

# Homework 6: Multilayer Feedforward Network - Dealing with Missing Data

Harvard University Fall 2018

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#### In [3]:

```
#RUN THIS CELL
import requests
from IPython.core.display import HTML
styles = requests.get("https://raw.githubusercontent.com/Harvard-IACS/2018-CS109A/mathralentary HTML(styles)
```

Out[3]:

#### **INSTRUCTIONS**

- To submit your assignment follow the <u>instructions given in canvas</u> (<a href="https://canvas.harvard.edu/courses/42693/pages/homework-policies-and-submission-instructions">https://canvas.harvard.edu/courses/42693/pages/homework-policies-and-submission-instructions</a>).
- This homework can be submitted in pairs.
- If you submit individually but you have worked with someone, please include the name of your one partner below.

Names of person you have worked with goes here:

#### In [4]:

```
%matplotlib inline
import numpy as np
import numpy.random as nd
import pandas as pd
import math
import matplotlib.pyplot as plt
import os
import seaborn as sns
sns.set(style="darkgrid")
from sklearn.linear model import LogisticRegressionCV
from sklearn.model selection import cross val score
from sklearn.metrics import accuracy score
from sklearn.metrics import confusion matrix
from sklearn.preprocessing import Imputer
from sklearn.metrics import mean squared error
from sklearn.model selection import train test split
from sklearn.preprocessing import StandardScaler
from IPython.display import display
```

# Overview

In this homework, you are free to explore different ways of solving the problems -within the restrictions of the questions. Your solutions should read like a report with figures to support your statements. Please include your code cells as usual but augment your solutions with written answers. We will also check for code readability and efficiency as we feel you have some experience now. In particular, for Q1, we expect you to write appropriate functions, such as your code can be generalized beyond the specified network architectures of his homework.

For this homework you may **not** use a machine learning library such as keras or tensorflow to build and fit the network. The objective is to build the network equations from scratch.

- Q1 explores approximating a function using a Multilayer Feedforward Network with one input layer, one hidden layer, and one output layer.
- Q2 deals with missing data in a medical dataset.

# Question 1: Construct a feed forward neural network [50 pts]

In this part of the homework you are to construct three feed forward neural networks consisting of an input layer, one hidden layer with 1, 2 and 4 nodes respectively, and an output layer. The hidden layer uses the sigmoid as the activation function and use a linear output node. You should code the equations from scratch.

You are given three datasets containing (x, y) points where y = f(x):

- In the first dataset, f(x) is a **single step** function (data in data/step df.csv),
- In the second dataset, f(x) is a **one hump** function (data in data/one\_hump\_df.csv),
- In the third dataset, f(x) is a **two equal humps** function (data in data/two hump df.csv).
- 1.1 Create a plot of each dataset and explore the structure of the data.
- **1.2** Give values to the weights **manually**, perform a forward pass using the data for the **single step** function and a hidden layer of **one** node, and plot the output from the network, in the same plot as the true *y* values. Adjust the weights (again manualy) until the plots match as closely as possible.
- **1.3** Do the same for the **one hump** function data, this time using a hidden layer consisting of **two** nodes.
- 1.4 Do the same for the two hump function data but this time increase the number of hidden nodes to four.
- **1.5** Choose the appropriate loss function and calculate and report the loss from all three cases. Derive the gradient of the output layer's weights for all three cases (step, one hump and two humps). Use the weights for the hidden layers you found in the previous question and perform gradient descent on the weights of this layer (output layer). What is the optimised weight value and loss you obtained? How many steps did you take to reach this value? What is the threshold value you used to stop?

## **Answers**

1.1

Single Step Data

#### In [5]:

```
# your code here
single_step = pd.read_csv('./data/step_df.csv')
single_step.head()
```

#### Out[5]:

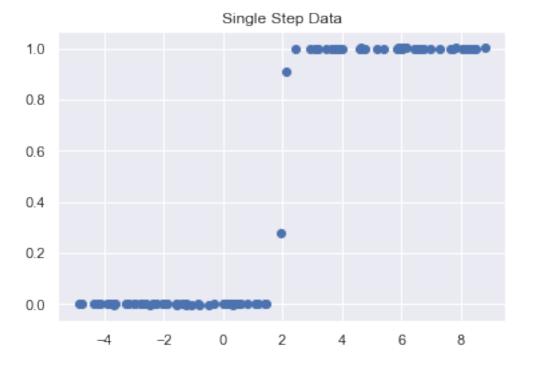
	^	У
0	-2.762886	0.000706
1	1.108371	-0.000376
2	-0.793581	-0.002845
3	-3.666329	-0.000031
4	8.805071	1.001807

#### In [6]:

```
plt.scatter(single_step.x, single_step.y)
plt.title('Single Step Data')
```

#### Out[6]:

Text(0.5,1,'Single Step Data')



# **One Hump Data**

#### In [7]:

```
one_hump = pd.read_csv('./data/one_hump_df.csv')
one_hump.head()
```

### Out[7]:

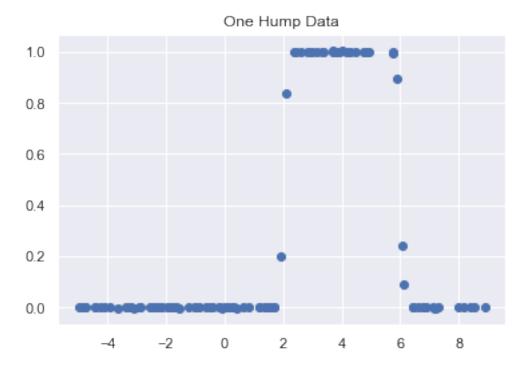
	^	У
0	3.734197	1.000226
1	6.890217	-0.000877
2	3.330365	0.999072
3	-4.250132	-0.000071
4	3.700311	1.002423

#### In [8]:

```
plt.scatter(one_hump.x, one_hump.y)
plt.title("One Hump Data")
```

# Out[8]:

Text(0.5,1,'One Hump Data')



# **Two Hump Data**

#### In [9]:

```
# your code here
two_hump = pd.read_csv('./data/two_hump_df.csv')
two_hump.head()
```

# Out[9]:

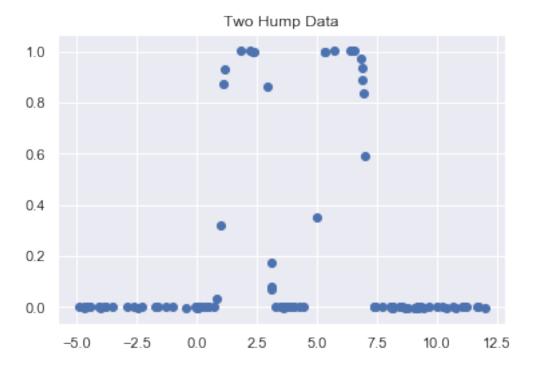
		y
0	-2.637720	0.000288
1	3.808384	0.000326
2	3.121579	0.080294
3	5.713059	1.000351
4	3.975868	0.000362

#### In [10]:

```
plt.scatter(two_hump.x, two_hump.y)
plt.title('Two Hump Data')
```

#### Out[10]:

Text(0.5,1,'Two Hump Data')



#### **Analysis**

In all three of the data sets, there is a strong non-linear relationship between the x and y variables.

#### **Coding the Neural Network**

```
In [51]:
class MLP(object):
    def init (self, input nodes, hidden nodes):
        self.l1 matrix = np.random.rand(input nodes + 1, hidden nodes)
        self.12 matrix = np.random.rand(hidden nodes+1, 1)
    def set l1(self, new param):
        if new_param.shape != self.l1_matrix.shape:
            raise ValueError("New parameters must be dimension {}".format(self.11 material)
        self.l1 matrix = new param
    def set 12(self, new param):
        if new_param.shape != self.12_matrix.shape:
            raise ValueError("New parameters must be dimension {}".format(self.12 material)
        self.12 matrix = new param
    def predict(self, x):
        # define sigmoid
        sigmoid = lambda x: 1/(1+np.exp(-x))
        # add bias to x
        x = np.array(x)
        x = x.reshape(-1,1)
        x = np.append(x, np.ones((x.shape[0],1)), axis = 1)
        # run forward mode
        self.layer 1 = x.dot(self.l1 matrix)
        self.activation 1 = sigmoid(self.layer 1)
        self.activation 1 = np.append(self.activation 1, np.ones(self.activation 1.s
        self.layer 2 = self.activation 1.dot(self.12 matrix)
        return self.layer 2
    def loss(self, x, y):
        y_hat = self.predict(x)
        y = y.values.reshape(-1,1)
        return np.mean((y-y hat)**2)
    def grad(self, x, y):
        y hat = self.predict(x)
        y = y.values.reshape(-1,1)
        grad = np.mean(-2*(y-y_hat)*self.activation_1, axis = 0)
        return grad.reshape(-1,1)
    def optimize_layer_2(self, x, y, epochs, lr, threshold = 1e-5):
        e = 0
```

```
while e < epochs and self.loss(x, y) > threshold:
    grad = self.grad(x, y)
    self.set_l2(self.l2_matrix - lr*grad)
    e += 1
print('converged in {} epochs'.format(e))
```

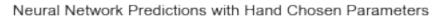
1.2

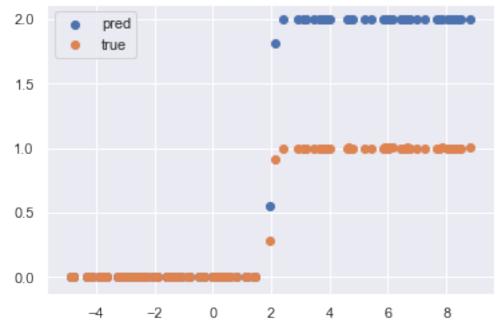
#### In [52]:

```
# initialize network
network_step = MLP(1, 1)
new_l1 = np.array([20,-40]).reshape(2,1)
network_step.set_l1(new_l1)
new_l2 = np.array([2,0]).reshape(2,1)
network_step.set_l2(new_l2)
```

#### In [53]:

```
plt.scatter(single_step.x, network_step.predict(single_step.x), label = 'pred')
plt.scatter(single_step.x, single_step.y, label = 'true')
plt.legend()
plt.title("Neural Network Predictions with Hand Chosen Parameters")
plt.show()
```



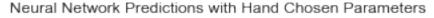


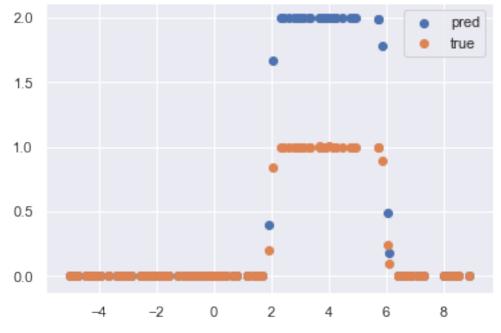
#### In [57]:

```
# initialize network
network_one_hump = MLP(1, 2)
new_l1 = np.array([[20,20],[-40,-120]])
network_one_hump.set_l1(new_l1)
new_l2 = np.array([2,-2,0]).reshape(3,1)
network_one_hump.set_l2(new_l2)
```

#### In [58]:

```
plt.scatter(one_hump.x, network_one_hump.predict(one_hump.x), label = 'pred')
plt.scatter(one_hump.x, one_hump.y, label = 'true')
plt.legend()
plt.title("Neural Network Predictions with Hand Chosen Parameters")
plt.show()
```





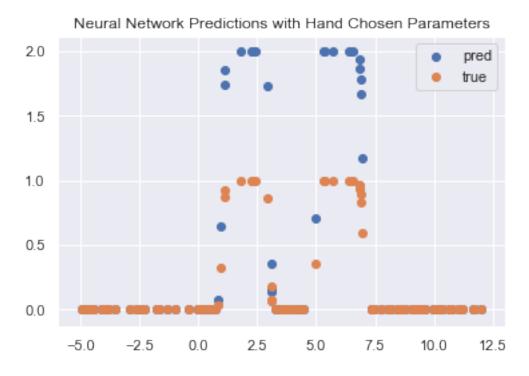
# 1.4

#### In [60]:

```
# initialize network
network_two_hump = MLP(1, 4)
new_l1 = np.array([[20,20,20,20],[-20,-60,-100,-140]])
network_two_hump.set_l1(new_l1)
new_l2 = np.array([2,-2,2,-2,0]).reshape(5,1)
network_two_hump.set_l2(new_l2)
```

#### In [61]:

```
plt.scatter(two_hump.x, network_two_hump.predict(two_hump.x), label = 'pred')
plt.scatter(two_hump.x, two_hump.y, label = 'true')
plt.legend()
plt.title("Neural Network Predictions with Hand Chosen Parameters")
plt.show()
```



**1.5** Choose the appropriate loss function and calculate and report the loss from all three cases.

I chose to implement a mean squared loss function

Hence, the gradient of the output layer's weights for all three cases (step, one hump and two humps) is  $\nabla L_2 = 1/n \sum_{i=1}^n \left( -2(y_i - \overset{\wedge}{y_i}) * \sigma(X_i L_1) \right)$ 

The threshold value I'm using is 1e-5.

#### **Gradient Descent Single Step**

```
In [62]:
network_step.optimize_layer_2(single_step.x, single_step.y, 10000, 0.1)
print('Layer 2 parameters')
network_step.12_matrix
converged in 122 epochs
Layer 2 parameters
Out[62]:
array([[ 1.00581744],
       [-0.00314928]]
In [63]:
network_one_hump.optimize_layer_2(one_hump.x, one_hump.y, 10000, 0.1)
print('Layer 2 parameters')
network_one_hump.12_matrix
converged in 283 epochs
Layer 2 parameters
Out[63]:
array([[ 1.00545105],
       [-1.00848556],
       [-0.00109126]]
In [64]:
network_two_hump.optimize_layer_2(two_hump.x, two_hump.y, 10000, 0.1)
print('Layer 2 parameters')
network_two_hump.12_matrix
converged in 889 epochs
Layer 2 parameters
Out[64]:
array([[ 1.01116114],
       [-1.01408857],
       [ 1.00698042],
       [-1.00331341],
       [-0.00106433]]
```

From these results, we can see that it takes more epochs for gradient descent to converge when the there are more parameters in the model.

# Question 2: Working with missing data. [50 pts]

In this exercise we are going to use the **Pima Indians onset of diabetes** dataset found in <code>pima-indians-diabetes.csv</code>. This dataset describes patient medical record data for Pima Indians and whether they had an onset of diabetes within five years. It is a binary classification problem (onset of diabetes as 1 or not as 0). The input variables that describe each patient are numerical and have varying scales. The list below shows the eight attributes plus the target variable for the dataset:

- Number of times pregnant.
- Plasma glucose concentration a 2 hours in an oral glucose tolerance test.
- Diastolic blood pressure (mm Hg).
- Triceps skin fold thickness (mm).
- 2-Hour serum insulin (mu U/ml).
- Body mass index.
- Diabetes pedigree function.
- Age (years).
- Outcome (1 for early onset of diabetes within five years, 0 for not), target class.

2.1. Load the dataset into a pandas dataframe named <code>pima\_df</code> . Clean the data by looking at the various features and making sure that their values make sense. Look for missing data including disguised missing data. The problem of disguised missing data arises when missing data values are not explicitly represented as such, but are coded with values that can be misinterpreted as valid data. Comment on your findings.

```
In [88]:
```

```
pima_df = pd.read_csv('./data/pima-indians-diabetes.csv')
pima_df.head()
```

#### Out[88]:

	Pregnancies	Glucose	BloodPressure	SkinThickness	Insulin	BMI	DiabetesPedigreeFunction
0	6	148	72	35	0	33.6	0.627
1	1	85	66	29	0	26.6	0.351
2	8	183	64	0	0	23.3	0.672
3	1	89	66	23	94	28.1	0.167
4	0	137	40	35	168	43.1	2.288

```
In [89]:
pima_df.dtypes
Out[89]:
Pregnancies
                                 int64
Glucose
                                 int64
BloodPressure
                                 int64
SkinThickness
                                 int64
Insulin
                                 int64
BMI
                               float64
DiabetesPedigreeFunction
                               float64
                                 int64
Age
Outcome
                                object
dtype: object
It's strange that Outcome is type object. Let's investigate further.
In [90]:
pima df.Outcome.unique()
Out[90]:
array(['1', '0', '0\\', '1\\', '0}'], dtype=object)
I'm assuming that these are data entry errors - I will remove the slashes and brackets
In [91]:
pima df.Outcome = pima df.Outcome.apply(lambda x : x[0]).astype('category')
pima_df.Outcome.unique()
```

Much better! Now let's turn our attention to the predictors.

Categories (2, object): [1, 0]

Out[91]:

[1, 0]

#### In [92]:

pima\_df.describe()

#### Out[92]:

	Pregnancies	Glucose	BloodPressure	SkinThickness	Insulin	ВМІ	Diabetes
count	764.000000	764.000000	764.000000	764.000000	764.000000	764.000000	
mean	3.853403	120.922775	69.111257	20.537958	80.070681	31.998429	
std	3.374327	32.039835	19.403339	15.970234	115.431087	7.899591	
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	
25%	1.000000	99.000000	62.000000	0.000000	0.000000	27.300000	
50%	3.000000	117.000000	72.000000	23.000000	34.000000	32.000000	
75%	6.000000	141.000000	80.000000	32.000000	128.250000	36.600000	
max	17.000000	199.000000	122.000000	99.000000	846.000000	67.100000	

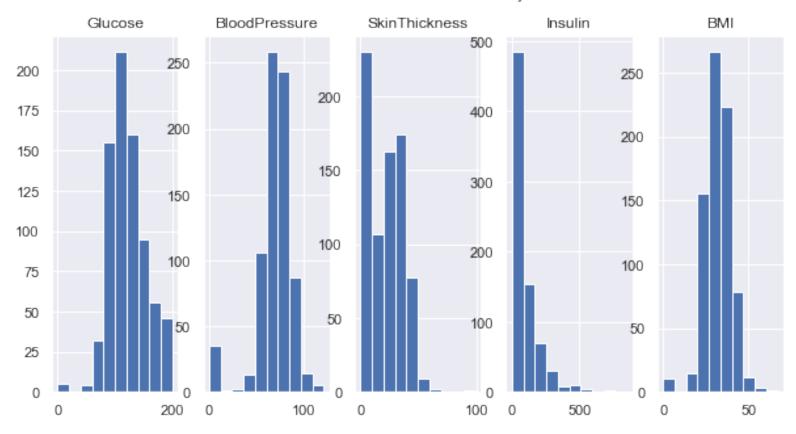
There are two issues that deserve further investigating.

- 1. Glucose, BloodPressure, SkinThickness, Insulin, and BMI should never be 0, yet they all have min 0.
- 2. Glucose, BloodPressure, SkinThickness, Insulin, and BMI have high maximums and these outliers might be errors.

#### In [93]:

/Users/joshfeldman/anaconda3/envs/py36/lib/python3.6/site-packages/mat plotlib/figure.py:457: UserWarning: matplotlib is currently using a no n-GUI backend, so cannot show the figure "matplotlib is currently using a non-GUI backend,"

Distribution of Predictors that Should Potentially be Non-Zero



These predictors seem to have an abnormal number of zeros, which makes me think that zeros are indeed missing values. I will replace them with None

#### In [94]:

```
non_zero_columns = ['Glucose', 'BloodPressure', 'SkinThickness', 'Insulin', 'BMI']
pima_df[non_zero_columns] = pima_df[non_zero_columns].replace(0,np.nan)
pima_df.describe()
```

#### Out[94]:

	Pregnancies	Glucose	BloodPressure	SkinThickness	Insulin	BMI	DiabetesF
count	764.000000	759.000000	729.000000	538.000000	393.000000	753.00000	
mean	3.853403	121.719368	72.429355	29.165428	155.659033	32.46587	
std	3.374327	30.597938	12.406940	10.502130	118.906865	6.93688	
min	0.000000	44.000000	24.000000	7.000000	14.000000	18.20000	
25%	1.000000	99.000000	64.000000	22.000000	76.000000	27.50000	
50%	3.000000	117.000000	72.000000	29.000000	125.000000	32.30000	
<b>75</b> %	6.000000	141.000000	80.000000	36.000000	190.000000	36.60000	
max	17.000000	199.000000	122.000000	99.000000	846.000000	67.10000	

The minimum values now make more sense. The maximum values do not seem completely out of the ordinary, so I will leave them as is.

2.2 Split the dataset into a 75-25 train-test split (use random\_state=9001). Fit a logistic regression classifier to the training set and report the accuracy of the classifier on the test set. You should use  $L_2$  regularization in logistic regression, with the regularization parameter tuned using cross-validation (LogisticRegressionCV). Report the overall classification rate.

```
In [95]:
```

```
def get train and test acc(df, impute):
    # create a training and test set
    print("Creating train and test sets...")
    pima train, pima test = train test split(pima df, random state=9001)
    # handle missing values
    print("Imputing missing values...")
    pima train impute, pima test impute = impute(pima train, pima test)
    print("Size of training data after imputation:",len(pima train impute))
    print("Size of test data after imputation:",len(pima test impute))
    #split into predictors and labels
   print("Preprocessing data")
    pima train X = pima train impute.drop("Outcome", axis = 1)
    pima train y = pima train impute["Outcome"]
    pima test X = pima test impute.drop("Outcome", axis = 1)
    pima test y = pima test impute["Outcome"]
    # we need to scale the data to ensure the 12 regularization performs better
    scaler = StandardScaler().fit(pima train X)
    pima_train_X_scaled = scaler.transform(pima_train_X)
    # fit logistic regression with L2 penalty
   print("Fitting model...")
    model = LogisticRegressionCV().fit(pima train X scaled, pima train y)
    print("The accuracy on the training set is", accuracy_score(pima_train_y, model
    # report the accuracy on the test set
   pima test X scaled = scaler.transform(pima test X)
    print("The accuracy on the test set is", accuracy_score(pima_test_y, model.pred;
    return (model.coef_, model.intercept_)
```

#### In [96]:

```
def impute_drop(df_train, df_test):
    df_train = df_train.dropna()
    dt_test = df_test.dropna()
    return df_train, dt_test
```

```
In [97]:
```

```
coefs_drop = get_train_and_test_acc(pima_df, impute_drop)
Creating train and test sets...
Imputing missing values...
```

```
Imputing missing values...
Size of training data after imputation: 287
Size of test data after imputation: 104
Preprocessing data
Fitting model...
The accuracy on the training set is 0.7804878048780488
The accuracy on the test set is 0.7692307692307693
```

2.3 Restart with a fresh copy of the whole dataset and impute the missing data via mean imputation. Split the data 75-25 (use random\_state=9001) and fit a regularized logistic regression model. Report the overall classification rate.

```
In [98]:
```

```
def impute_mean(df_train, df_test):
    predictors = df_train.drop('Outcome',axis =1).columns
    df_train[predictors] = df_train[predictors].fillna(df_train[predictors].mean())
    df_test[predictors] = df_test[predictors].fillna(df_train[predictors].mean())
    return df_train, df_test
```

```
In [99]:
coefs_mean = get_train_and_test_acc(pima_df, impute_mean)

Creating train and test sets...
Imputing missing values...

/Users/joshfeldman/anaconda3/envs/py36/lib/python3.6/site-packages/pan das/core/frame.py:3140: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead
```

See the caveats in the documentation: http://pandas.pydata.org/pandas-docs/stable/indexing.html#indexing-view-versus-copy
(http://pandas.pydata.org/pandas-docs/stable/indexing.html#indexing-view-versus-copy)
self[k1] = value[k2]

```
Size of training data after imputation: 573
Size of test data after imputation: 191
Preprocessing data
Fitting model...
The accuracy on the training set is 0.7731239092495636
The accuracy on the test set is 0.7591623036649214
```

**2.4** Again restart with a fresh copy of the whole dataset and impute the missing data via a model-based imputation method. Once again split the data 75-25 (same random\_state=9001) and fit a regularized logistic regression model. Report the overall classification rate.

For the model-based inputation, we will use the rows for which we have no missing values to train KNN predictors. For each combination of missing and non-missing covariates in the dataset, we will train a KNN predictor to impute the missing elements.

```
In [100]:
```

```
from sklearn.neighbors import KNeighborsRegressor
```

```
In [101]:
```

```
def get_missing_in_row(row):
    row_na = row.isna()
    row_na_names = row[row_na].index
    return row_na_names
```

```
In [102]:
```

#### In [103]:

```
def impute KNN single df(df to impute, df train):
    count = 0
    models = {}
    for idx, row in df to impute.iterrows():
        if count % 10 == 0:
            print("Imputed {}/{}".format(count, len(df to impute)))
        all missing cols = list(get missing in row(row))
        for missing col in all missing cols:
            if str(missing col) + str(all missing cols) in models.keys():
                model = models[str(missing col) + str(all missing cols)]
            else:
                model = fit_KNN(missing_col, all_missing_cols, df_train)
                models[str(missing col) + str(all missing cols)] = model
            value to impute = model.predict(row
                                             .drop('Outcome')
                                             .drop(all missing cols)
                                             .values
                                             \cdotreshape(1,-1)
            row[missing col] = value to impute[0]
        df to impute.loc[idx] = row
        count += 1
    return df to impute
```

```
In [104]:
```

ew-versus-copy)

Imputed 10/573 Imputed 20/573

self.obj[item] = s

```
def impute KNN(df train, df test):
    print("Imputing training data...")
    df train = impute KNN single df(df train, df train)
    print("Imputing testing data...")
    dt test = impute KNN single df(df test, df train)
    return df train, dt test
In [105]:
coefs knn = get train and test acc(pima df, impute KNN)
Creating train and test sets...
Imputing missing values...
Imputing training data...
Imputed 0/573
/Users/joshfeldman/anaconda3/envs/py36/lib/python3.6/site-packages/pan
das/core/indexing.py:543: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row indexer,col indexer] = value instead
See the caveats in the documentation: http://pandas.pydata.org/pandas-
docs/stable/indexing.html#indexing-view-versus-copy
(http://pandas.pydata.org/pandas-docs/stable/indexing.html#indexing-vi
```

2.5 Compare the results in the 3 previous parts of this problem. Prepare a paragraph (5-6 sentences) discussing the results, the computational complexity of the methods, and explain why you get the results that you see.

For all three of the imputation methods, we achieve a test set accuracy of 76%. This might be because the missing values are missing completely at random. When data is missing completely at random, our remaining dataset is a representative sample of the original data. Mean and model based imputation shouldn't introduce any bias and lead to a similar result as simply dropping the rows with missing data.

Unfortunately, without knowing anything about how the data was collected or the underlying true data generating processes, we cannot test this hypothesis.

The model based imputation was much slower than the other methods.

2.6 This question does not have one answer and requires some experimentation. Check which coefficients changed the most between the model in 2.1-2.2 and the models in 2.3 and 2.4. Are they the coefficients you expected to change given the imputation you performed? If not explain why (supporting your explanation using the data is always a good idea).

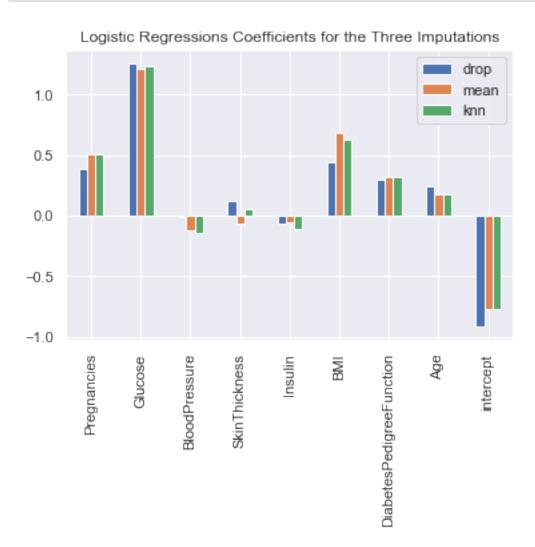
```
In [106]:
```

```
drop = list(coefs_drop[0][0])
drop.append(coefs_drop[1][0])
mean = list(coefs_mean[0][0])
mean.append(coefs_mean[1][0])
knn = list(coefs_knn[0][0])
knn.append(coefs_knn[1][0])

coefs_df = pd.DataFrame([drop,mean,knn])
covariates = list(pima_df.columns[:-1])
covariates.append("intercept")
coefs_df.columns = covariates
coefs_df.index = ['drop', 'mean', 'knn']
```

#### In [107]:

```
coefs_df.T.plot(kind = 'bar')
plt.title('Logistic Regressions Coefficients for the Three Imputations')
plt.show()
```



We should expect the coefficients resulting from mean or model-based imputation to differ from the coefficients attained through drop imputation. When we drop samples with missing data, it makes our dataset smaller, leading to a larger standard error on our coefficients. This means that for drop imputation there is a greater probability that the estimated coefficients are further from the true coefficients. Alternatively, mean imputation and model-based imputation should lead to estimates closer to the true coefficients. We see this in the graph above, with the mean and model-based imputation giving similar results, whereas drop imputation gives different estimates.

This analysis, however, rests upon the assumption that our imputation method does not introduce bias in our estimates. This is almost certainly not the case, but as mentioned above, without knowledge of how the data was collected or the data generating process we cannot assess this claim.

It does appear, however, that blood pressure, skin thickness, and insulin are not related to the onset of diabetes (all the models, regardless of the imputation method, have blood pressure, skin thickness, and insulin coefficients close to zero).