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Exercise Sheet 09

Machine Learning
December 15, 2019

.

Problem 1

Proof:

$$y = log \sum_{e=1}^{N} e^{x_i}$$

$$e^y = \sum_{i=1}^{N} e^{x_i}$$

$$e^{-a} e^y = e^{-a} \sum_{i=1}^{N} e^{x_i}$$

$$e^{y-a} = \sum_{i=1}^{N} e^{x_i} e^{-a}$$

$$e^{y-a} = \sum_{i=1}^{N} e^{x_i - a}$$

$$y - a = log \sum_{i=1}^{N} e^{x_i - a}$$

$$y = a + log \sum_{i=1}^{N} e^{x_i - a}$$

Problem 2

Proof:

$$\frac{e^{x_i - a}}{\sum_{i=1}^{N} e^{x_i - a}} = \frac{e^{x_i} e^{-a}}{\sum_{i=1}^{N} e^{x_1} e^{-a}}$$

$$\frac{e_i^x e^{-a}}{e^{-a} \sum_{i=1}^{N} e^{x_i}} = \frac{e^{x_i}}{\sum_{i=1}^{N} e^{x_i}}$$

Alternative Proof:

$$y = \frac{e^{x_i}}{\sum_{i=1}^{N} e^{x_i}}$$

$$ye^{-a} = \frac{e^{x_i}}{\sum_{i=1}^{N} e^{x_i}} e^{-a}$$

$$ye^{-a} = \frac{e^{x_i - a}}{\sum_{i=1}^{N} e^{x_i}}$$

$$y = \frac{e^{x_i - a}}{e^{-a} \sum_{i=1}^{N} e^{x_i}}$$

$$y = \frac{e^{x_i - a}}{\sum_{i=1}^{N} e^{x_i - a}}$$

In [177]:
```
import numpy as np
import matplotlib.pyplot as plt

from sklearn.datasets import load_digits
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import label_binarize
from sklearn.metrics import accuracy_score

from scipy.special import softmax
```

In [178]:
```
X, y = load_digits(return_X_y=True)
# Convert a categorical vector y (shape [N]) into a one-hot encoded mat
rix (shape [N, K])
Y = label_binarize(y, np.unique(y)).astype(np.float64)

np.random.seed(123)
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=0.2
5)
```

In [179]:
```
N, K = Y.shape  # N - num_samples, K - num_classes
D = X.shape[1] # num_features
```

Remember from the tutorial:

1. No for loops! Use matrix multiplication and broadcasting whenever possible.
2. Think about numerical stability

In [180]:
```
import nn_utils  # module containing helper functions for checking the
 correctness of your code
```

Task 1: Affine layer

Implement `forward` and `backward` functions for `Affine` layer

In [181]:
```
class Affine:
    def forward(self, inputs, weight, bias):
        """Forward pass of an affine (fully connected) layer.

        Args:
            inputs: input matrix, shape (N, D)
            weight: weight matrix, shape (D, H)
            bias: bias vector, shape (H)

        Returns
            out: output matrix, shape (N, H)
        """
        self.cache = (inputs, weight, bias)
        #############################################################
        # TODO
        b = bias[None, :]
        out = inputs.dot(weight) + b
        #############################################################
        assert out.shape[0] == inputs.shape[0]
        assert out.shape[1] == weight.shape[1] == bias.shape[0]
        return out

    def backward(self, d_out):
        """Backward pass of an affine (fully connected) layer.

        Args:
            d_out: incoming derivaties, shape (N, H)

        Returns:
            d_inputs: gradient w.r.t. the inputs, shape (N, D)
            d_weight: gradient w.r.t. the weight, shape (D, H)
            d_bias: gradient w.r.t. the bias, shape (H)
        """
        inputs, weight, bias = self.cache
        #############################################################
        # TODO
        d_inputs = d_out.dot(weight.T)
```

```
        d_weight = inputs.T.dot(d_out)
        d_bias   = np.sum(d_out, 0)

        #############################################################
        assert np.all(d_inputs.shape == inputs.shape)
        assert np.all(d_weight.shape == weight.shape)
        assert np.all(d_bias.shape == bias.shape)
        return d_inputs, d_weight, d_bias
```

In [182]:
```
affine = Affine()
nn_utils.check_affine(affine)
```

```
All checks passed succesfully!
```

Task 2: ReLU layer

Implement `forward` and `backward` functions for `ReLU` layer

In [183]:
```
class ReLU:

    def forward(self, inputs):
        """Forward pass of a ReLU layer.

        Args:
            inputs: input matrix, arbitrary shape

        Returns:
            out: output matrix, has same shape as inputs
        """
        self.cache = inputs
        #############################################################
        # TODO

        out = np.maximum(0,inputs)

        #############################################################
        assert np.all(out.shape == inputs.shape)
```

```
        return out

    def backward(self, d_out):
        """Backward pass of an ReLU layer.

        Args:
            d_out: incoming derivatives, same shape as inputs in forwar
d

        Returns:
            d_inputs: gradient w.r.t. the inputs, same shape as d_out
        """
        inputs = self.cache
        ############################################################
        # TODO
        d_i = np.where(inputs >= 0, 1, 0)
        d_inputs = d_i * d_out

        ############################################################
        assert np.all(d_inputs.shape == inputs.shape)
        return d_inputs
```

In [184]:
```
relu = ReLU()
nn_utils.check_relu(relu)
```

```
All checks passed succesfully!
```

Task 3: CategoricalCrossEntropy layer

Implement `forward` and `backward` for `CategoricalCrossEntropy` layer

In [185]:
```
class CategoricalCrossEntropy:
    def forward(self, logits, labels):
        """Compute categorical cross-entropy loss.

        Args:
            logits: class logits, shape (N, K)
```

```
            labels: target labels in one-hot format, shape (N, K)

        Returns:
            loss: loss value, float (a single number)
        """
        ################################################################
        # TODO
        N = logits.shape[0]
        logits_shifted = logits - logits.max(axis=1, keepdims=True)

        probs = softmax(logits_shifted, axis = 1)

        log_sum_exp = np.log(np.sum(np.exp(logits_shifted), axis=1, kee
pdims=True))
        probs_L = logits_shifted - log_sum_exp
        loss = -np.sum(labels * probs_L) / N
        ################################################################
        # probs is the (N, K) matrix of class probabilities
        self.cache = (probs, labels)
        assert isinstance(loss, float)
        return loss

    def backward(self, d_out=1.0):
        """Backward pass of the Cross Entropy loss.

        Args:
            d_out: Incoming derivatives. We set this value to 1.0 by de
fault,
                since this is the terminal node of our computational gr
aph
                (i.e. we usually want to compute gradients of loss w.r.
t.
                other model parameters).

        Returns:
            d_logits: gradient w.r.t. the logits, shape (N, K)
            d_labels: gradient w.r.t. the labels
                we don't need d_labels for our models, so we don't
                compute it and set it to None. It's only included in th
```

```
e
                function definition for consistency with other layers.
        """
        probs, labels = self.cache
        ##############################################################
        # TODO
        N = labels.shape[0]
        d_logits = ((probs - labels)/N)*d_out

        ##############################################################
        d_labels = None
        assert np.all(d_logits.shape == probs.shape == labels.shape)
        return d_logits, d_labels
```

In [186]:

```
cross_entropy = CategoricalCrossEntropy()
nn_utils.check_cross_entropy(cross_entropy)
```

```
All checks passed succesfully!
```

Logistic regression (with backpropagation) --- nothing to do in this section

In [187]:

```
class LogisticRegression:
    def __init__(self, num_features, num_classes, learning_rate=1e-2):
        """Logistic regression model.
        Gradients are computed with backpropagation.


        The model consists of the following sequence of opeartions:

        input -> affine -> softmax
        """
        self.learning_rate = learning_rate

        # Initialize the model parameters
        self.params = {
```

```
            'W': np.zeros([num_features, num_classes]),
            'b': np.zeros([num_classes])
        }

        # Define layers
        self.affine = Affine()
        self.cross_entropy = CategoricalCrossEntropy()

    def predict(self, X):
        """Generate predictions for one minibatch.

        Args:
            X: data matrix, shape (N, D)

        Returns:
            Y_pred: predicted class probabilities, shape (N, D)
            Y_pred[n, k] = probability that sample n belongs to class k
        """
        logits = self.affine.forward(X,self.params['W'], self.params[
'b'])
        Y_pred = softmax(logits, axis=1)
        return Y_pred

    def step(self, X, Y):
        """Perform one step of gradient descent on the minibatch of dat
a.

        1. Compute the cross-entropy loss for given (X, Y).
        2. Compute the gradients of the loss w.r.t. model parameters.
        3. Update the model parameters using the gradients.

        Args:
            X: data matrix, shape (N, D)
            Y: target labels in one-hot format, shape (N, K)

        Returns:
            loss: loss for (X, Y), float, (a single number)
        """
        # Forward pass - compute the loss on training data
```

```
        logits = self.affine.forward(X, self.params['W'], self.params[
'b'])
        loss = self.cross_entropy.forward(logits, Y)

        # Backward pass - compute the gradients of loss w.r.t. all the
 model parameters
        grads = {}
        d_logits, _ = self.cross_entropy.backward()
        _, grads['W'], grads['b'] = self.affine.backward(d_logits)

        # Apply the gradients
        for p in self.params:
            self.params[p] = self.params[p] - self.learning_rate * grad
s[p]
        return loss
```

In [188]:

```
# Specify optimization parameters
learning_rate = 1e-2
max_epochs = 501
report_frequency = 50
```

In [189]:

```
log_reg = LogisticRegression(num_features=D, num_classes=K)
```

In [190]:

```
for epoch in range(max_epochs):
    loss = log_reg.step(X_train, Y_train)
    if epoch % report_frequency == 0:
        print(f'Epoch {epoch:4d}, loss = {loss:.4f}')
```

```
Epoch    0, loss = 2.3026
Epoch   50, loss = 0.2275
Epoch  100, loss = 0.1599
Epoch  150, loss = 0.1306
Epoch  200, loss = 0.1130
Epoch  250, loss = 0.1009
Epoch  300, loss = 0.0918
Epoch  350, loss = 0.0846
Epoch  400, loss = 0.0788
```

```
Epoch  450, loss = 0.0738
Epoch  500, loss = 0.0696
```

In [191]:

```
y_test_pred = log_reg.predict(X_test).argmax(1)
y_test_true = Y_test.argmax(1)
```

In [192]:

```
print(f'test set accuracy = {accuracy_score(y_test_true, y_test_pred):.3f}')
```

```
test set accuracy = 0.953
```

Feed-forward neural network (with backpropagation)

In [193]:

```
def xavier_init(shape):
    """Initialize a weight matrix according to Xavier initialization.

    See pytorch.org/docs/stable/nn.init#torch.nn.init.xavier_uniform_ for details.
    """
    a = np.sqrt(6.0 / float(np.sum(shape)))
    return np.random.uniform(low=-a, high=a, size=shape)
```

Task 4: Implement a two-layer `FeedForwardNeuralNet` model

You can use the `LogisticRegression` class for reference

In [194]:

```
class FeedforwardNeuralNet:
    def __init__(self, input_size, hidden_size, output_size, learning_rate=1e-2):
        """A two-layer feedforward neural network with ReLU activations.
```

```
        (input_layer -> hidden_layer -> output_layer)


        The model consists of the following sequence of opeartions:

        input -> affine -> relu -> affine -> softmax

        """
        self.learning_rate = learning_rate

        # Initialize the model parameters
        self.params = {
            'W1': xavier_init([input_size, hidden_size]),
            'b1': np.zeros([hidden_size]),
            'W2': xavier_init([hidden_size, output_size]),
            'b2': np.zeros([output_size]),
        }

        # Define layers
        ############################################################
        # TODO
        self.affine = Affine()
        self.affine_1 = Affine()
        self.categorical_cross_entropy = CategoricalCrossEntropy()
        self.relu = ReLU()
        ############################################################

    def predict(self, X):
        """Generate predictions for one minibatch.

        Args:
            X: data matrix, shape (N, D)

        Returns:
            Y_pred: predicted class probabilities, shape (N, D)
            Y_pred[n, k] = probability that sample n belongs to class k
        """
        ############################################################
        # TODO
```

```
        logits_1    = self.affine.forward(X, self.params['W1'], self.pa
rams['b1'])
        logits_reLU = self.relu.forward(logits_1)
        logits_2    = self.affine_1.forward(logits_reLU, self.params['W
2'], self.params['b2'])
        Y_pred      = softmax(logits_2, axis=1)
        ############################################################
        return Y_pred

    def step(self, X, Y):
        """Perform one step of gradient descent on the minibatch of dat
a.

        1. Compute the cross-entropy loss for given (X, Y).
        2. Compute the gradients of the loss w.r.t. model parameters.
        3. Update the model parameters using the gradients.

        Args:
            X: data matrix, shape (N, D)
            Y: target labels in one-hot format, shape (N, K)

        Returns:
            loss: loss for (X, Y), float, (a single number)
        """
        ############################################################
        # TODO
        # Forward pass - compute the loss on training data
        logits_1    = self.affine.forward(X, self.params['W1'], self.pa
rams['b1'])
        logits_reLU = self.relu.forward(logits_1)
        logits_2    = self.affine_1.forward(logits_reLU, self.params['W
2'], self.params['b2'])
        loss        = self.categorical_cross_entropy.forward(logits_2,
Y)

        # Backward pass - compute the gradients of loss w.r.t. all the
 model parameters
        grads = {}
        d_logits, _ = self.categorical_cross_entropy.backward()
```

```
        d_inputs, grads['W2'], grads['b2'] = self.affine_1.backward(d_l
ogits)
        d_relu = self.relu.backward(d_inputs)
        _, grads['W1'], grads['b1'] = self.affine.backward(d_relu)


        # Apply the gradients
        for p in self.params:
            self.params[p] = self.params[p] - self.learning_rate * grad
s[p]
        ############################################################
        return loss
```

In [195]:

```
H = 32  # size of the hidden layer

# Specify optimization parameters
learning_rate = 1e-2
max_epochs = 501
report_frequency = 50
```

In [196]:

```
model = FeedforwardNeuralNet(input_size=D, hidden_size=H, output_size=K
, learning_rate=learning_rate)
```

In [197]:

```
for epoch in range(max_epochs):
    loss = model.step(X_train, Y_train)
    if epoch % report_frequency == 0:
        print(f'Epoch {epoch:4d}, loss = {loss:.4f}')
```

```
Epoch    0, loss = 8.5876
Epoch   50, loss = 0.6002
Epoch  100, loss = 0.3517
Epoch  150, loss = 0.2510
Epoch  200, loss = 0.1975
Epoch  250, loss = 0.1631
Epoch  300, loss = 0.1401
Epoch  350, loss = 0.1231
Epoch  400, loss = 0.1098
```

```
Epoch  450, loss = 0.0989
Epoch  500, loss = 0.0897
```

In [198]:
```
y_test_pred = model.predict(X_test).argmax(1)
y_test_true = Y_test.argmax(1)
```

In [199]:
```
print(f'test set accuracy = {accuracy_score(y_test_true, y_test_pred):.
3f}')
```

```
test set accuracy = 0.938
```