding the optimal step size at each iteration of the algorithm, However gradient descent step sizes are constant meaning one of the situations represented by the above figures may occur , either step is too long (fig1) or too short (fig2) i.e. decrease in f is not proportional to the size of the directional derivative

Why would you prefer gradient descent over steepest descent?

There can be many issues with steepest descent (exact line search) such as Exact line search requires univariate minimization it's also generally very expensive and not cost effective. Also exact line search may not be much better than an approximate line search methods.

Finally, explain why this is a reasonable condition to terminate use to terminate the algorithm.

The termination condition is reasonable as $||\nabla f(x^k)||$ is describing the gradient at each x if $\nabla f(x^k) = 0$ then we have found the minimum as in our case the gradient may never converge to zero a small value is needed such as 0.0001 so that algorithm stops and we can achieve a 'good' enough estimate to the true minimum.

Q2 d)

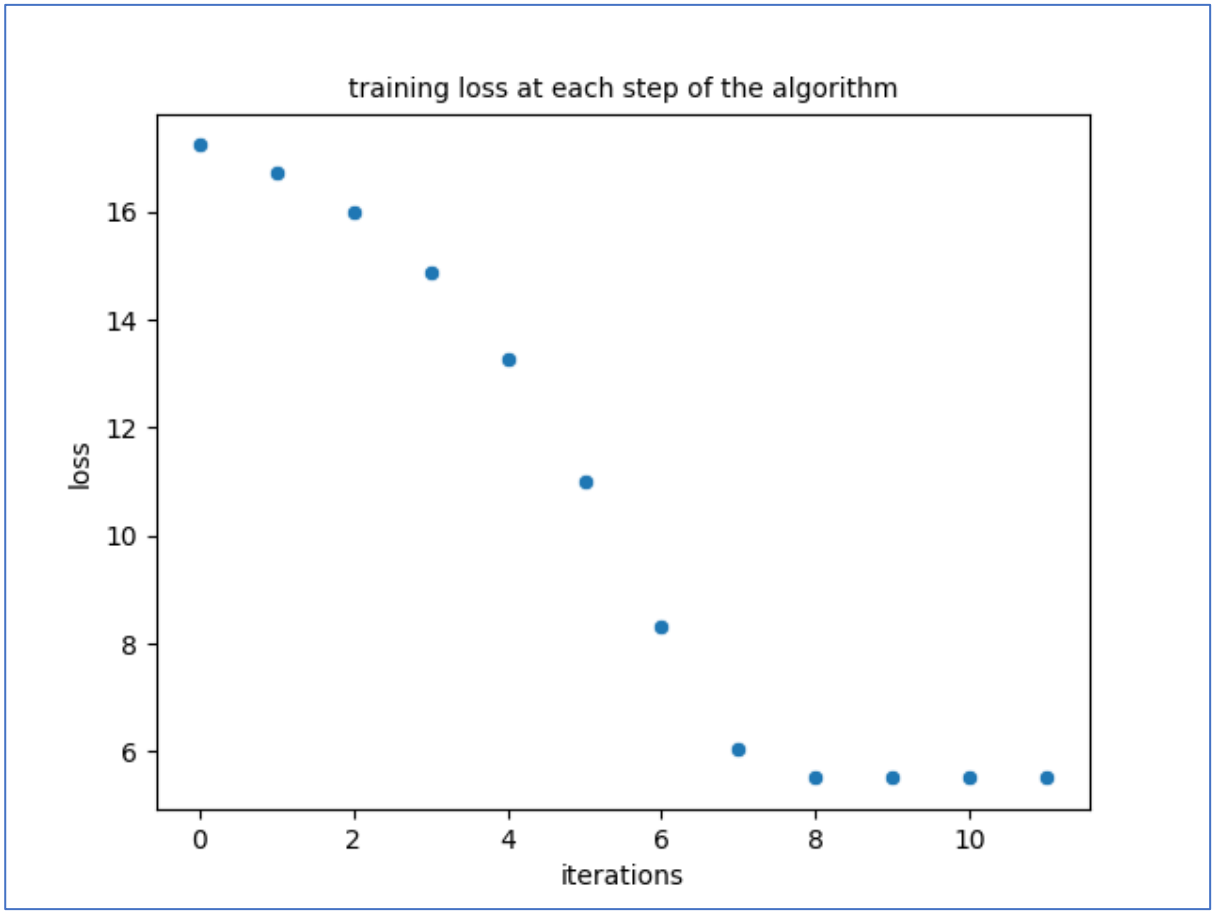
Code used for data pre-processing

```
#Q2d

df = pd.read_csv("Q2.csv")
df = df.dropna()
x_df = df.drop(columns=['transactiondate','latitude','longitude','price'])
y_df = df[["price"]]
scaler = MinMaxScaler()
scaled_x_df = scaler.fit_transform(x_df)

print(scaled_x_df)

scaled_x_df = pd.DataFrame(data=scaled_x_df)
print(scaled_x_df)
scaled_x_df["1"] = 1
first_col = scaled_x_df.pop("1")
scaled_x_df.insert(0, "1", first_col)

print(scaled_x_df)

x_train, x_test, y_train, y_test = train_test_split(scaled_x_df, y_df, test_size=0.5, shuffle=False)
print(x_train)

y_train = np.asarray(y_train)
y_test = np.asarray(y_test)
x_train = np.asarray(x_train)
x_test = np.asarray(x_test)
print(f"x trian first row  {x_train[0]}")
print(f"x trian last row  {x_train[-1]}")
print(f"x test first 1 {x_test[0]}")
print(f"x test last row 1 {x_test[-1]}")

print(f"y trian first row  {y_train[0]}")
print(f"y trian last row  {y_train[-1]}")
print(f"y test first 1 {y_train[0]}")
print(f"y test last row 1 {y_train[-1]}")
```

Q2 e)

Training loss 5.532811641693115
Testing loss 5.052703857421875
Final Iteration: 11
Absolute loss difference between final weight vector and vector before it: 6.4373016e-05
Final weight vector: [18.337734 18.337734 18.337734 18.337734]

Plot produced:



See code next page

Code used to produce results

```python
# Q2e
def get_loss(x,y,w):
    WtX = jnp.matmul(w, jnp.transpose(x))
    sqrt_loss = 0.25*((y-WtX)**2)
    sqrt_loss += 1
    loss = jnp.sqrt(sqrt_loss)
    loss -= 1

    return jnp.sum(loss) # changes the shape of the array its just 1 number still

def get_loss_sum(x,y,w):
    k = x.shape[0]
    losses = []
    res = []
    for i in range(k):
        loss = get_loss(x[i],y[i],w)
        losses.append(loss)
    res = jnp.mean(jnp.array(losses))
    return res

def get_gradient(x,y,w):
    k = x.shape[0]
    losses = []
    res = []
    for i in range(k):
        loss = grad(get_loss)(x[i],y[i],w)
        losses.append(loss)
    res = jnp.mean(jnp.array(losses))
    return res
loss_all = []
def gradient_descent_train(w, x, y, step=1,termination_val=0.0001):
    results = {}

    converged = False
    wk = w
    k=0
    inital_loss = get_loss_sum(x, y, wk)
    cond = inital_loss
    while cond >= 0.0001:
        grad = get_gradient(x, y, wk)
        wk_new = wk - step * grad
        results[k] = wk_new

        cond = abs(get_loss_sum(x, y, wk_new) - get_loss_sum(x, y, wk))
        loss_for_wk = get_loss_sum(x, y, wk)
        numpy_array = float(np.asarray(loss_for_wk))

        loss_all.append(numpy_array)
        print("Iteration: ", k)
        #jnp mean is just changing shape of result here
        print("weight_diff: ", jnp.mean(cond))
        wk = wk_new
        k+=1
    return results, wk
```

```python
w0 = np.array([1,1,1,1])
initial_step = 1
res, final_w = gradient_descent_train(w0, x_train, y_train, initial_step)
print(final_w)
print("-------loss all ")
print(loss_all)

#getting train loss
train_loss = float(np.asarray(get_loss_sum(x_train, y_train, final_w)))
test_loss = float(np.asarray(get_loss_sum(x_test, y_test, final_w)))

print(f"train_loss {train_loss}")
print(f"test_loss {test_loss}")



sns.scatterplot(data = loss_all)
plt.title('training loss at each step of the algorithm', fontsize=10)
plt.xlabel('iterations')
plt.ylabel('loss')
plt.show()
```

Q2 g) Gradient Boosting Algorithms

Another broad category of gradient based algorithms is gradient boost algorithms. In boosting, we build an ensemble of classifiers or regressors incrementally. In each step, we add a new sub-model that tries to compensate for the errors made by the previous sub-models. To avoid overfitting, boosting is typically done using simple sub-models: the classical choice is small decision trees ("decision stumps"). Gradient boosting is when we optimize the boosted ensemble with respect to some loss function. different types of loss functions can be used resulting in a flexible technique that can be applied to regression, multi-class classification.

The difference between gradient descent and gradient boosting is that inn GD you modify the predictions by e.g., adding a delta to the model coefficients; in gradient boosting you modify the predictions by adding a delta directly to the predictions. An example of a weak learner used is Decision trees. Trees are added together one at a time based on minimizing some loss, and existing trees in the model are not changed. XGBoost is one of the most popular variants of gradient boosting.