8E and 8F: Finding the Probability P(Y==1|X)

8E: Implementing Decision Function of SVM RBF Kernel

After we train a kernel SVM model, we will be getting support vectors and their corresponsing coefficients α_i

Check the documentation for better understanding of these attributes:

https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html

Attributes:

support_ : *array-like, shape = [n_SV]*
Indices of support vectors.

support_vectors_ : *array-like, shape = [n_SV, n_features]*
Support vectors.

n_support_ : *array-like, dtype=int32, shape = [n_class]*
Number of support vectors for each class.

dual_coef_ : *array, shape = [n_class-1, n_SV]*
Coefficients of the support vector in the decision function. For multiclass, coefficient for all 1-vs-1 classifiers. The layout of the coefficients in the multiclass case is somewhat non-trivial. See the section about multi-class classification in the SVM section of the User Guide for details.

coef_ : *array, shape = [n_class * (n_class-1) / 2, n_features]*
Weights assigned to the features (coefficients in the primal problem). This is only available in the case of a linear kernel.

coef_ is a readonly property derived from `dual_coef_` and `support_vectors_`.

intercept_ : *array, shape = [n_class * (n_class-1) / 2]*
Constants in decision function.

fit_status_ : *int*
0 if correctly fitted, 1 otherwise (will raise warning)

probA_ : *array, shape = [n_class * (n_class-1) / 2]*

probB_ : *array, shape = [n_class * (n_class-1) / 2]*
If probability=True, the parameters learned in Platt scaling to produce probability estimates from decision values. If probability=False, an empty array. Platt scaling uses the logistic function `1 / (1 + exp(decision_value * probA_ + probB_))` where `probA_` and `probB_` are learned from the dataset [R20c70293ef72-2]. For more information on the multiclass case and training procedure see section 8 of [R20c70293ef72-1].

As a part of this assignment you will be implementing the `decision_function()` of kernel SVM, here decision_function() means based on the value return by `decision_function()` model will classify the data point either as positive or negative

Ex 1: In logistic regression After traning the models with the optimal weights w we get, we will find the value $\frac{1}{1+\exp(-(wx+b))}$, if this value comes out to be < 0.5 we will mark it as negative class, else its positive class

Ex 2: In Linear SVM After traning the models with the optimal weights w we get, we will find the value of $sign(wx+b)$, if this value comes out to be -ve we will mark it as negative class, else its positive class.

Similarly in Kernel SVM After traning the models with the coefficients α_i we get, we will find the value of $sign(\sum_{i=1}^{n}(y_i\alpha_i K(x_i,x_q)) + intercept)$, here $K(x_i,x_q)$ is the RBF kernel. If this value comes out to be -ve we will mark x_q as negative class, else its positive class.

RBF kernel is defined as: $K(x_i,x_q)$ = $exp(-\gamma|$

For better understanding check this link: https://scikit-learn.org/stable/modules/svm.html#svm-mathematicalformulation

Task E

> 1. Split the data into X_{train} (60), X_{cv} (20), X_{test} (20)
>
> 2. Train $SVC(gamma = 0.001, C = 100.)$ on the (X_{train} , y_{train})
>
> 3. Get the decision boundry values f_{cv} on the X_{cv} data i.e. f_{cv} `= decision_function(` X_{cv} `)` you need to implement this decision_function()

In [1]:

```
import numpy as np
import pandas as pd
import numpy as np

from sklearn.svm import SVC
from tqdm import tqdm
from matplotlib import pyplot as plt

from sklearn.datasets import make_classification
from sklearn.model_selection import train_test_split


plt.style.use('fivethirtyeight')
```

In [2]:

```
X, y = make_classification(n_samples=5000, n_features=5, n_redundant=2,
                           n_classes=2, weights=[0.7], class_sep=0.7, random_state=15)
```

Pseudo code

clf = SVC(gamma=0.001, C=100.)
clf.fit(Xtrain, ytrain)

def decision_function(Xcv, ...): #use appropriate parameters
    for a data point x_q in Xcv:
        #write code to implement $(\sum_{i=1}^{\text{all the support vectors}}(y_i\alpha_iK(x_i, x_q)) + intercept)$, here the values y_i , α_i , and $intercept$ can be obtained from the trained model
    return *# the decision_function output for all the data points in the Xcv*

fcv = decision_function(Xcv, ...) *# based on your requirement you can pass any other parameters*

Note: Make sure the values you get as fcv, should be equal to outputs of clf.decision_function(Xcv)

In [3]:
```
# https://scikit-learn.org/stable/modules/generated/sklearn.model_selection.train_test_split.html
# https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html

# 1. Split the data into Xtrain(60), Xcv(20), Xtest(20)
x_tr, x_test, y_tr, y_test = train_test_split(X, y, test_size = 0.2,
                                               stratify = y, random_state = 2)
x_train, x_cv, y_train , y_cv = train_test_split(x_tr, y_tr, test_size = 0.25,
                                               stratify = y_tr, random_state = 2)

print('X_Train shape',x_train.shape )
print('X_Test shape',x_test.shape )
print('X_Cv shape',x_cv.shape )

# 2. Train SVC(gamma=0.001,C=100.) on the (Xtrain, ytrain)

gamma_ = 0.001
svc_clf = SVC(gamma = gamma_, C = 100)
svc_clf.fit(x_train, y_train)
```

```
X_Train shape (3000, 5)
X_Test shape (1000, 5)
X_Cv shape (1000, 5)
```

Out[3]:
```
▾ SVC
SVC(C=100, gamma=0.001)
```

def decision_function(Xcv, ...): #use appropriate parameters

for a data point x_q in Xcv:

#write code to implement $(\sum_{i=1}^{\text{all the support vectors}}(y_i\alpha_i K(x_i, x_q)) + intercept)$, here the values y_i, α_i, and $intercept$ can be obtained from the trained model

return *# the decision_function output for all the data points in the Xcv*

fcv = decision_function(Xcv, ...) # *based on your requirement you can pass any other parameters*

Similarly in Kernel SVM After traning the models with the coefficients α_i we get, we will find the value of $sign(\sum_{i=1}^{n}(y_i\alpha_i K(x_i, x_q)) + intercept)$, here $K(x_i, x_q)$ is the RBF kernel. If this value comes out to be -ve we will mark x_q as negative class, else its positive class.

RBF kernel is defined as: $K(x_i, x_q)$ = $exp(-\gamma|$

In [4]:
```
# https://towardsdatascience.com/radial-basis-function-rbf-kernel-the-go-to-kernel-acf0d22c798a
# https://towardsdatascience.com/support-vector-machines-learning-data-science-step-by-step-f2a569d90f76
# https://github.com/eriklindernoren/ML-From-Scratch/blob/master/
#         mlfromscratch/supervised_learning/support_vector_machine.py

def decision_function(x, intercept, coeff, support_vector, gamma ):

#     RBF kernel is defined as: K(xi,xq) = exp(-γ||xi-xq||2)
    kernel = np.zeros((x.shape[0], support_vector.shape[0]))
    for id_x, pt in enumerate(x):
        for id_y, vec in enumerate(support_vector):
            k_value = np.exp(-gamma * np.sum((pt- vec)**2))
```

```
            kernel[id_x][id_y] = k_value

#    yi*αi*K(xi,xq)) + intercept
    custom_decision = np.sum(coeff * kernel, axis = 1) + intercept

    return custom_decision
```

In [5]:

```
fcv = decision_function(x_cv, svc_clf.intercept_, svc_clf.dual_coef_,
                                                    svc_clf.support_vectors_, gamma_ )
```

Comparing Custom implementation and Native SVC implementation

In [6]:

```
print(f'Shape at Native SVC implementation\t : {fcv.shape}')
print(f'Shape at Custom implementation\t\t : {fcv.shape}')
```

```
Shape at Native SVC implementation       : (1000,)
Shape at Custom implementation           : (1000,)
```

In [7]:

```
# https://numpy.org/doc/stable/reference/generated/numpy.around.html

result_ = all(np.round(svc_clf.decision_function(x_cv), 7) == np.round(fcv, 7))
print(f"'True' if all values are same, other-wise 'False'\t: {result_}")

n_ = 180

print(f'\nComparison of 1st {n_} values :\
            \n{np.round(svc_clf.decision_function(x_cv)[:n_], 7) == np.round(fcv[:n_], 7)}')

fcv[:20]
```

```
'True' if all values are same, other-wise 'False'       : True

Comparison of 1st 180 values :
[ True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True]
```

Out[7]:

```
array([-3.2630509 ,  1.84661142, -3.92647752, -1.67949529, -2.14324374,
       -3.05654121, -3.31298576, -1.56365973, -3.76088812, -3.70935314,
        1.71459596, -2.87275849, -2.57540088, -3.01488941, -3.46797186,
       -0.73400885, -1.33553508,  0.24029827, -1.53850604, -1.13269479])
```

8F: Implementing Platt Scaling to find P(Y==1|X)

Let the output of a learning method be $f(x)$. To get calibrated probabilities, pass the output through a sigmoid:

$$P(y=1|f) = \frac{1}{1+exp(Af+B)} \qquad (1)$$

where the parameters A and B are fitted using maximum likelihood estimation from a fitting training set (f_i, y_i). Gradient descent is used to find A and B such that they are the solution to:

$$\underset{A,B}{argmin}\{-\sum_i y_i log(p_i) + (1-y_i)log(1-p_i)\}, \qquad (2)$$

where

$$p_i = \frac{1}{1+exp(Af_i+B)} \qquad (3)$$

Two questions arise: where does the sigmoid train set come

Two questions arise: where does the sigmoid train set come from? and how to avoid overfitting to this training set?

If we use the same data set that was used to train the model we want to calibrate, we introduce unwanted bias. For example, if the model learns to discriminate the train set perfectly and orders all the negative examples before the positive examples, then the sigmoid transformation will output just a 0,1 function. So we need to use an independent calibration set in order to get good posterior probabilities. This, however, is not a draw back, since the same set can be used for model and parameter selection.

To avoid overfitting to the sigmoid train set, an out-of-sample model is used. If there are N_+ positive examples and N_- negative examples in the train set, for each training example Platt Calibration uses target values y_+ and y_- (instead of 1 and 0, respectively), where

$$y_+ = \frac{N_+ + 1}{N_+ + 2}; \; y_- = \frac{1}{N_- + 2} \tag{4}$$

For a more detailed treatment, and a justification of these particular target values see (Platt, 1999).

Check this PDF

TASK F

1. Apply SGD algorithm with (f_{cv} , y_{cv}) and find the weight W intercept b `Note: here our data is of one dimensional so we will have a one dimensional weight vector i.e W.shape (1,)`

Note1: Don't forget to change the values of y_{cv} as mentioned in the above image. you will calculate y+, y- based on data points in train data

Note2: the Sklearn's SGD algorithm doesn't support the real valued outputs, you need to use the code that was done in the `'Logistic Regression with SGD and L2'` Assignment after modifying loss function, and use same parameters that used in that assignment.

```
def log_loss(w, b, X, Y):
    N = len(X)
    sum_log = 0
    for i in range(N):
        sum_log += Y[i]*np.log10(sig(w, X[i], b)) + (1-Y[i])*np.log10(1-sig(w, X[i], b))
    return -1*sum_log/N
```

if Y[i] is 1, it will be replaced with y+ value else it will replaced with y- value

1. For a given data point from X_{test} , $P(Y = 1|$ where f_{test} `= decision_function(` X_{test} `)` , W and b will be learned as metioned in the above step

In [8]:

```
# https://www.delftstack.com/howto/numpy/numpy-count-zero/
# https://numpy.org/doc/stable/reference/generated/numpy.count_nonzero.html

n_pos = np.count_nonzero(y_train)
print(f'Positive counts : {n_pos}')

n_neg = len(y_train) - n_pos
```

```
print(f'Negative counts : {n_neg}')

calibrated_y_pos = (n_pos + 1) / (n_pos + 2)
calibrated_y_neg = 1 / (n_neg + 2)

print(f"\nCalibrated 'y' positives : {round(calibrated_y_pos, 4)}")
print(f"Calibrated 'y' negatives : {round(calibrated_y_neg, 4)}")
```

```
Positive counts : 908
Negative counts : 2092

Calibrated 'y' positives : 0.9989
Calibrated 'y' negatives : 0.0005
```

In [9]:

```
# changing $y\_cv$ values

updated_y_cv = []

for p in y_cv:
    if p == 1:
        updated_y_cv.append(calibrated_y_pos)
    else:
        updated_y_cv.append(calibrated_y_neg)
```

In [10]:

```
def sigmoid(w, x, b):
    z = np.dot(w, x) + b
    return (1 / (1 + np.exp(-z)))

def log_loss(w, b, X, Y):

    N = len(X)
    sum_log = 0

    for i in range(N):
        sum_log += Y[i] * np.log10(sigmoid(w, X[i], b)) + \
                        (1 - Y[i]) * np.log10(1 - sigmoid(w, X[i], b))

    return (-1 * sum_log / N)
```

$dw^{(t)} = x_n(y_n - \sigma$

$db^{(t)} = y_n - \sigma$

In [11]:

```
N = len(fcv)
w = np.zeros_like(fcv[0])
b = 0

eta0 = 0.0001
alpha = 0.0001
epochs = 25

cv_loss = []

y = updated_y_cv

for epoch in tqdm(range(epochs)):
    for j in range(N):

        dw = fcv[j] * (y[j] - sigmoid(w, fcv[j], b)) - (( alpha / N) * w)
        w = w + (eta0 * dw)

        db = y[j] - sigmoid(w, fcv[j], b)
        b = b + (eta0 * db)

    loss = log_loss(w, b, fcv, y)
    cv_loss.append(loss)
```

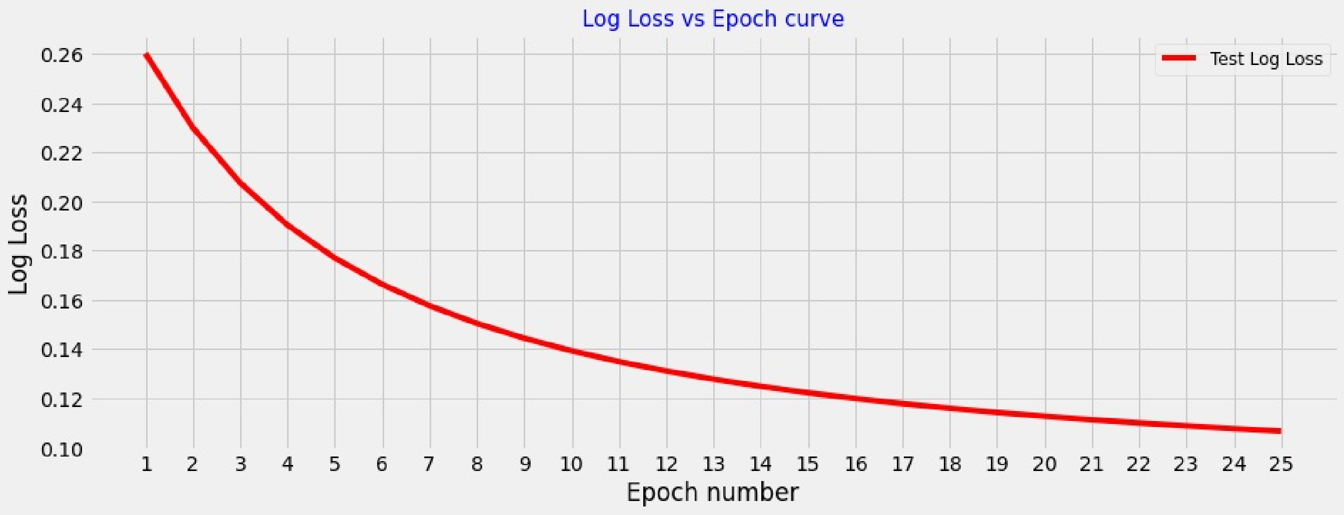
```
100%|████████████████████████████████████████████| 25/25 [00:00<00:00, 64.59it/s]
```

In [12]:

```
epoch = np.arange(epochs) + 1
plt.figure(figsize = (14,5))

plt.plot(epoch, cv_loss, c = 'r',label='Test Log Loss')
plt.xticks(epoch)
plt.title('Log Loss vs Epoch curve', fontsize = 15, c = 'b')
plt.xlabel("Epoch number")
plt.ylabel('Log Loss')
plt.legend(fontsize = 12)
```

```
plt.show()
```



In [13]:

```
print(f"Optimized 'w' : {w}\nOptimized 'b' : {b}")
```

```
Optimized 'w' : 0.8964154031692937
Optimized 'b' : -0.1059103765770649
```

In [14]:

```
f_test = decision_function(x_test, svc_clf.intercept_, svc_clf.dual_coef_,
                           svc_clf.support_vectors_, gamma_ )
```

In [15]:

```
probas = sigmoid(w, f_test, b)

print('Probability scores corresponding to $X\_test$ :\n')

for i in range(0, len(probas),2):
    print(f'{i+1} : {round(probas[i], 7)}\t\t{i+2} : {round(probas[i+1],7)}')
```

Probability scores corresponding to X_test :

```
1 : 0.4165747           2 : 0.0190188
3 : 0.6271969           4 : 0.1733171
5 : 0.4585853           6 : 0.799688
7 : 0.061171            8 : 0.7661707
9 : 0.872142            10 : 0.1896545
11 : 0.007809           12 : 0.7174306
13 : 0.0637876          14 : 0.3933717
15 : 0.7223651          16 : 0.1927996
17 : 0.6349105          18 : 0.0931003
19 : 0.0616461          20 : 0.0680393
21 : 0.0444377          22 : 0.1406477
23 : 0.0845875          24 : 0.771343
25 : 0.1622533          26 : 0.0483245
27 : 0.0572729          28 : 0.0372025
29 : 0.0634906          30 : 0.0449975
31 : 0.0204865          32 : 0.0643757
33 : 0.0752368          34 : 0.8300568
35 : 0.8632498          36 : 0.0898285
37 : 0.1689578          38 : 0.0968646
39 : 0.0377977          40 : 0.0439399
41 : 0.1686636          42 : 0.5903914
43 : 0.1012054          44 : 0.0364759
45 : 0.1035759          46 : 0.0853356
47 : 0.3474237          48 : 0.734585
49 : 0.8377354          50 : 0.0791457
51 : 0.2379581          52 : 0.1557444
53 : 0.8181413          54 : 0.8582482
55 : 0.0376176          56 : 0.8714598
57 : 0.2167779          58 : 0.4265603
59 : 0.8862525          60 : 0.1085779
61 : 0.8320746          62 : 0.2660353
63 : 0.3004638          64 : 0.1759626
65 : 0.0781887          66 : 0.0840931
67 : 0.1108084          68 : 0.0670411
69 : 0.0320749          70 : 0.1243772
71 : 0.3193777          72 : 0.0513671
73 : 0.1228921          74 : 0.222336
75 : 0.5904902          76 : 0.0273043
77 : 0.0422021          78 : 0.1293486
79 : 0.7925336          80 : 0.7626793
```

81 : 0.4540692 82 : 0.8104249
83 : 0.0339327 84 : 0.1973169
85 : 0.0600657 86 : 0.5915985
87 : 0.8741682 88 : 0.050328
89 : 0.712379 90 : 0.7569324
91 : 0.0883039 92 : 0.7131215
93 : 0.0603754 94 : 0.0538948
95 : 0.2360916 96 : 0.4144056
97 : 0.0588722 98 : 0.0207701
99 : 0.059212 100 : 0.8445676
101 : 0.1336626 102 : 0.7559836
103 : 0.0535805 104 : 0.0894821
105 : 0.1089454 106 : 0.0778952
107 : 0.1479503 108 : 0.4765982
109 : 0.4084003 110 : 0.1946074
111 : 0.0752162 112 : 0.0724592
113 : 0.0388725 114 : 0.1393005
115 : 0.7437013 116 : 0.8559409
117 : 0.9405504 118 : 0.01187
119 : 0.0386836 120 : 0.7375065
121 : 0.8537572 122 : 0.8279527
123 : 0.7271689 124 : 0.8609402
125 : 0.1156322 126 : 0.0763227
127 : 0.0645989 128 : 0.7809083
129 : 0.1959797 130 : 0.3050527
131 : 0.1394914 132 : 0.0248915
133 : 0.1093614 134 : 0.0797313
135 : 0.0506046 136 : 0.052886
137 : 0.1602985 138 : 0.1562373
139 : 0.1211836 140 : 0.8560652
141 : 0.0644889 142 : 0.8732613
143 : 0.6216455 144 : 0.6537779
145 : 0.1515319 146 : 0.4720842
147 : 0.5101588 148 : 0.0361035
149 : 0.0651236 150 : 0.0365127
151 : 0.1603164 152 : 0.0772473
153 : 0.4065972 154 : 0.0618147
155 : 0.1079551 156 : 0.8017678
157 : 0.0654119 158 : 0.0865315
159 : 0.0389689 160 : 0.0599703
161 : 0.1068038 162 : 0.8007216
163 : 0.8566436 164 : 0.8592045
165 : 0.8767332 166 : 0.0974953
167 : 0.8390979 168 : 0.8616407
169 : 0.4779008 170 : 0.0110815
171 : 0.7360725 172 : 0.5669181
173 : 0.7032836 174 : 0.0506348
175 : 0.140132 176 : 0.6594581
177 : 0.1203434 178 : 0.0501157
179 : 0.2488659 180 : 0.8782152
181 : 0.337796 182 : 0.0470368
183 : 0.375333 184 : 0.0856449
185 : 0.1884772 186 : 0.6981141
187 : 0.773522 188 : 0.4481496
189 : 0.1838304 190 : 0.0309949
191 : 0.3250267 192 : 0.0264273
193 : 0.7616043 194 : 0.5134539
195 : 0.0915411 196 : 0.1052337
197 : 0.0876359 198 : 0.0875543
199 : 0.9076548 200 : 0.658391
201 : 0.0886875 202 : 0.8277083
203 : 0.0358457 204 : 0.3073069
205 : 0.0894901 206 : 0.0684587
207 : 0.9029777 208 : 0.4794582
209 : 0.0750636 210 : 0.1538429
211 : 0.3483755 212 : 0.6269176
213 : 0.0595161 214 : 0.1172843
215 : 0.2153521 216 : 0.1063794
217 : 0.6738411 218 : 0.8259964
219 : 0.1219957 220 : 0.0763856
221 : 0.0756919 222 : 0.4506184
223 : 0.0082704 224 : 0.0849395
225 : 0.0467083 226 : 0.0565634
227 : 0.3385379 228 : 0.157075
229 : 0.1099592 230 : 0.724935
231 : 0.0677357 232 : 0.4785039
233 : 0.0605863 234 : 0.8224583
235 : 0.0673795 236 : 0.8102354
237 : 0.085959 238 : 0.0562769
239 : 0.063391 240 : 0.4028321
241 : 0.0712631 242 : 0.3572159
243 : 0.2528688 244 : 0.1605152
245 : 0.2132797 246 : 0.0879745
247 : 0.4117907 248 : 0.0686321
249 : 0.8522116 250 : 0.8470699
251 : 0.0870581 252 : 0.0299667
253 : 0.0682861 254 : 0.094072
255 : 0.8211114 256 : 0.7539697
257 : 0.0766636 258 : 0.0527095

259 : 0.1247695	260 : 0.0119229
261 : 0.0448903	262 : 0.4206795
263 : 0.1376104	264 : 0.1925248
265 : 0.0541856	266 : 0.2913851
267 : 0.0365775	268 : 0.8759429
269 : 0.3873152	270 : 0.7429233
271 : 0.0515601	272 : 0.0112652
273 : 0.3541725	274 : 0.0422214
275 : 0.0862784	276 : 0.7896495
277 : 0.2402622	278 : 0.067064
279 : 0.0768621	280 : 0.906774
281 : 0.0941425	282 : 0.8288583
283 : 0.7729672	284 : 0.0982036
285 : 0.771636	286 : 0.7625684
287 : 0.0121517	288 : 0.0599596
289 : 0.8437346	290 : 0.8763085
291 : 0.3387254	292 : 0.0559814
293 : 0.8589955	294 : 0.0639958
295 : 0.1184041	296 : 0.0483672
297 : 0.9640836	298 : 0.0629093
299 : 0.0777332	300 : 0.3732268
301 : 0.1020436	302 : 0.0974396
303 : 0.8926577	304 : 0.0936333
305 : 0.0826159	306 : 0.0478238
307 : 0.1900002	308 : 0.1185805
309 : 0.1595389	310 : 0.2584356
311 : 0.605381	312 : 0.0364777
313 : 0.1458784	314 : 0.1645338
315 : 0.0617619	316 : 0.0476603
317 : 0.0682152	318 : 0.1112186
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```

Note: in the above algorithm, the steps 2, 4 might need hyper parameter tuning, To reduce the complexity of the assignment we are excluding the hyerparameter tuning part, but intrested students can try that

If any one wants to try other calibration algorithm istonic regression also please check these tutorials

1. http://fa.bianp.net/blog/tag/scikit-learn.html#fn:1
2. https://drive.google.com/open?id=1MzmA7QaP58RDzocB0RBmRiWfl7Co_VJ7
3. https://drive.google.com/open?id=133odBinMOIVb_rh_GQxxsyMRyW-Zts7a
4. https://stat.fandom.com/wiki/Isotonic_regression#Pool_Adjacent_Violators_Algorithm