

Fully connected networks

In the previous notebook you implemented a simple two-layer neural network class. However, this class is not modular. If you wanted to change the number of layers, you would need to write a new loss and gradient function. If you wanted to optimize the network with different optimizers, you'd need to write new training functions. If you wanted to incorporate regularizations, you'd have to modify the loss and gradient function.

Instead of having to modify functions each time, for the rest of the class, we'll work in a more modular framework where we define forward and backward layers that calculate losses and gradients respectively. Since the forward and backward layers share intermediate values that are useful for calculating both the loss and the gradient, we'll also have these function return "caches" which store useful intermediate values.

The goal is that through this modular design, we can build different sized neural networks for various applications.

In this HW #3, we'll define the basic architecture, and in HW #4, we'll build on this framework to implement different optimizers and regularizations (like BatchNorm and Dropout).

Modular layers

This notebook will build out the forward and backward passes in the following manner. First, there will be a forward pass for a given layer with inputs (\mathbf{x}) and return the output of that layer (\mathbf{out}) as well as cached values (\mathbf{cache}) that will be used to calculate the gradient in the backward pass.

```
def layer_forward(x, w):
    """ Receive inputs x and weights w """
    # Some intermediate values
    z = # ... some intermediate value
    # Do some more computations ...
    out = # the output

    cache = (x, w, z, out) # Values we need to compute gradients

    return out, cache
```

The backward pass will receive upstream derivatives and the `cache` object, and will return gradients with respect to the inputs and weights, like this:

```
def layer_backward(dout, cache):
    """
    Receive derivative of loss with respect to outputs and cache,
    and compute derivatives with respect to inputs.
    """
    # Unpack cache values
    x, w, z, out = cache

    # Use values in cache to compute derivatives
    dx = # Derivative of loss with respect to x
    dw = # Derivative of loss with respect to w

    return dx, dw
```

```
In [1]: ## Import and setups

import time
import numpy as np
import matplotlib.pyplot as plt
from nnutils.fc_net import *
from utils.data_utils import get_CIFAR10_data
from utils.gradient_check import eval_numerical_gradient, eval_numerical_gradient_array
from utils.solver import Solver

# For auto-reloading external modules
# See: http://stackoverflow.com/questions/1907993/autoreload-of-modules-in-python
%load_ext autoreload
%autoreload 2

def rel_error(x, y):
    """ returns relative error """
    return np.max(np.abs(x - y) / (np.maximum(1e-8, np.abs(x) + np.abs(y))))
```

```
In [2]: # Load the (preprocessed) CIFAR10 data.

data = get_CIFAR10_data()
for k in data.keys():
    print('! (%s)' % k, data[k].shape)

X_train: (49000, 3, 32, 32)
y_train: (49000,)
X_val: (1000, 3, 32, 32)
y_val: (1000,)
X_test: (1000, 3, 32, 32)
y_test: (1000,)

# Test affine forward function:
dx_error: 8.393418893437644e-11
dw_error: 5.78953207031032e-11
db_error: 4.39959789021158e-08
```

Linear layers

In this section, we'll implement the forward and backward pass for the linear layers.

The linear layer forward pass is the function `affine_forward` in `nnutils/layers.py` and the backward pass is `affine_backward`.

After we have implemented these, test your implementation by running the cell below.

Affine layer forward pass

Implement `affine_forward` and then test your code by running the following cell.

```
In [3]: # Test the affine_forward function

num_inputs = 2
input_shape = (4, 3, 6)
output_dim = 3

input_size = num_inputs * np.prod(input_shape)
weight_size = output_dim * np.prod(input_shape)

w = np.linspace(-0.1, 0.5, num=input_size).reshape(input_shape)
w = np.linspace(-0.2, 0.3, num=weight_size).reshape((np.prod(input_shape), output_dim))
b = np.linspace(-0.3, 0.1, num=output_dim)

out, cache = affine_forward(x, w, b)
correct_out = np.array([1.49834967, 1.70660132, 1.91485297],
                        [ 3.25553139, 3.9143127, 3.7727342])

# Compare your output with ours. The error should be around 1e-9.
print('Testing affine_forward function:')
print('Difference: (%s)' % format(rel_error(out, correct_out)))

Testing affine_forward function:
Difference: 3.76800047988e-10
```

Affine layer backward pass

Implement `affine_backward` and then test your code by running the following cell.

```
In [4]: # Test the affine_backward function

x = np.random.randn(10, 2, 3)
w = np.random.randn(6, 5)
b = np.random.randn(5)
dout = np.random.randn(10, 5)

dx_num = eval_numerical_gradient_array(lambda x: affine_forward(x, w, b)[0], x, dout)
dw_num = eval_numerical_gradient_array(lambda x: affine_forward(x, w, b)[0], w, dout)
db_num = eval_numerical_gradient_array(lambda b: affine_forward(x, w, b)[0], b, dout)

_, cache = affine_forward(x, w, b)
dx, dw, db = affine_backward(dout, cache)

# The error should be around 1e-10
print('Testing affine_backward function:')
print('dx error: (%s)' % format(rel_error(dx_num, dx)))
print('dw error: (%s)' % format(rel_error(dw_num, dw)))
print('db error: (%s)' % format(rel_error(db_num, db)))

Testing affine backward function:
dx error: 8.393418893437644e-11
dw error: 5.78953207031032e-11
db error: 4.39959789021158e-08
```

Activation layers

In this section you'll implement the ReLU activation.

ReLU forward pass

Implement the `relu_forward` function in `nnutils/layers.py` and then test your code by running the following cell.

```
In [5]: # Test the relu_forward function

dx_num = np.linspace(-0.5, 0.5, num=12).reshape(3, 4)

out, cache = relu_forward(x)
correct_out = np.array([0., 0., 0., 0., ],
                       [ 0., 0., 0.0454545, 0.13636364, ],
                       [ 0.22727273, 0.31618182, 0.40909091, 0.5, ])

# Compare your output with ours. The error should be around 1e-8
print('Testing relu_forward function:')
print('Difference: (%s)' % format(rel_error(out, correct_out)))

Testing relu_forward function:
Difference: 4.39959789021158e-08
```

ReLU backward pass

Implement the `relu_backward` function in `nnutils/layers.py` and then test your code by running the following cell.

```
In [6]: x = np.random.randn(10, 10)
dout = np.random.randn(*x.shape)

dx_num = eval_numerical_gradient_array(lambda x: relu_forward(x)[0], x, dout)

_, cache = relu_forward(x)
dx = relu_backward(dout, cache)

# The error should be around 1e-12
print('Testing relu_backward function:')
print('dx error: (%s)' % format(rel_error(dx_num, dx)))

Testing relu backward function:
dx error: 3.27562444787486e-12
```

Combining the affine and ReLU layers

Often times an affine layer will be followed by a ReLU layer. So let's make one that puts them together. Layers that are combined are stored in `nnutils/layer_utils.py`.

Affine-ReLU layers

We've implemented `affine_relu_forward()` and `affine_relu_backward` in `nnutils/layer_utils.py`. Take a look at them to make sure you understand what's going on. Then run the following cell to ensure its implemented correctly.

```
In [7]: from nnutils.layer_utils import affine_relu_forward, affine_relu_backward

x = np.random.randn(2, 3, 4)
w = np.random.randn(12, 10)
b = np.random.randn(10)
dout = np.random.randn(2, 10)

out, cache = affine_relu_forward(x, w, b)
dx, dw, db = affine_relu_backward(dout, cache)

dx_num = eval_numerical_gradient_array(lambda x: affine_relu_forward(x, w, b)[0], x, dout)
dw_num = eval_numerical_gradient_array(lambda x: affine_relu_forward(x, w, b)[0], w, dout)
db_num = eval_numerical_gradient_array(lambda b: affine_relu_forward(x, w, b)[0], b, dout)

print('Testing affine_relu_forward and affine_relu_backward:')
print('dx error: (%s)' % format(rel_error(dx_num, dx)))
print('dw error: (%s)' % format(rel_error(dw_num, dw)))
print('db error: (%s)' % format(rel_error(db_num, db)))

Testing affine_relu forward and affine_relu backward:
dx error: 2.21764296235752e-10
dw error: 2.6133840810927e-09
db error: 7.826729316297815e-12
```

Softmax losses

You've already implemented it, so we have written it in `layers.py`. The following code will ensure its working correctly.

```
In [8]: num_classes, num_inputs = 10, 50
x = 0.001 * np.random.randn(num_inputs, num_classes)
y = np.random.randint(num_classes, size=num_inputs)

dx_num = eval_numerical_gradient(lambda x: softmax_loss(x, y)[0], x, verbose=False)
loss, dx = softmax_loss(x, y)

# Test softmax_loss function. Loss should be 2.3 and dx error should be 1e-8
print('Testing softmax_loss:')
print('Loss: (%s)' % format(loss))
print('dx error: (%s)' % format(rel_error(dx_num, dx)))

Testing softmax loss:
loss: 2.302599297115487
dx error: 6.65901943244728e-09
```

Implementation of a two-layer NN

In `nnutils/net.py`, implement the class `TwoLayerNet` which uses the layers you made here. When you have finished, the following cell will test your implementation.

```
In [9]: N, D, H, C = 3, 5, 50, 7
x = np.random.randn(N, D)
y = np.random.randint(C, size=N)

std = 1e-2
model = TwoLayerNet(input_dim=D, hidden_dim=H, num_classes=C, weight_scale=std)

print('Testing initialization ...')
W1_std = abs(model.params['W1'].std() - std)
b1 = model.params['b1']
W2_std = abs(model.params['W2'].std() - std)
b2 = model.params['b2']
assert W1_std < std / 10, 'First layer weights do not seem right'
assert np.all(b1 == 0), 'First layer biases do not seem right'
assert W2_std < std / 10, 'Second layer weights do not seem right'
assert np.all(b2 == 0), 'Second layer biases do not seem right'

print('Testing test-time forward pass ...')
model.params['W1'] = np.linspace(-0.7, 0.3, num=D*H).reshape(D, H)
model.params['b1'] = np.linspace(-0.1, 0.9, num=H)
model.params['W2'] = np.linspace(-0.3, 0.4, num=H*C).reshape(H, C)
model.params['b2'] = np.linspace(-0.9, 0.1, num=C)
x_num = np.linspace(-0.5, 0.5, num=N*D).reshape(N, D)
scores = model.loss(x)
correct_scores = np.asarray([
    1.15165108, 1.2591344, 1.05181371, 13.81190102, 14.57186424, 15.33204765, 16.09215061,
    12.05760081, 12.76614105, 13.43459113, 14.12304412, 14.81149128, 15.49994135, 16.18839143,
    12.58373087, 13.2054771, 13.81736455, 14.43418138, 15.05099822, 15.66781506, 16.2846319 ]])
scores_diff = np.abs(scores - correct_scores).sum()
assert scores_diff < 1e-5, 'Problem with test-time forward pass'

print('Testing training loss (no regularization)')
# It's with the Solver. Choose hyperparameters so that your validation
# accuracy is at least 50%. We won't have you optimize this further
# since you did it in the previous notebook.

model.loss(x) - correct_loss) < 1e-10, 'Problem with training-time loss'

model.reg = 1.0
loss, grads = model.loss(x, y)
correct_loss = 3.4702243556
assert abs(loss - correct_loss) < 1e-10, 'Problem with regularization loss'

for reg in [0.0, 0.7]:
    print('Running numeric gradient check with reg = (%s)' % format(reg))
    model.reg = reg
    loss, grads = model.loss(x, y)
    for name in sorted(grads):
        f = lambda: model.loss(x, y)[0]
        grad_num = eval_numerical_gradient(f, model.params[name], verbose=False, h=1e-5)
        print('! %s relative error: (%s)' % (name, rel_error(grad_num, grads[name])))

Testing initialization ...
Testing test-time forward pass ...
Testing training loss (no regularization)
Running numeric gradient check with reg = 0.0
W1 relative error: 1.289701627275205e-06
W2 relative error: 2.81281705614754e-06
b1 relative error: 1.42404896128542e-08
b2 relative error: 1.72889405813046e-09
W2 relative error: 4.329128523396134e-10
Running numeric gradient check with reg = 0.7
W1 relative error: 2.57791528613156e-07
W2 relative error: 1.36783572210513e-07
b1 relative error: 1.534680149611563e-08
b2 relative error: 1.03896115567809e-10
```

Solver

We will now use the `utils Solver` class to train these networks. Familiarize yourself with the API in `utils/solver.py`. After you have done so, declare an instance of a `TwoLayerNet` with 200 units and then train it with the Solver. Choose parameters so that your validation accuracy is at least 50%.

```
In [10]: model = TwoLayerNet()
solver = Solver(model, data,
                update_rule='sgd',
                learning_rate=8.5e-4,
                lr_decay=0.95,
                num_epochs=10, batch_size=25,
                print_every=100)

solver.train()

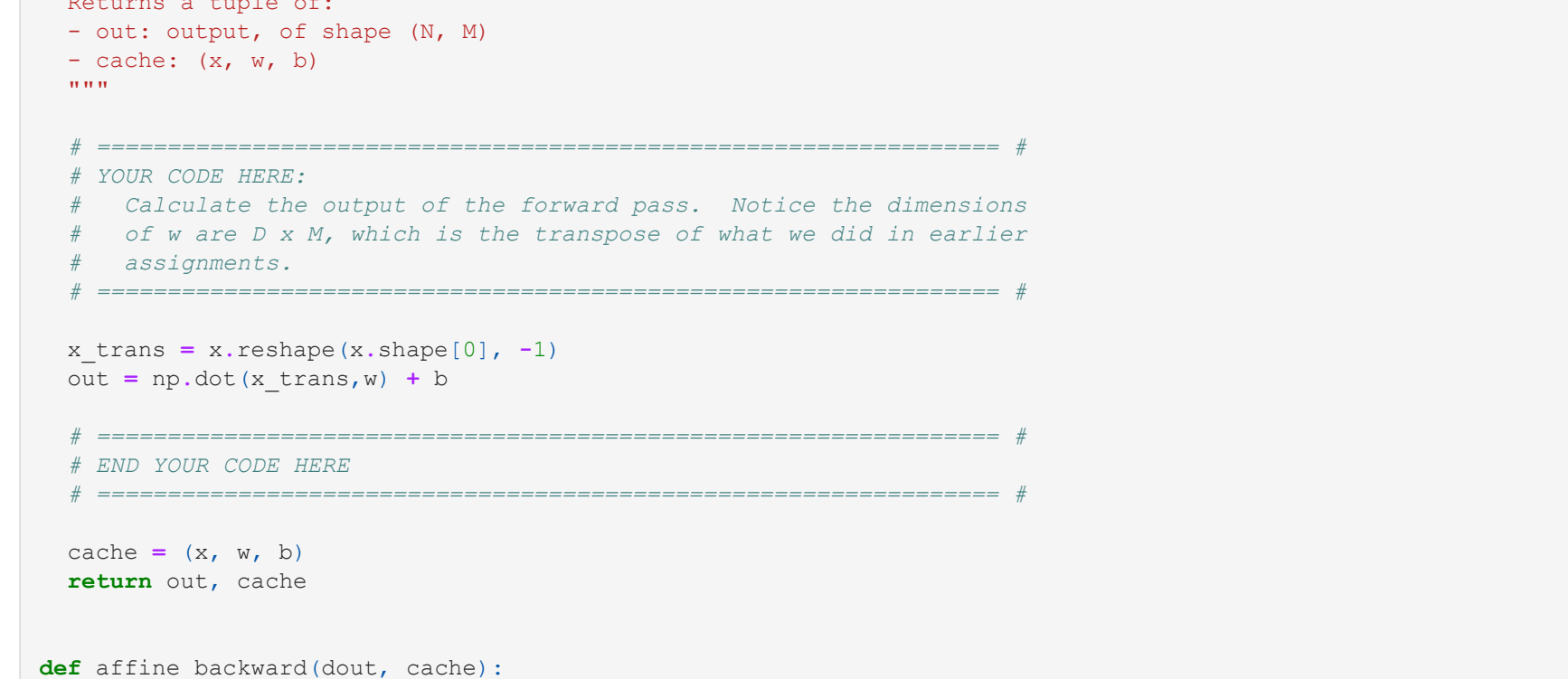
# ===== YOUR CODE HERE =====
# ===== YOUR CODE HERE =====

(iteration 1 / 2770) loss: 2.386164
(Epoch 0 / 10) train acc: 0.127000; val_acc: 0.123000
(iteration 101 / 2770) loss: 1.49602
(iteration 201 / 2770) loss: 1.817794
(Epoch 1 / 10) train acc: 0.440000; val_acc: 0.429000
(iteration 301 / 2770) loss: 1.68315
(iteration 401 / 2770) loss: 1.652731
(Epoch 2 / 10) train acc: 0.472000; val_acc: 0.480000
(iteration 501 / 2770) loss: 1.681828
(iteration 601 / 2770) loss: 1.552158
(Epoch 3 / 10) train acc: 0.510000; val_acc: 0.465000
(iteration 701 / 2770) loss: 1.631960
(iteration 801 / 2770) loss: 1.484787
(Epoch 4 / 10) train acc: 0.506000; val_acc: 0.471000
(iteration 901 / 2770) loss: 1.538187
(iteration 1001 / 2770) loss: 1.486124
(iteration 1101 / 2770) loss: 1.434921
(Epoch 5 / 10) train acc: 0.543000; val_acc: 0.511000
(iteration 1201 / 2770) loss: 1.356131
(iteration 1301 / 2770) loss: 1.462831
(Epoch 6 / 10) train acc: 0.547000; val_acc: 0.513000
(iteration 1401 / 2770) loss: 1.301775
(iteration 1501 / 2770) loss: 1.302279
(Epoch 7 / 10) train acc: 0.553000; val_acc: 0.497000
(iteration 1601 / 2770) loss: 1.366449
(iteration 1701 / 2770) loss: 1.385570
(iteration 1801 / 2770) loss: 1.342451
(Epoch 8 / 10) train acc: 0.563000; val_acc: 0.529000
(iteration 1901 / 2770) loss: 1.313358
(iteration 2001 / 2770) loss: 1.538187
(Epoch 9 / 10) train acc: 0.562000; val_acc: 0.521000
(iteration 2101 / 2770) loss: 1.400173
(iteration 2201 / 2770) loss: 1.350052
(Epoch 10 / 10) train acc: 0.609000; val_acc: 0.540000
```

```
In [11]: # Run this cell to visualize training loss and train / val accuracy

plt.subplot(2, 1, 1)
plt.title('Training loss')
plt.plot(solver.loss_history, 'o')
plt.xlabel('Iteration')

plt.subplot(2, 1, 2)
plt.title('Accuracy')
plt.plot(solver.train_acc_history, '-o', label='train')
plt.plot(solver.val_acc_history, '-o', label='val')
plt.plot([0.5] * len(solver.val_acc_history), 'k-')
plt.xlabel('Epoch')
plt.legend(loc='lower right')
plt.gcf().set_size_inches(15, 12)
plt.show()
```



Multilayer Neural Network

Now, we implement a multi-layer neural network.

Read through the `FullyConnectedNet` class in the file `nnutils/net.py`.

Implement the initialization, the forward pass, and the backward pass. There will be lines for batchnorm and dropout layers and caches; ignore these all for now. That'll be in HW #4.

```
In [49]: N, D, H1, H2, C = 2, 15, 20, 30, 10
x = np.random.randn(N, D)
y = np.random.randint(C, size=N)

for reg in [0, 3.14]:
    print('Running check with reg = (%s)' % format(reg))
    model = FullyConnectedNet([H1, H2], input_dim=D, num_classes=C,
                              reg=reg, weight_scale=5e-2, dtype=np.float64)

    loss, grads = model.loss(x, y)
    print('Initial loss: (%s)' % format(loss))

    f = lambda: model.loss(x, y)[0]
    grad_num = eval_numerical_gradient(f, model.params[name], verbose=False, h=1e-5)
    print('! %s relative error: (%s)' % (name, rel_error(grad_num, grads[name])))

Running check with reg = 0
Initial loss: 2.302599297115487
W1 relative error: 1.289701627275205e-06
W2 relative error: 2.81281705614754e-06
b1 relative error: 1.42404896128542e-08
b2 relative error: 1.72889405813046e-09
b3 relative error: 1.210598878662188e-10
Running check with reg = 3.14
Initial loss: 7.20831810593218
W1 relative error: 1.3895236383682937e-08
W2 relative error: 1.692782141920887e-08
b3 relative error: 1.42404896128542e-08
b1 relative error: 3.10368835503096e-08
b2 relative error: 1.52959204602356e-09
b3 relative error: 1.6222947517855002e-10
```

```
In [50]: # Use the three layer neural network to overfit a small dataset.

num_train = 50
small_data = {
    'X_train': data['X_train'][:num_train],
    'y_train': data['y_train'][:num_train],
    'X_val': data['X_val'],
    'y_val': data['y_val'],
}

### !!!!!!
# Play around with the weight_scale and learning_rate so that you can overfit a small dataset.
# It's with the Solver. Choose hyperparameters so that you receive full credit on this part.
weight_scale = 2e-2
learning_rate = 3e-3

model = FullyConnectedNet([100, 100],
                          weight_scale=weight_scale, dtype=np.float64)
solver = Solver(model, small_data,
                update_rule='sgd',
                learning_rate=learning_rate,
                num_epochs=20, batch_size=25,
                print_every=10)

solver.train()
```

```
Plot(solver.loss_history, 'o')
plt.title('Training loss history')
plt.xlabel('Iteration')
plt.ylabel('Training loss')
plt.show()
```

```
(iteration 1 / 40) loss: 3.446991
(Epoch 0 / 20) train acc: 0.240000; val_acc: 0.090000
(Epoch 1 / 20) train acc: 0.240000; val_acc: 0.160000
(Epoch 2 / 20) train acc: 0.360000; val_acc: 0.151000
(Epoch 3 / 20) train acc: 0.680000; val_acc: 0.141000
(Epoch 4 / 20) train acc: 0.740000; val_acc: 0.141000
(Epoch 5 / 20) train acc: 0.860000; val_acc: 0.179000
(iteration 11 / 40) loss: 0.987222
(Epoch 6 / 20) train acc: 0.880000; val_acc: 0.180000
(Epoch 7 / 20) train acc: 0.940000; val_acc: 0.175000
(Epoch 8 / 20) train acc: 0.940000; val_acc: 0.187000
(Epoch 9 / 20) train acc: 0.940000; val_acc: 0.191000
(Epoch 10 / 20) train acc: 0.940000; val_acc: 0.182000
(iteration 21 / 40) loss: 0.240758
(Epoch 11 / 20) train acc: 0.980000; val_acc: 0.179000
(Epoch 12 / 20) train acc: 1.000000; val_acc: 0.182000
(Epoch 13 / 20) train acc: 1.000000; val_acc: 0.182000
(Epoch 14 / 20) train acc: 1.000000; val_acc: 0.185000
(Epoch 15 / 20) train acc: 1.000000; val_acc: 0.190000
(iteration 31 / 40) loss: 0.103356
(Epoch 16 / 20) train acc: 1.000000; val_acc: 0.182000
(Epoch 17 / 20) train acc: 1.000000; val_acc: 0.175000
(Epoch 18 / 20) train acc: 1.000000; val_acc: 0.182000
(Epoch 19 / 20) train acc: 1.000000; val_acc: 0.181000
(Epoch 20 / 20) train acc: 1.000000; val_acc: 0.181000
```



layers.py

```
In [51]: import numpy as np
import pdb

def affine_forward(x, w, b):
    """ Computes the forward pass for an affine (fully-connected) layer.

    The input x has shape (N, d1, ..., dN) and contains a minibatch of N
    examples, where each example x[i] has shape (d1, ..., dN). We will
    reshape each input into a vector of dimension D = d1 * ... * dN, and
    then transform it to an output vector of dimension M.

    Inputs:
    - x: A numpy array containing input data, of shape (N, d1, ..., dN)
    - w: A numpy array of weights, of shape (D, M)
    - b: A numpy array of biases, of shape (M,)

    Returns a tuple of:
    - out: output, of shape (N, M)
    - cache: (x, w, b)
    """
    # ===== YOUR CODE HERE =====
    # Calculate the output of the forward pass. Notice the dimensions
    # of w are D x M, which is the transpose of what we did in earlier
    # assignments.
    # ===== YOUR CODE HERE =====

    x_trans = x.reshape(x.shape[0], -1)
    out = np.dot(x_trans, w) + b

    # ===== YOUR CODE HERE =====

    cache = (x, w, b)
    return out, cache

def affine_backward(dout, cache):
    """ Computes the backward pass for an affine layer.

    Inputs:
    - dout: Upstream derivative, of shape (N, M)
    - cache: tuple of:
      - x: Input data, of shape (N, d1, ..., dN)
      - w: Weights, of shape (D, M)

    Returns a tuple of:
    - dx: Gradient with respect to x, of shape (N, d1, ..., dN)
    - dw: Gradient with respect to w, of shape (D, M)
    - db: Gradient with respect to b, of shape (M,)
    """
    x, w, b = cache
    dx, dw, db = None, None, None

    # ===== YOUR CODE HERE =====
    # Calculate the gradients for the backward pass.

    # dout is N x M
    # dx should be N x d1 x ... x dN; it relates to dout through multiplication with w, which is D x M
    # dw should be D x M; it relates to dout through multiplication with x, which is N x D after reshaping
    # db should be M; it is just the sum over dout examples

    x_trans = x.reshape(x.shape[0], -1)
    dx = np.dot(dout, w.T)
    dx = dx.reshape(x.shape)
    dw = np.dot(x_trans, dout)
    db = np.sum(dout, axis=0)

    # ===== YOUR CODE HERE =====

    return dx, dw, db

def relu_forward(x):
    """ Computes the forward pass for a layer of rectified linear units (ReLUs).

    Inputs:
    - x: Inputs, of any shape

    Returns a tuple of:
    - out: Output, of the same shape as x
    - cache: x
    """
    # ===== YOUR CODE HERE =====
    # Implement the ReLU forward pass.

    f = lambda x: x * (x > 0)
    out = f(x)

    # ===== YOUR CODE HERE =====

    cache = x
    return out, cache

def relu_backward(dout, cache):
    """ Computes the backward pass for a layer of rectified linear units (ReLUs).

    Inputs:
    - dout: Upstream derivatives, of any shape
    - cache: Input x, of same shape as dout

    Returns:
    - dx: Gradient with respect to x
    """
    # ===== YOUR CODE HERE =====
    # Implement the ReLU backward pass.

    f = lambda x: x * (x > 0)
    out = f(x)

    # ===== YOUR CODE HERE =====

    return dx

def svm_loss(x, y):
    """ Computes the loss and gradient using multiclass SVM classification.

    Inputs:
    - x: Input data, of shape (N, C) where x[i, j] is the score for the jth class
      for the ith input.
    - y: Vector of labels, of shape (N,) where y[i] is the label for x[i] and
      0 <= y[i] < C

    Returns a tuple of:
    - loss: scalar giving the loss
    - dx: Gradient of the loss with respect to x
    """
    N = x.shape[0]
    correct_class_scores = x[np.arange(N), y]
    margins = np.maximum(0, x - correct_class_scores[:, np.newaxis] + 1.0)
    margins[np.arange(N), y] = 0
    loss = np.sum(margins) / N
    num_pos = np.sum(margins > 0, axis=1)
    dx = np.zeros_like(x)
    dx[np.arange(N), y] += num_pos
    return loss, dx

def softmax_loss(x, y):
    """ Computes the loss and gradient for softmax classification.

    Inputs:
    - x: Input data, of shape (N, C) where x[i, j] is the score for the jth class
      for the ith input.
    - y: Vector of labels, of shape (N,) where y[i] is the label for x[i] and
      0 <= y[i] < C

    Returns a tuple of:
    - loss: scalar giving the loss
    - dx: Gradient of the loss with respect to x
    """
    probs = np.exp(x - np.max(x, axis=-1, keepdims=True))
    probs /= np.sum(probs, axis=-1, keepdims=True)
    N = x.shape[0]
    loss = -np.sum(np.log(probs[np.arange(N), y])) / N
    dx = probs.copy()
    dx[np.arange(N), y] -= 1
    dx /= N
    return loss, dx
```

neural_net.py

