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Q1 . Solution.

Following is method for Double Cross Validation on Dataset D with folds k and hyperparameter set H.

Please find doDoubleCrossValidation.py for the source code.

```

1  def doCrossValidation (D, k, h):
2
3      allIdxs = np.arange(len(D))
4      # Randomly split dataset into k folds
5      idxs = np.random.permutation(allIdxs)
6      idxs = idxs.reshape(k, -1)
7      accuracies = []
8      h_best=INT_MAX
9      acc=0
10     for fold in range(k):
11         # Get all indexes for this fold
12         testIdxs = idxs[fold,:]
13         # Get all the other indexes
14         trainIdxs = np.array(set(allIdxs) - set(testIdxs)).flatten()
15         # Train the model on the training data
16         model = trainModel(D[trainIdxs], h)
17         accuracy=testModel(model, D[testIdxs])
18         if accuracy>acc:
19             acc=accuracy
20             h_best=h
21         # # Test the model on the testing data
22         # accuracies.append(testModel(model, D[testIdxs]))
23
24     return h_best
25
26
27
28 def doDoubleCrossValidation(D, k, H):
29
30     allIdxs = np.arange(len(D))
31     # Randomly split dataset into k folds
32     idxs = np.random.permutation(allIdxs)
33     idxs = idxs.reshape(k, -1)
34
35     accuracies = []
36
37     #Outer loop
38     for outer_fold in range(k):
39         # Get all indexes for this fold
40         testIdxs_outer = idxs[outer_fold,:]
41         # Get all the other indexes
42         trainIdxs_outer = idxs[list(set(allIdxs) - set(testIdxs)),:].flatten()
43         # Train the model on the training data
44
45
46         h_best = doCrossValidation(D[trainIdxs_outer], k, H[outer_fold])
47         accuracies.append(testModel(model, D[testIdxs_outer]))
48
49     return np.mean(accuracies)

```

Q2 a. Solution.

We have $f(x, y) = x^4 + xy + x^2$
we take,

$$\frac{\partial f}{\partial x} = 4x^3 + y + 2x \quad (1)$$

$$\frac{\partial f}{\partial y} = x \quad (2)$$

We calculate Hessian matrix H_f

$$H_f = \begin{bmatrix} \frac{\partial^2 f}{\partial x \partial x} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y \partial y} \end{bmatrix} \quad (3)$$

$$H_f = \begin{bmatrix} 12x^2 + 2 & 1 \\ 1 & 0 \end{bmatrix} \quad (4)$$

So,

$$\det(H_f) = -1 \quad (5)$$

Thus as the $\det(H_f)$ is -1 the given function is not convex for $\in \mathbb{R}$

Moreover we can also check for the eigen values to be $\lambda_j \geq 0$

Q2 b. Solution.

We have f_{mse} for two layer neural network ,

$$f_{mse} = \frac{1}{2}(X^T w - y)^T (X^T w - y) \quad (6)$$

y is the n-dimensional vector of ground-truth labels and X is the design matrix and weight vector w .

For simplifying we ignore the $\frac{1}{2n}$ for now but will use it later.

$$f_{mse} = (X^T w - y)^T (X^T w - y) \quad (7)$$

From 3.d in HW 1 we know

$$\nabla_x [(Ax + b)^T (Ax + b)] = 2A^T (Ax + b) \quad (8)$$

Similarly we get,

$$\nabla_w [(x^T w - y)^T (x^T w - y)] = 2(X^T)^T X^T w \quad (9)$$

We get,

$$\nabla_w = 2X X^T w \quad (10)$$

Now taking the Hessian H of the f_{mse} i.e ∇_w^2

Thus we get

$$H = 2X X^T \quad (11)$$

Considering $\frac{1}{2n}$ from eq. 5 we get,
we get

$$H = \frac{1}{n} X X^T \quad (12)$$

For any vector $v \in \mathbb{R}$,

$$v^T H v = v^T (H) v \quad (13)$$

$$v^T H v = v^T (X X^T) v \quad (14)$$

$$v^T H v = (X v)^T (X v) \quad (15)$$

$$v^T H v = \|X v\|_2^2 \geq 0 \quad (16)$$

Therefore we have,

$$v^T H v \geq 0 \quad (17)$$

Thus the given Hessian matrix H is Positive semi definite and $v^T H v \geq 0$ for any real vector v .

Q3 . Solution.

The final MSE loss for the test data set is Dte is 83.99095638911503.

Q4 . Solution.

We have

$$\sigma(x) = \frac{1}{1 + e^{-x}} \forall x \quad (18)$$

Solution a.

$$\sigma(-x) = \frac{1}{1 + e^x} \quad (19)$$

So,

$$\begin{aligned} 1 - \sigma(-x) &= 1 - \frac{1}{1 + e^x} \\ &= \frac{1 + e^x - 1}{1 + e^x} \\ &= \frac{e^x}{1 + e^x} \\ &= \frac{1}{1 + e^{-x}} \end{aligned} \quad (20)$$

From Eq. 18 and 20 we get

$$\sigma(-x) = 1 - \sigma(x) \quad (21)$$

Hence Proved.

Solution b.

For calculating $\sigma'(x)$ we take

$$\begin{aligned} \frac{\partial \sigma(x)}{\partial x} &= \frac{\partial}{\partial x} \left(\frac{1}{1 + e^{-x}} \right) \\ &= \frac{\partial}{\partial x} (1 + e^{-x})^{-1} \\ &= -(1 + e^{-x})^{-2} \cdot (-e^{-x}) \\ &= \frac{e^{-x}}{(1 + e^{-x})^2} \\ &= \frac{1}{1 + e^{-x}} \cdot \frac{e^{-x}}{1 + e^{-x}} \end{aligned} \quad (22)$$

We get ,

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x) \cdot \sigma(-x) \quad (23)$$

From equation 21 we get,

$$\sigma'(x) = \sigma(x) \cdot (1 - \sigma(x)) \quad (24)$$

Hence Proved.
