School of Data and Computer Science, Sun Yat-sen University

E14 BP Algorithm (C++/Python)

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Contents

1 Horse Colic Data Set 2
2 Reference Materials 2
3 Tasks 5
4 Codes and Results 6

1 Horse Colic Data Set

The description of the horse colic data set (http://archive.ics.uci.edu/ml/datasets/Horse+Colic) is as follows:

Data Set Characteristics:	Multivariate	**Number of Instances:**	368	**Area:**	Life
Attribute Characteristics:	Categorical, Integer, Real	**Number of Attributes:**	27	**Date Donated**	1989-08-06
Associated Tasks:	Classification	**Missing Values?**	Yes	**Number of Web Hits:**	108569

We aim at trying to predict if a horse with colic will live or die.
Note that we should deal with missing values in the data! Here are some options:

- Use the features mean value from all the available data.
- Fill in the unknown with a special value like -1.
- Ignore the instance.
- Use a mean value from similar items.
- Use another machine learning algorithm to predict the value.

2 Reference Materials

1. Stanford: **CS231n: Convolutional Neural Networks for Visual Recognition** by Fei-Fei Li,etc.
   - Course website: http://cs231n.stanford.edu/2017/syllabus.html
   - Video website: https://www.bilibili.com/video/av17204303/?p=9&tdsourcetag=s_pctim_aiomsg
2. **Machine Learning** by Hung-yi Lee
   - Course website: http://speech.ee.ntu.edu.tw/~tlkagk/index.html
   - Video website: https://www.bilibili.com/video/av9770302/from=search
3. A Simple neural network code template

```python
# -*- coding: utf-8 -*
import random
import math

# Shorthand:
# "pd_" as a variable prefix means "partial derivative"
# "d_" as a variable prefix means "derivative"
# "_wrt_" is shorthand for "with respect to"
# "w_ho" and "w_ih" are the index of weights from hidden to output layer neurons and input to hidden layer neurons respectively

class NeuralNetwork:
    LEARNING_RATE = 0.5
    def __init__(self, num_inputs, num_hidden, num_outputs, hidden_layer_weights = None, hidden_layer_bias = None, output_layer_weights = None, output_layer_bias = None):
    #Your Code Here

    def init_weights_from_inputs_to_hidden_layer_neurons(self, hidden_layer_weights):
    #Your Code Here

    def init_weights_from_hidden_layer_neurons_to_output_layer_neurons(self, output_layer_weights):
```

```
    #Your Code Here

    def inspect(self):
        print('------')
        print('* Inputs: {}'.format(self.num_inputs))
        print('------')
        print('Hidden Layer')
        self.hidden_layer.inspect()
        print('------')
        print('* Output Layer')
        self.output_layer.inspect()
        print('------')

    def feed_forward(self, inputs):
        #Your Code Here

    # Uses online learning, ie updating the weights after each training case
    def train(self, training_inputs, training_outputs):
        self.feed_forward(training_inputs)

        # 1. Output neuron deltas
        #Your Code Here
        #  E /  z

        # 2. Hidden neuron deltas
        # We need to calculate the derivative of the error with respect to the output of each hidden layer neuron
        # dE/ dy  =    E /  z   * z /  y   =    E /  z   *   w
        #  E /  z   = dE/ dy  *  z  /
        #Your Code Here

        # 3. Update output neuron weights
        #   E  /   w    =  E /  z   *   z  /   w
        # w =   *   E  /  w
        #Your Code Here

        # 4. Update hidden neuron weights
        #   E  /  w   =  E /  z   *   z  /  w
        # w =   *   E  /  w
        #Your Code Here

    def calculate_total_error(self, training_sets):
        #Your Code Here
        return total_error

class NeuronLayer:
    def __init__(self, num_neurons, bias):

        # Every neuron in a layer shares the same bias
        self.bias = bias if bias else random.random()

        self.neurons = []
        for i in range(num_neurons):
            self.neurons.append(Neuron(self.bias))

    def inspect(self):
```

```
        print('Neurons:', len(self.neurons))
        for n in range(len(self.neurons)):
            print(' Neuron', n)
            for w in range(len(self.neurons[n].weights)):
                print(' Weight:', self.neurons[n].weights[w])
            print(' Bias:', self.bias)

    def feed_forward(self, inputs):
        outputs = []
        for neuron in self.neurons:
            outputs.append(neuron.calculate_output(inputs))
        return outputs

    def get_outputs(self):
        outputs = []
        for neuron in self.neurons:
            outputs.append(neuron.output)
        return outputs

class Neuron:
    def __init__(self, bias):
        self.bias = bias
        self.weights = []

    def calculate_output(self, inputs):
    #Your Code Here

    def calculate_total_net_input(self):
    #Your Code Here

    # Apply the logistic function to squash the output of the neuron
    # The result is sometimes referred to as 'net' [2] or 'net' [1]
    def squash(self, total_net_input):
    #Your Code Here

    # Determine how much the neuron's total input has to change to move closer to the expected output
    #
    # Now that we have the partial derivative of the error with respect to the output (E/y) and
    # the derivative of the output with respect to the total net input (dy/dz) we can calculate
    # the partial derivative of the error with respect to the total net input.
    # This value is also known as the delta () [1]
    #    =  E /  z   =  E /  y   *  dy / dz
    #
    def calculate_pd_error_wrt_total_net_input(self, target_output):
    #Your Code Here

    # The error for each neuron is calculated by the Mean Square Error method:
    def calculate_error(self, target_output):
    #Your Code Here

    # The partial derivate of the error with respect to actual output then is calculated by:
    # = 2 * 0.5 * (target output - actual output) ^ (2 - 1) * -1
```

```
    # = -(target output - actual output)
    #
    # The Wikipedia article on backpropagation [1] simplifies to the following, but most other learning material does not [2]
    # = actual output - target output
    #
    # Alternative, you can use (target - output), but then need to add it during backpropagation [3]
    #
    # Note that the actual output of the output neuron is often written as y and target output as t so:
    # =  E /  y   = -( t  -  y )
    def calculate_pd_error_wrt_output(self, target_output):
    #Your Code Here

    # The total net input into the neuron is squashed using logistic function to calculate the neuron's output:
    #  y  =   = 1 / (1 + e^(-z))
    # Note that where  represents the output of the neurons in whatever layer we're looking at and  represents the layer below it
    #
    # The derivative (not partial derivative since there is only one variable) of the output then is:
    #  dy / dz  =  y  * (1 -  y )
    def calculate_pd_total_net_input_wrt_input(self):
    #Your Code Here

    # The total net input is the weighted sum of all the inputs to the neuron and their respective weights:
    # =  z  =  net  =   xw   +   xw   ...
    #
    # The partial derivative of the total net input with respective to a given weight (with everything else held constant) then is:
    # =   z  /  w   = some constant + 1 *  xw  ^(1-0) + some constant ... = x
    def calculate_pd_total_net_input_wrt_weight(self, index):
    #Your Code Here

# An example:

nn = NeuralNetwork(2, 2, 2, hidden_layer_weights=[0.15, 0.2, 0.25, 0.3], hidden_layer_bias=0.35, output_layer_weights=[0.4, 0.45, 0.5, 0.55], output_layer_bias=0.6)
for i in range(10000):
    nn.train([0.05, 0.1], [0.01, 0.99])
    print(i, round(nn.calculate_total_error([[[0.05, 0.1], [0.01, 0.99]]]), 9))
```

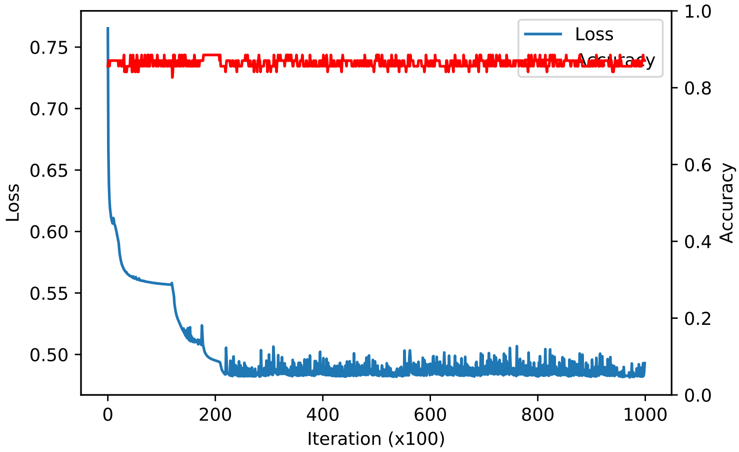
3 Tasks

- Given the training set `horse-colic.data` and the testing set `horse-colic.test`, implement the BP algorithm and establish a neural network to predict if horses with colic will live or die. In addition, you should calculate the accuracy rate.
- Please submit a file named `E14_YourNumber.pdf` and send it to `ai_201901@foxmail.com`

4 Codes and Results

This experiment costs me three full days to finish (finetune the hyperparameters), but I still cannot figure out why my accuracy is so awkward. Sad :(

The following figure gives the training loss and the accuracy (without early stopping).



The training log is shown below (with early stopping), and the best accuracy I can get is 92% accuracy on test set. (Notice the two figures are not in the same training process.)

```
Iter 1000/100000 Loss: 0.6910220450181086 Accuracy: 87.58823529411765%
Iter 1100/100000 Loss: 0.6750272830662208 Accuracy: 87.58823529411765%
Iter 1200/100000 Loss: 0.665812515211816 Accuracy: 87.58823529411765%
Iter 1300/100000 Loss: 0.6597815957555795 Accuracy: 87.58823529411765%
Iter 1400/100000 Loss: 0.6545913532922571 Accuracy: 90.5294117647059%
Iter 1500/100000 Loss: 0.6480593287768979 Accuracy: 92.0%
Iter 1600/100000 Loss: 0.6427443958094696 Accuracy: 92.0%
Iter 1700/100000 Loss: 0.6384380537773697 Accuracy: 92.0%
Iter 1800/100000 Loss: 0.6353141344986356 Accuracy: 92.0%
Iter 1900/100000 Loss: 0.6330266213543354 Accuracy: 92.0%
Iter 2000/100000 Loss: 0.6312329687173412 Accuracy: 92.0%
Iter 2100/100000 Loss: 0.6296858360830062 Accuracy: 92.0%
Iter 2200/100000 Loss: 0.6282317805795642 Accuracy: 92.0%
Iter 2300/100000 Loss: 0.6268011951659986 Accuracy: 92.0%
Early stop at iter 2400/100000 Loss: 0.625693064579745 Accuracy: 90.5294117647059%
Time: 3.130645275115967s
```

Please refer to `nn.py` and `bp.ipynb` (or the generated `bp.py`) for the codes.

Highlight some used techniques:

- The network structure is n_i-8-3.
- Used Kaiming He's method to initialize the network
- A pytorch-like network class with `forward` method is designed.
- L2-regulization and weight decay are used for training.
- All computation are based on tensor, and only the numpy package is used.
- `np.einsum` is used for accelerating the tensor product in backpropagation.
- Heavy preprocessing methods are used, including one-hot encoding, missing data complement, and useless attributes removal. please refer to `bp.ipynb` file for details.
- Early stopping is used to avoid overfitting, and learning rate decay is used for better convergence.
- Batch SGD is used to accelerate training.
- Checkpoints and logging make training more controlable.

Following gives the code of `nn.py`.

```
import numpy as np

class FullyConnectedLayer(object):
    """
    Linear transformation: y = x W^T + b
    Input: (N, in_features), i.e. a row vector, in this example, N = 1
    Output: (N, out_features)

    Attributes:
      Weight: (in_features, out_features)
      Bias: (out_features)

    Ref:
    http://cs231n.stanford.edu/vecDerivs.pdf
    """

    def __init__(self, in_features, out_features, bias=True):
        self.in_features = in_features
        self.out_features = out_features
        """
        Xavier initialization
        # https://www.deeplearning.ai/ai-notes/initialization/
        W^{[l]} &\sim \mathcal{N}(\mu=0,\sigma^2 = \frac{1}{n^{[l-1]}})
        b^{[l]} &= 0

        Kaiming He initialization
        # https://medium.com/@shoray.goel/kaiming-he-initialization-a8d9ed0b5899
        """
        self.weight = np.random.normal(0,np.sqrt(2/in_features),(out_features,in_features))
        if bias:
            self.bias = np.random.rand(out_features)
        else:
            self.bias = None

    def forward(self, inputs):
        """
        Forward propagation
        """
        if type(self.bias) != type(None):
            return np.dot(inputs, self.weight.T) + self.bias
        else:
            return np.dot(inputs, self.weight.T)

    def __call__(self,x):
        """
        Syntax sugar for forward method
        """
        return self.forward(x)

class Network(object):

    def __init__(self,in_features,hidden_features,out_features,learning_rate=0.01):
        """
        Here three-layer network architecture is used

```

```
        The number of neurons in each layer is listed below:
        in_features -> hidden_features -> out_features
        """
        self.fc1 = FullyConnectedLayer(in_features,hidden_features,True)
        self.fc2 = FullyConnectedLayer(hidden_features,out_features,True)
        self.learning_rate = learning_rate
        self.memory = {} # used for store intermediate results
        self.train_flag = True

    def train(self):
        """
        When training, memory is set to remember the intermediate results
        """
        self.train_flag = True

    def eval(self):
        """
        When inferencing, memory is no need to set
        """
        self.train_flag = False

    def relu(self,x):
        """
        Relu(x) = x, x > 0
                  0, x <= 0
        """
        return np.maximum(0,x)

    def d_relu(self,x):
        x[x <= 0] = 0
        x[x > 0] = 1
        return x

    def sigmoid(self,x):
        """
        Element-wise function
        \Sigma(x) = 1/(1+\ee^{-x})
        """
        return 1 / (1 + np.exp(-x))

    def d_sigmoid(self,x):
        """
        Derivative of sigmoid function
        \Sigma'(x) = \Sigma(x) * (1 - \Sigma(x))
        """
        return self.sigmoid(x) * (1 - self.sigmoid(x))

    def tanh(self,x):
        return np.tanh(x)

    def d_tanh(self,x):
        return 1 - np.tanh(x) ** 2

    def MSE(self,y_hat,y):
        """
        Mean-square error (MSE)
```

```
        """
        return np.linalg.norm(y_hat - y) # 2-norm

    def cross_entropy(self,y_hat,y):
        """
        Cross entropy loss
        """
        return y * np.log(y_hat) + (1 - y) * np.log(1 - y_hat)

    def forward(self,x):
        """
        w/o activation: z^{(l+1)} = W^{(l)}a^{(l)} + b^{(l)}
        w/ activation : a^{(l+1)} = f(z^{(l+1)})
        """
        # training
        if self.train_flag:
            self.memory["a0"] = np.copy(x)
            x = self.fc1(x) # N * hidden
            self.memory["z1"] = np.copy(x)
            x = self.sigmoid(x)
            self.memory["a1"] = np.copy(x)
            x = self.fc2(x) # N * out
            self.memory["z2"] = np.copy(x)
            x = self.sigmoid(x)
        # inferencing
        else:
            x = self.fc1(x) # N * hidden
            x = self.sigmoid(x)
            x = self.fc2(x) # N * out
            x = self.sigmoid(x)
        return x

    def backward(self,y_hat,y,lamb=0):
        """
        Use Mean-Squared Error (MSE) as error function

        lambda is used for weight decay

        Ref: http://ufldl.stanford.edu/tutorial/supervised/MultiLayerNeuralNetworks/
        """
        batch_size = y.shape[0]
        # Calculate \delta
        # output layer: \delta(n_l) = -(y - a(n_l)) * f'(z(n_l))
        # other layers: \delta(l) = W(l)^T\delta(l+1) * f'(z(l))
        delta = [0] * 3
        delta[2] = (y_hat - y) * self.d_sigmoid(self.memory["z2"]) # N * out_features
        delta[1] = np.dot(delta[2],self.fc2.weight) * self.d_sigmoid(self.memory["z1"]) # N
            ↪ * hidden_features
        # print(delta[2].shape,delta[1].shape)

        # Calculat \nabla
        # output layer: \nabla_{W(l)}J(W,b;x,y) = \delta(l+1)(a(l))^T # outer product
        # other layers: \nabla_{b(l)}J(W,b;x,y) = \delta(l+1)
        nabla_W = [0] * 2
        nabla_W[1] = np.einsum("ij,ik->ijk",delta[2],self.memory["a1"]) # N * out_features
            ↪ * hidden_features
```

```
        nabla_W[0] = np.einsum("ij,ik->ijk",delta[1],self.memory["a0"]) # N * hidden_features * in_features
        nabla_b = [0] * 2
        nabla_b[1] = delta[2] # N * out_features
        nabla_b[0] = delta[1] # N * hidden_features
        # print(nabla_W[1].shape,nabla_W[0].shape,nabla_b[1].shape,nabla_b[0].shape)

        # Update parameters
        # W(l) = W(l) - \alpha((1/m \Delta W(l)) + \lambda W(l))
        # b(l) = b(l) - \alpha(1/m \Delta b(l))
        # Use einsum to accelerate
        # https://rockt.github.io/2018/04/30/einsum
        nabla_W[1] = nabla_W[1].mean(axis=0)
        nabla_W[0] = nabla_W[0].mean(axis=0)
        nabla_b[1] = nabla_b[1].mean(axis=0)
        nabla_b[0] = nabla_b[0].mean(axis=0)

        # weight decay, lambda is the L2 regularization term
        self.fc2.weight -= self.learning_rate * (nabla_W[1] + lamb * self.fc2.weight / batch_size)
        self.fc1.weight -= self.learning_rate * (nabla_W[0] + lamb * self.fc1.weight / batch_size)
        self.fc2.bias -= self.learning_rate * nabla_b[1]
        self.fc1.bias -= self.learning_rate * nabla_b[0]
```