3F8 Coursework: Classification With Logistic Regression Probabilistic Model

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***Abstract*—This coursework investigates the Logistic Classification model. The model is implemented as a binary classifier, and is tested on a set of two dimensional non-linearly separable data points. The effect of under-fitting is observed through only using linear features. Non-linear feature expansion using radial basis functions is performed on the model with F1=92%.**

I. Probabilistic Model and Gradient Ascent

Consider the Logistic Classification model, aimed to classify a dataset $\mathcal{D}\{\mathcal{X},\mathcal{Y}\}$ consisting of N datapoints. The nth datapoint within the dataset is denoted $\{\boldsymbol{x}^{(n)}, y^{(n)}\}$, where $\{\boldsymbol{x}^{(n)} \in \mathbb{R}^M\}$, where M is the number of datapoint features. $y^{(n)}$ is the binary label to be predicted by the classifier.
To incorporate a bias within the model, the inputs are augmented with a fixed unit input $\hat{\boldsymbol{x}}^{(n)} = (1, \boldsymbol{x}^{(n)})$. The task of classification can therefore be expressed as:

$$\hat{\boldsymbol{y}}^{(n)} = \boldsymbol{\beta}^{\boldsymbol{T}}\hat{\boldsymbol{x}}^{(n)} = \beta_0 + \sum_{m=0}^{M}\beta_m x_m^{(n)} \tag{1}$$

In equation 1, $\hat{y}^{(n)}$ represents the model predication for the nth datapoint, $\boldsymbol{\beta}$ is the model parameter vector. The probability of the dataset is therefore a product of Bernoulli distributions, with σ being a sigmoid function:

$$\mathbb{P}(\mathcal{Y}|\mathcal{X},\boldsymbol{\beta}) = \prod_{n=1}^{N}\mathbb{P}(y^{(n)}|\hat{\boldsymbol{x}}^{(n)}) \tag{2}$$

$$= \prod_{n=1}^{N}\sigma(\boldsymbol{\beta}^{\boldsymbol{T}}\hat{\boldsymbol{x}}^{(n)})^{y^{(n)}}(1-\sigma(\boldsymbol{\beta}^{\boldsymbol{T}}\hat{\boldsymbol{x}}^{(n)}))^{1-y^{(n)}} \tag{3}$$

The gradients of the log-likelihood of the parameters $\frac{\partial}{\partial\boldsymbol{\beta}}\mathcal{L}(\boldsymbol{\beta})$ where $\mathcal{L}(\boldsymbol{\beta}) = \log\mathbb{P}(\mathcal{Y}|\mathcal{X},\boldsymbol{\beta})$ are derived. Letting $u = \boldsymbol{\beta}^{\boldsymbol{T}}\hat{\boldsymbol{x}}$:

$$\mathcal{L}(\boldsymbol{\beta}) = \log\mathbb{P}(\mathcal{Y}|\mathcal{X},\boldsymbol{\beta}) \tag{4}$$

$$= \sum_{n=1}^{N} y^{(n)}\log\sigma(u) + (1-y^{(n)})\log(1-\sigma(u)) \tag{5}$$

Taking the derivative with respect to a single parameter β_j, $\frac{\partial}{\partial\beta_j}$ is:

$$\sum_{n=1}^{N} y^{(n)}\frac{\partial}{\partial\beta_j}\log\sigma(u) + (1-y^{(n)})\frac{\partial}{\partial\beta_j}\log(1-\sigma(u)) \tag{6}$$

$$= \sum_{n=1}^{N} y^{(n)}A + (1-y^{(n)})B \tag{7}$$

The partial derivatives A and B are computed separately, applying chain rule:

$$A = \frac{\partial}{\partial\beta_j}\log\sigma(u) = \frac{\partial}{\partial\beta_j}\log K \tag{8}$$

$$= \frac{\partial}{\partial K}\frac{\partial K}{\partial u}\frac{\partial u}{\partial\beta_j} \tag{9}$$

$$= \frac{1}{K}\sigma(u)(1-\sigma(u))x_j^{(n)} \tag{10}$$

$$= (1-\sigma(u))x_j^{(n)} \tag{11}$$

Equation 10 can be written since the derivative of a sigmoid function is $\sigma(u)(1-\sigma(u))$. Repeating the same procedure to B:

$$B = \frac{\partial}{\partial\beta_j}\log(1-\sigma(u)) \tag{12}$$

$$= \frac{1}{1-\sigma(u)}\sigma(u)(\sigma(u)-1)x_j^{(n)} \tag{13}$$

$$= -\sigma(u)x_j^{(n)} \tag{14}$$

Substituting A and B into equation 7 the partial derivative with respect to one of the parameters is computed:

$$\frac{\partial\mathcal{L}}{\partial\beta_j} = \sum_{n=1}^{N}[y^{(n)} - \sigma(\beta^T\hat{x}^{(n)})]\hat{x_j}^{(n)} \tag{15}$$

$$= \sum_{n=1}^{N}[y^{(n)} - \hat{y}^{(n)}]\hat{x_j}^{(n)} \tag{16}$$

Intuitively, equation 16 states that the likelihood gradient with respect to β_j equals to the error term $y^{(n)} - \hat{y}^{(n)}$ multiplied by the datapoint's feature $\hat{x_j}^{(n)}$ that the parameter is responsible for, summed over all datapoints in the dataset.
Denoting the new parameter vector $\hat{\boldsymbol{\beta}}$, the parameter update procedure can therefore be written as:

$$\hat{\boldsymbol{\beta}} = \boldsymbol{\beta} + \eta\frac{\partial}{\partial\boldsymbol{\beta}}\mathcal{L}(\boldsymbol{\beta}) \tag{17}$$

The parameter update can be done incorporating the vectorized format of equation 16, using the dataset matrices $\mathcal{X}$ and $\mathcal{Y}$:

$$\hat{\boldsymbol{\beta}} = \boldsymbol{\beta} + \eta\mathcal{X}^T(\mathcal{Y} - \sigma(\mathcal{X}\boldsymbol{\beta})) \tag{18}$$

The pseudocode implementation of the gradient ascent algorithm is shown in algorithm 1.

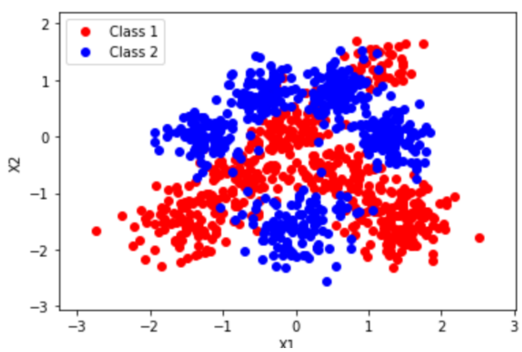
Algorithm 1 β Gradient Ascent

procedure SIGMOID($\{x_i\}_{j=1}^{N}$) **return** $1/(1+exp(-x))$
procedure PAD_ONES($\{x_{i,j}\}_{i,j=1}^{N,M}$)
  $\{y_{i,j}\}_{i,j=1}^{N,M+1} \leftarrow 0$
  $\{y_{i,j}\}_{i,j=1,2}^{N,M+1} \leftarrow \{x_{i,j}\}_{i,j=1}^{N,M}$ **return** $\{y_{i,j}\}_{i,j=1}^{N,M+1}$
procedure LOGISTIC_REGRESSION(X, Y, l_rate, max_iter)
  loss $\leftarrow$ [ ]
  $X \leftarrow$ Pad_ones(X)
  $\boldsymbol{\beta} \leftarrow$ random uniform vector
  for $i <$ max_iter **do**
    y_pred $\leftarrow$ sigmoid($X^T\boldsymbol{\beta}$)
    loss $\leftarrow$ compute_average_loss($X, Y, \boldsymbol{\beta}$)
    $\boldsymbol{\beta} \leftarrow \boldsymbol{\beta} +$ l_rate $* X^t(Y -$ y_pred) **return** $\boldsymbol{\beta}$, loss

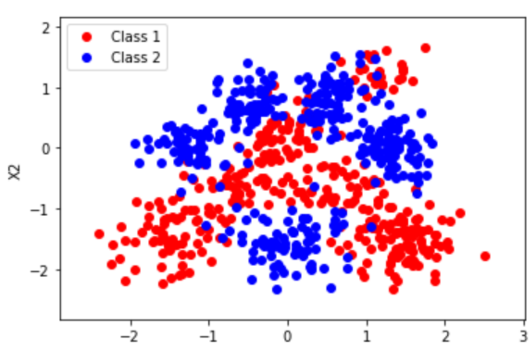
II. Exploratory Data Analysis

As the dimension of the input dataset is two, the exploratory data analysis (EDA) is carried out by simply plotting all data points with axis being the two features, coloured according to the class of the datapoint shown in figure 1(a). From the plot, it is clear that to classify the datapoints, a linear boundary is not suitable for this purpose. Non linear transformation on features of the datapoints should be used (discussed in section IV).

The data is then split into training and test sets, using existing train_test_split() function provided by the sklearn.metrics library, a split ratio of 70:30 is used as there is no need to cross validate the hyper parameters (a split ratio of 60:20:20 would have been used if a validation set is needed). A random seed is chosen to ensure the randomization step is reproducible (for debug and result sharing purposes). Figure shown in 1(b) is the plot of the training set, it is clear that the training set is representative of all datapoints.



(a) All datapoints



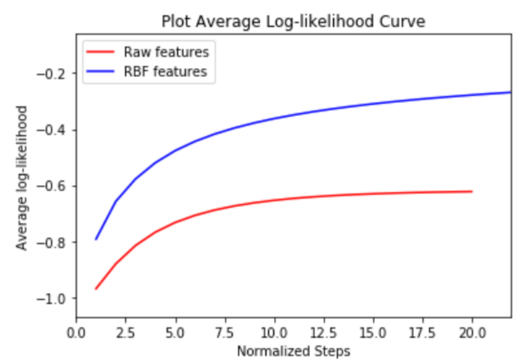
(b) Training sets

Fig. 1. EDA

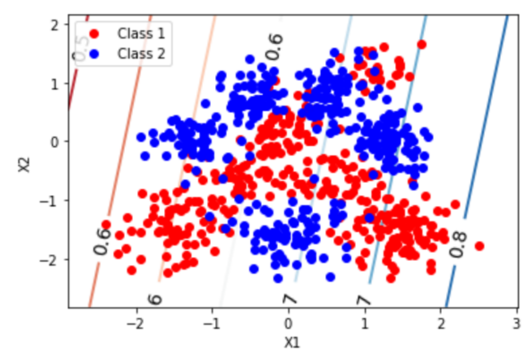
III. Python Implementation

The code described in 1 is implemented in python and is used to train the Logistic Classification method on the dataset.The red line from figure 2(a) shows the average log-likelihood obtained when the classifier is only trained on the raw input features. The predictions are visualized by adding probability contours to the plots made in figure 1(b). It is clear that by using the linear model, it is impossible for the solution space to be reached. The final training and testing log-likelihoods per datapoint is -0.62 and -0.63 respectively. The fact that the testing error is slightly less than training error indicates that underfitting may be present.

The 2x2 confusion matrix is constructed through the standard confusion_matrix() function provided by the sklearn.metrics library shown in table III, this table is obtained by setting no



(a) All datapoints



(b) Training sets

Fig. 2. Training on raw input features

		predicted label, $\hat{y}$ 0	predicted label, $\hat{y}$ 1
y	0	$P(\hat{y}=0\|y=0)$=0.752	$P(\hat{y}=0\|y=1)$ = 0.321
	1	$P(\hat{y}=0\|y=1)$ = 0.248	$P(\hat{y}=1\|y=1)$ = 0.679

TABLE I
Confusion Matrix for Raw Features Input

bias in the prediction threshold, i.e if the prediction probability is greater than 0.5, the output gets mapped to class label $\hat{y} = 1$. The F1 score calculated from the confusion matrix is 0.715.

IV. Feature Expansion

In order to reach the solution space, non-linearities are introduced to the input features. Instead of feature crossing, the inputs are expanded through a set of radial basis functions (RBFs) centred on the training datapoints. The $m+1$th feature of a datapoint therefore represents the amount of deviation of the datapoint from the mth datapoint in the training set, calculated as:

$$\hat{x}_{m+1}^{(n)} = exp\left(-\frac{1}{2l^2}\sum_{d=1}^{2}(x_d^{(n)} - x_d^{(m)})^2\right) \tag{19}$$

Where l is a hyperparameter denoting the width of the radial basis function, as it is observed later, this parameter determines whether the model is overfitting or underfitting the data. Figure 3 shows different decision boundaries drawn by varying the width $l = \{0.01, 0.1, 1\}$, it is clear that for $l = 0.01, 0.1$ the decision boundaries are over complicated therefore resulting in an over-fitted model. On the contrary, when $l = 1$, the decision boundaries are too wide, resulting in an under-fitted model. The optimum parameter for l therefore lies somewhere around 0.1 and 1, a grid search in space $\{l, \eta\}$ where η is the learning rate, can be used to determine the close-to-optimum hyper-parameters.

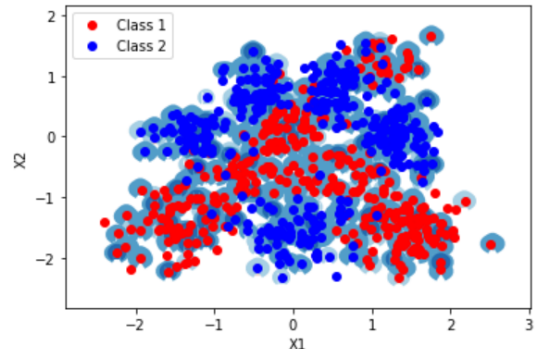
	train loss	**test loss**	C_{00}	C_{01}	C_{10}	C_{11}	$F1$
raw	-0.62	-0.633	124	53	41	112	0.714
$l = 0.01$	-0.055	-0.661	12	165	2	151	0.385
$l = 0.1$	-0.0786	-0.31	154	23	17	136	0.874
$l = 1$	-0.243	-0.239	161	16	0	143	0.92
$l = 08$	-0.211	-0.205	162	15	8	145	0.93

TABLE II
Performance table of RBF width

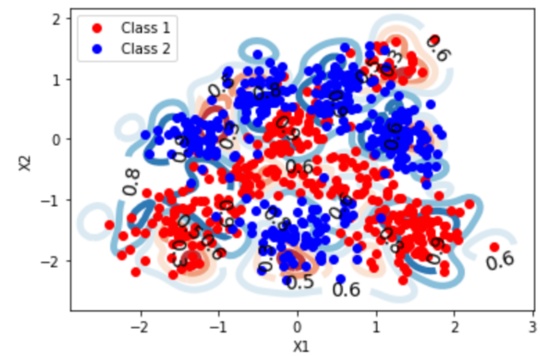
Table II shows the performance metrics with different RBF widths. Note that both the training and test set losses are in log-likelihood (closer to 0 the better), $C_{i,j}$ is a member in the **un-normalized** confusion matrix denoting $P(\hat{y} = i|y = j)$. Note that all RBF expansions except for when $l = 0.01$ beat raw input features. When $l = 0.01$, training loss is a lot less negative than test loss, indicating overfitting which is observed in figure 3(a), which corresponds the extremely poor performance on the test set when $y = 1$. Similar situation albeit less severe is observed when $l = 0.1$. Test loss is slightly above the training loss when $l = 1$, hence some degree of underfitting is present, this is validated in figure 3(c). Through experimentation (grid search not implemented), the solution of $l = 0.8$ seems to be close to optimum.

V. Conclusion and Discussion

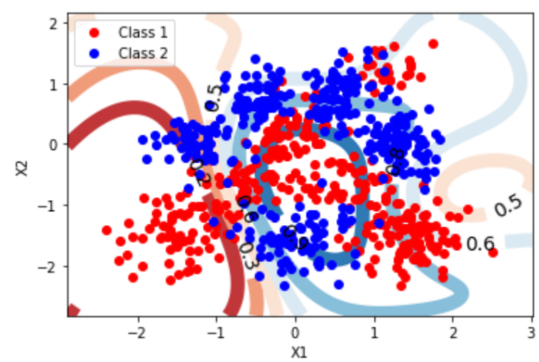
The coursework investigated a Logistic Regression model, with gradient ascent derived from taking the gradient of log-likelihood of data generation, with respect to the parameters representing the weights of the input features. The aspects of a Logistic Regression model are demonstrated on a simple binary classification of two dimensional datapoints.
Without feature engineering, it is observed that linear combination of raw input features is unable to reach the solution space, caused by underfitting. RBF is used to add non linearities and expand the feature dimension, one hyper-parameter is the width of the RBF function. Significant overfitting is observed when the width is too low ($l = 0.01$), some degree of underfitting is observed when the with is large ($l = 1$). Overall, a F1 score of 93% is achieved on the dataset using $l = 0.8, \eta = 0.001$, where η is the learning rate. Logistic regression can therefore provide good estimation on classification problems.



(a) $l = 0.01$



(b) $l = 0.1$



(c) $l = 1$

Fig. 3. RBF features learning devision boundaries

VI. Appendix: Jupyter Notebook

```
#!/usr/bin/env python
# coding: utf-8

# # 3F8 Logistic Regression Lab
# #### *Submitted by Tom Lu xl402 on
    ↪ 1/17/2019*

# In[1]:

import numpy as np
from python_code import *
from sklearn.model_selection import
    ↪ train_test_split
from sklearn.metrics import
    ↪ confusion_matrix
from sklearn.metrics import f1_score

# ## EDA

# In[2]:

# Load data, X is the input featire matrix
    ↪ , y is the one-hot encoded label
X = np.loadtxt('X.txt')
y = np.loadtxt('y.txt')
print("X␣has␣shape:␣{},␣y␣has␣shape:␣{}".
    ↪ format(X.shape, y.shape))


# **c) Using the given function *plot_data
    ↪ ()*, the dataset is visualised in
    ↪ the two dimensional input space
    ↪ displaying each datapoint's class
    ↪ label**

# In[3]:

plot_data(X,y)

# Clearly this problem cannot be linearly
    ↪ seperated, feature crossings should
    ↪ be used (later on) to improve
    ↪ classification accuracy

# **d) Split the data into training and
    ↪ test sets**
# Using the *train_test_split()* function
    ↪ already provided by sklearn, with a
    ↪ fixed random seed to make the
    ↪ results reproducable each time, the
    ↪ test/train dataset ratio is set to
    ↪ be 33% V 67%, this is because our
    ↪ dataset is sufficiently large

# In[4]:

X_train, X_test, y_train, y_test =
    ↪ train_test_split(X, y, test_size
    ↪ =0.33, random_state=69)
# Visualize it just to be sure it is
    ↪ representative of the actual data
    ↪ set
plot_data(X_train,y_train)
print("X_train␣has␣shape:␣{},␣y_train␣has␣
    ↪ shape:␣{}".format(X_train.shape,
    ↪ y_train.shape))

# **e) Transform the pseudocode from the
    ↪ perperation exercise into python
    ↪ code**


# Define sigmoid function
def sigmoid(x):
    return 1/(1+np.exp(-x))

def pad_bias(X):
    return np.append(np.ones((X.shape[0],
        ↪ 1)), X, axis = 1)

def logistic_regression(X_data, y_data,
    ↪ l_rate = 0.001, max_iter = 1000):

    loss = []
    # Add bias to training set
    X_data = pad_bias(X_data)

    # Initialize weights
    b = np.random.uniform(-1, 1, X_data.
        ↪ shape[1])

    for i in range (0, max_iter):
        # Compute sigmoid(Xb)
        y_pred = sigmoid(np.dot(X_data, b))

        # Compute log liklihood
        loss.append(compute_average_ll(
            ↪ X_data, y_data, b))

        # Weights update
        b = b + l_rate * np.dot(np.transpose
            ↪ (X_data), y_data-y_pred)
    return b, loss

# In[29]:
def plot_ll_2(ll, ll2):
    plt.figure()
    ax = plt.gca()
    plt.xlim(0, len(ll) + 2)
    plt.ylim(min(ll) - 0.1, max(ll2) + 0.1)
    ll2 = np.asarray(ll2)
    ax.plot(np.arange(1, len(ll) + 1), ll,'
        ↪ r-')
```

```
    ll2 = ll2.reshape(-1,len(ll)).mean(axis
        =1)
    ax.plot(np.arange(1, len(ll2) + 1), ll2
        ,'b-')
    plt.legend(['Raw features', 'RBF
        features'], loc='upper left')
    plt.xlabel('Normalized Steps')
    plt.ylabel('Average log-likelihood')
    plt.title('Plot Average Log-likelihood
        Curve')
    plt.show()

# Report the average log likelihood after
    each training step

# In[26]:

b, loss_array = logistic_regression(
    X_train, y_train, 0.001, max_iter =
    20)
plot_ll(loss_array)


# Visualise the predictions by adding
    probability contours to the plots
    made in part c)

# In[10]:

plot_predictive_distribution(X_train,
    y_train, b, predict_for_plot)

# Two helper functions which return the
    predicted label for given input
    features and parameters, if *thresh*
     is set to a value, then for all
    probabilities above the threshold,
    the label returns 1, otherwise 0.

# In[11]:


def predict_threshold(y_pred, thresh):
    y_pred[y_pred > thresh] = 1
    y_pred[y_pred <= thresh] = 0
    return y_pred

def predict_y(X_data, param, thresh = None
    ):
    X_data = np.append(np.ones((X_data.
        shape[0], 1)), X_data, axis = 1)
    if thresh != None:
        return predict_threshold(sigmoid(np.
            dot(X_data, param)), thresh)
    else:
        return sigmoid(np.dot(X_data, param)
            )

# Report the final traning and test log-
    likelihoods per datapoint.

# In[12]:

ll_train = compute_average_ll(pad_bias(
    X_train), y_train, b)
print("Final training log-likelihood: {}".
    format(ll_train))

ll_test = compute_average_ll(pad_bias(
    X_test), y_test, b)
print("Final test set log-likelihood: {}".
    format(ll_test))

# **f) For the test data, apply a
    threshold to the probabilistic
    predictions. Confusion matrix and f1
     score are calculated**

y_pred = predict_y(X_test, b, 0.5)
c = confusion_matrix(y_test, y_pred)
f1 = f1_score(y_test, y_pred, average='
    macro')
print("Test Set Confusion matrix: {}".
    format(c))
print("f1 score: {}".format(f1))

# **g) Expand the inputs through a set of
    RBFs centred on the training
    datapoints**

# In[241]:

def expand_inputs(l, X, Z):
    X2 = np.sum(X**2, 1)
    Z2 = np.sum(Z**2, 1)
    ones_Z = np.ones(Z.shape[ 0 ])
    ones_X = np.ones(X.shape[ 0 ])
    r2 = np.outer(X2, ones_Z) - 2 * np.dot(
        X, Z.T) + np.outer(ones_X, Z2)
    return np.exp(-0.5 / l**2 * r2)

rbf_kernel_size = 0.01
X_train_rbf = expand_inputs(
    rbf_kernel_size, X_train, X_train)

# Train the logistic classification model
    on the feature expanded inputs and
    display the new predictions

b_rbf, loss_array_rbf =
    logistic_regression(X_train_rbf,
    y_train, 0.01, max_iter = 2000)
plot_ll(loss_array_rbf)
loss_array_rbf[-1]
```

```
# In[244]:

plot_ll_2(loss_array,loss_array_rbf)

# In[175]:
def plot_predictive_distribution_expanded(
    ↪ X, y, b):
    xx, yy = plot_data_internal(X, y)
    ax = plt.gca()
    X_predict = np.concatenate((xx.ravel().
        ↪ reshape((-1, 1)),
                               yy.ravel().reshape
                                   ↪ ((-1, 1))),
                                   ↪ 1)
    x_expanded = expand_inputs(
        ↪ rbf_kernel_size, X_predict,
        ↪ X_train)
    x_tilde = np.concatenate((x_expanded,
        ↪ np.ones((x_expanded.shape[ 0 ], 1
        ↪  ))), 1)
    Z = logistic(np.dot(x_tilde, b))
    Z = Z.reshape(xx.shape)
    cs2 = ax.contour(xx, yy, Z, cmap = '
        ↪ RdBu', linewidths = 5)
    plt.clabel(cs2, fmt = '%2.1f', colors =
        ↪  'k', fontsize = 14)
    plt.show()

# Visualise the predictions using
    ↪ probability contours as in part e)

# In[176]:

plot_predictive_distribution_expanded(
    ↪ X_train, y_train, b_rbf)

# **h) Report the final training and test
    ↪ log-likelihoods per datapoint, the 2
    ↪ x2 confusion matricies are generated
    ↪  for rbf kernel size = {0.01, 0.1,
    ↪ 1}**

# In[170]:
X_test_rbf = expand_inputs(rbf_kernel_size
    ↪ , X_test, X_train)
y_pred = predict_y(X_test_rbf, b_rbf, 0.5)
c = confusion_matrix(y_test, y_pred)
f1 = f1_score(y_test, y_pred, average='
    ↪ macro')
print("Test␣set␣confusion␣matrix:␣{},␣
    ↪ kernel␣size␣is␣{}".format(c,
    ↪ rbf_kernel_size))
print("f1␣score:␣{}".format(f1))

# kerne = 0.001, f1: 0.410; kernel = 1, f1
    ↪ :0.909; kernel = 0.1, f1:0.896
```

```
# In[245]:

def compute_average_ll_2(y, y_pred, w):
    return np.mean(y * np.log(y_pred)
                   + (1 - y) * np.log(1.0 -
                       ↪ y_pred))
# In[246]:
X_test_rbf = expand_inputs(rbf_kernel_size
    ↪ , X_test, X_train)
y_pred_test = predict_y(X_test_rbf, b_rbf)
y_pred_train = predict_y(X_train_rbf,
    ↪ b_rbf)
ll_train = compute_average_ll_2(y_train,
    ↪ y_pred_train, b_rbf)
ll_test_1 = compute_average_ll_2(y_test,
    ↪ y_pred_test, b_rbf)
print(ll_train)
print(ll_test_1)
y_pred = predict_y(X_test_rbf, b_rbf, 0.5)

c = confusion_matrix(y_test, y_pred)
f1 = f1_score(y_test, y_pred, average='
    ↪ macro')
print("Test␣set␣confusion␣matrix:␣{},␣
    ↪ kernel␣size␣is␣{}".format(c,
    ↪ rbf_kernel_size))
print("f1␣score:␣{}".format(f1))
```