Machine Learning

Assignment 3

Due: May 17

Lecture 5 Model Selection and Evaluation

1 Short Answers [必做，不用提交不算分数，后续公布答案后自行核对]

(1) [2pts] Explain overfitting and underfitting of machine learning models.
[2pts] Write down two aspects affecting the risk the overfitting.
[2 pt] What strategies do decision trees use to reduce the risk of overfitting?
[2 pt] What strategies do NNs use to reduce the risk of overfitting?

(2) [6pts] Derive Precision and Recall from confusion matrix (i.e., TP, TN, FP, FN). Write down the definition of F1 score given precision and recall.

(3) [6pts] Describe K-fold cross-validation. Are the error rates of different folds independent when K>2 and why?

Solutions

2 AUC [证明题，选做]

对于有限样例，请证明

$$\mathrm{AUC} = \frac{1}{m^+ m^-} \sum_{x^+ \in D^+} \sum_{x^- \in D^-} \left(\mathbb{I}(f(x^+) > f(x^-)) + \frac{1}{2} \mathbb{I}(f(x^+) = f(x^-)) \right)$$

Proof. 此处用于写证明(中英文均可)

3. Friedman 检验 [编程题，选做]

在数据集D_1、D_2、D_3、D_4、D_5 上运行了A、B、C、D、E 五种算法，算法比较序值表如表1所示:

表 1: 算法比较序值表

数据集	算法 A	算法 B	算法 C	算法 D	算法 E
D_1	2	3	1	5	4
D_2	5	4	2	3	1
D_3	4	5	1	2	3
D_4	2	3	1	5	4
D_5	3	4	1	5	2
平均序值	3.2	3.8	1.2	4	2.8

使用Friedman检验($\alpha = 0.05$) 判断这些算法是否性能都相同。若不相同，进行Nemenyi后续检验($\alpha = 0.05$)，并说明性能最好的算法与哪些算法有显著差别。本题需编程实现Friedman检验和Nemenyi后续检验。(预计代码行数小于50 行)

Solution. 此处用于写解答(中英文均可)

Lecture 6 Neural Networks

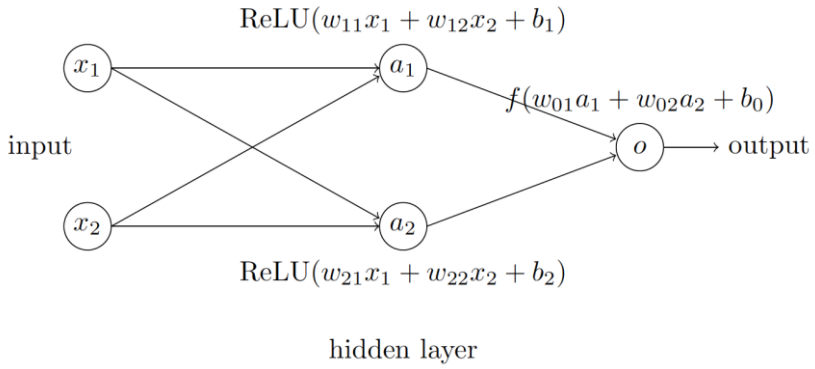
0. BP 算法推导 [必做，不提交不算分数，可根据南瓜书自行核对]

请将西瓜书教材中的标准 BP 算法的推导过程进行完整的推导，注意符号的一致性。

Solution（中英文均可）

1. [25pts] Multi-layer Perception

Suppose that we apply neural networks on a problem which has boolean inputs $x \in \{0,1\}^p$ and boolean output $y \in \{0,1\}$. The network structure example is showed as below. In this example we set $p = 2$, single hidden layer with 2 neurons, activation function $ReLU(u) = u$ if $u > 0$ otherwise 0, and an additional threshold function (e.g., $f(v) = 1$ if $v > 0$, otherwise $f(v) = 0$) for output layer.

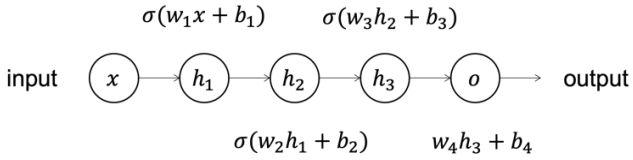


(1) [5pts] Using the structure and settings of neural network above, show that such a simple neural network could output the function $x_1 XOR\, x_2$ (equals to 0 if $x_1 = x_2$ and otherwise 1), which is impossible for linear models. State the values of parameters (i.e., w_{ij} and b_i) you found.

(2) [20pts] Now we allow the number of neurons in the hidden layer to be more than 2 but finite. Retain the structure and other settings. Show that such a neural network with single hidden layer could output an arbitrary binary function $h: \{0,1\}^p \mapsto \{0,1\}$. You can apply threshold function after each neuron in the hidden layer.

2. [10pts] Gradient explosion and gradient vanishing

As shown in the figure below, the neural network has three hidden layers, each with only one neuron, and the activation function is the sigmoid function $\sigma(x) = \frac{1}{1+e^{-x}}$. Let the input be $x = 3$. Use backpropagation to calculate the gradient, and experience the gradient explosion and gradient vanishing issues [1].

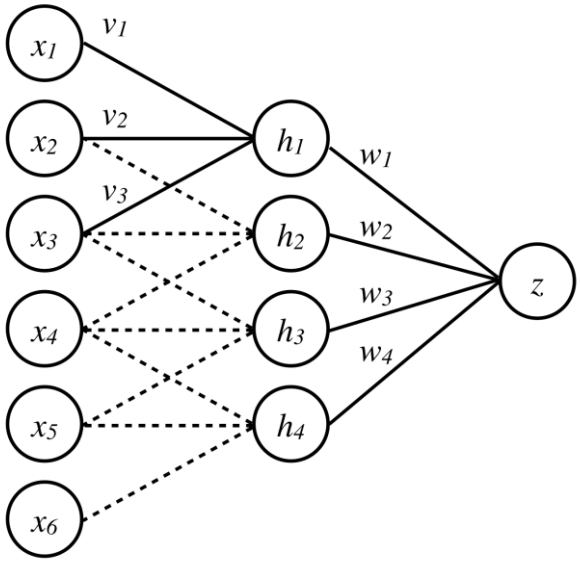


(1) [5pts] If $w_1 = 100, w_2 = 150, w_3 = 200, w_4 = 200, b_1 = -300, b_2 = -75, b_3 = -100, b_4 = 10$, calculate the gradient $\frac{\partial o}{\partial b_1}$.

(2) [5pts] If $w_1 = 0.2, w_2 = 0.5, w_3 = 0.3, w_4 = 0.6, b_1 = 1, b_2 = 2, b_3 = 2, b_4 = 1$, calculate the gradient $\frac{\partial o}{\partial b_1}$.

3. [25pts] CNN

Consider this **one-dimensional** convolutional neural network architecture.



In the first layer, we have a one-dimensional convolution with a single filter of size 3 such that $h_i = \sigma\left(\sum_{j=1}^{3} v_j\, x_{i+j-1}\right)$. The second layer is fully connected, such that $z = \sigma(\sum_{i=1}^{4} w_i\, h_i)$. The hidden units and output unit's activation function $\sigma(x)$ is the logistic (sigmoid) function with derivative $\sigma'(x) = \sigma(x)\big(1 - \sigma(x)\big)$. We perform gradient descent on the loss function $L = (y - z)^2$, where y is the training label for x.

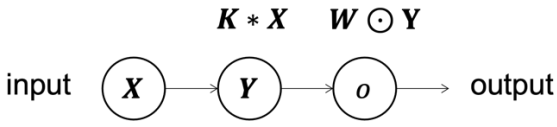
a) [5pts] What is the total number of parameters in this neural network? Recall that convolutional layers share weights. There are no bias terms.

b) [10pts] Compute $\frac{\partial L}{\partial w}$

c) [10pts] Compute $\frac{\partial L}{\partial v_i}$

4. [30pts] CNN

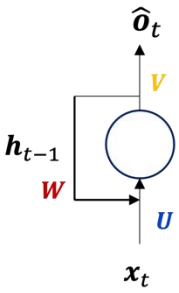
As shown in the figure below, the neural network consists of a convolutional layer and a fully connected layer, with input as $\boldsymbol{X} = \begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix}$, convolutional kernel (filter) as $\boldsymbol{K} = \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{pmatrix}$, convolution result as $\boldsymbol{Y}=\boldsymbol{K} * \boldsymbol{X} = \begin{pmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{pmatrix}$, and output as $o = \sigma(w_{11}y_{11} + w_{12}y_{12} + w_{21}y_{21} + w_{22}y_{22}), \sigma$ is sigmoid function. The sample label is z, and E is the mean squared error ($E = \frac{1}{2}\|z - o\|^2$). Find the derivative of the convolutional kernel [2].



Where, "*" is convolution, "⊙" is Hadamard product which is element-wise product.

5. [30pts] RNN: BPTT

Provide the detailed derivation process of the BPTT (Backpropagation Through Time) algorithm, ensuring that the symbols are consistent with those in the Lecture PPT.



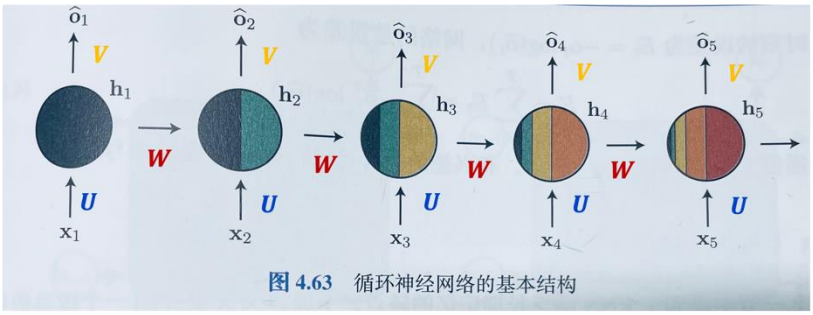


图 4.63 循环神经网络的基本结构

Reference

[1] 王贝伦, “习题 4.24,” 出处 *机器学习*, 东南大学, 2021.

[2] 王贝伦, “习题 4.25,” 出处 *机器学习*, 东南大学, 2021.