Tensor (aka multidimensional array) manipulation

Lecture 05 — CS 577 Deep Learning

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Multiclass classification

Let i = 1, ..., N (the sample index)

- Training samples $\mathbf{x}^{(i)} \in \mathcal{X} \subseteq \mathbb{R}^d$
- Labels $y^{(i)} \in \mathcal{Y} = \{1, ..., K\}$
- $f(\cdot; \boldsymbol{\theta}) : \mathcal{X} \to \mathcal{Y}$

Multiclass classification

```
import numpy as np
from sklearn.datasets import load_iris

n_classes = 3  # Number of classes

X, y = load_iris(return_X_y = True)
n = X.shape[0]
X = X[:,:2]  # Keep only the first two features
X = X - np.mean(X, axis=0)  # Center the data
```

Note: Shape of data

1-layer neural network

```
To define f(\cdot; \boldsymbol{\theta}) : \mathcal{X} \to \mathcal{Y}

\mathbf{h}^{(i)} = \mathbf{W}^{(1)\top} \mathbf{x}^{(i)} + \mathbf{b}^{(1)} \quad \text{and} \quad \mathbf{z}^{(i)} = \mathbf{W}^{(2)\top} q(\mathbf{h}^{(i)}) + \mathbf{b}^{(2)}
```

```
def init_params(input_dim, hidden_dim, output_dim):
    np.random.seed(0) # Ensure reproducibility

W1 = np.random.randn(input_dim, hidden_dim)

b1 = np.random.randn(hidden_dim)

W2 = np.random.randn(hidden_dim,output_dim)

b2 = np.random.randn(output_dim)

return W1, b1, W2, b2
```

1-layer neural network

```
\mathbf{h}^{(i)} = \mathbf{W}^{(1)\top} \mathbf{x}^{(i)} + \mathbf{b}^{(1)} and \mathbf{z}^{(i)} = \mathbf{W}^{(2)\top} g(\mathbf{h}^{(i)}) + \mathbf{b}^{(2)}
```

```
input_dim = 2  # Number of input dimension/features
2 hidden_dim = 10  # Number of hidden neurons
3 output_dim = 3  # Number of classes
 W1, b1, W2, b2 = init_params(input_dim, hidden_dim, output_dim)
6
7 \text{ theta} = \{
  "W1": W1,
9 "b1": b1,
"W2": W2,
  "b2": b2
1.1
12 }
```

Relu

$$\mathbf{h}^{(i)} = \mathbf{W}^{(1)\top} \mathbf{x}^{(i)} + \mathbf{b}^{(1)}$$
 and $\mathbf{z}^{(i)} = \mathbf{W}^{(2)\top} g(\mathbf{h}^{(i)}) + \mathbf{b}^{(2)}$

```
def relu(z):
    return np.maximum(0, z)
```

Note: What is the difference between np.max vs np.maximum?

Pairwise vs Reduction operations

• np.maximum is a type of pairwise operation like + and *

```
np.max(a,b) # will throw an error
```

Pairwise operations between tensors

What is a tensor (aka multidimensional array) anyways?

What is a tensor (aka multidimensional array) anyways?

```
1 a = np.arange(3*2*4).reshape([3,2,4])
2 b = np.arange(3*4).reshape([3,4])
3 a + b
4 # error
5 #
6 #
7 #
8 #
9 #
10 #
11 #
```

What is a tensor (aka multidimensional array) anyways?

```
1 a = np.arange(3*2*4).reshape([3,2,4])
2 b = np.arange(3).reshape([3,1])
3 a + b
4 # ?
5 #
6 #
7 #
8 #
9 #
10 #
11 #
```

```
1 a = np.arange(3*2*4).reshape([3,2,4])
2 b = np.arange(3).reshape([3,1,1])
3 a + b
4 # ?
5 #
6 #
7 #
8 #
9 #
10 #
11 #
```

Which of these two works?

```
1 a = np.arange(3*2*4).reshape([3,2,4])
2 b = np.arange(2).reshape([2,1])
3 a + b
4 # ?
5 #
6 a = np.arange(3*2*4).reshape([3,2,4])
7 b = np.arange(2).reshape([1,2,1])
8 a + b
9 # ?
10 #
```

```
Note: Back to np.maximum...
```

```
a = np.expand_dims(np.array([2,6,9]), axis=1)
b = np.arange(12).reshape((3,4))
# array([[0, 1, 2, 3],
# [4, 5, 6, 7],
# [8, 9, 10, 11]])
np.maximum(a,b)
# array([[2, 2, 2, 3],
# [6, 6, 6, 7],
9 # [9, 9, 10, 11]])
```

 \bullet np.maximum is a type of pairwise operation like + and *

Note: Breakout session: explain the output.

```
a = np.arange(3*2*4).reshape([3,2,4])
2 # array([[[ 0, 1, 2, 3],
         [4, 5, 6, 7]],
         [[ 8, 9, 10, 11],
          [12, 13, 14, 15]],
          [[16, 17, 18, 19],
        [20, 21, 22, 23]])
np.\max(a, axis=0)
11 \# a.shape == (2,4)
12 # array([[16, 17, 18, 19],
13 # [20, 21, 22, 23]])
```

```
a = np.arange(3*2*4).reshape([3,2,4])
2 # array([[[ 0, 1, 2, 3],
         [4, 5, 6, 7]],
         [[ 8, 9, 10, 11],
          [12, 13, 14, 15]],
          [[16, 17, 18, 19],
        [20, 21, 22, 23]]])
10 np.max(a, axis=1)
11 \# a.shape == (3,4)
12 # array([[ 4, 5, 6, 7],
13 # [12, 13, 14, 15],
          [20, 21, 22, 23]])
14 #
```

```
a = np.arange(3*2*4).reshape([3,2,4])
2 # array([[[ 0, 1, 2, 3],
        [4, 5, 6, 7]],
         [[ 8, 9, 10, 11],
          [12, 13, 14, 15]],
          [[16, 17, 18, 19],
        [20, 21, 22, 23]]])
np.max(a, axis=-1)
11 \# a.shape == (3,2)
12 # array([[ 3, 7],
13 # [11, 15],
          [19, 23]])
14 #
```

Forward

$$\mathbf{h}^{(i)} = \mathbf{W}^{(1)\top} \mathbf{x}^{(i)} + \mathbf{b}^{(1)}$$
 and $\mathbf{z}^{(i)} = \mathbf{W}^{(2)\top} g(\mathbf{h}^{(i)}) + \mathbf{b}^{(2)}$

```
def relu(z):
    return np.maximum(0, z)

def forward(X,theta):
    W1, b1, W2, b2 = theta["W1"], theta["b1"], theta["W2"], theta["b2"]
    h = relu(np.dot(X, W1) + b1)
    z = np.dot(h, W2) + b2
    return h,z
```

Note: Batched or vectorized operation

Forward (Non-vectorized)

$$\mathbf{h}^{(i)} = \mathbf{W}^{(1)\top} \mathbf{x}^{(i)} + \mathbf{b}^{(1)}$$
 and $\mathbf{z}^{(i)} = \mathbf{W}^{(2)\top} g(\mathbf{h}^{(i)}) + \mathbf{b}^{(2)}$

```
def forward_nonvectorized(X, theta):
    W1, b1, W2, b2 = theta["W1"], theta["b1"], theta["W2"], theta["b2"]
    h = np.zeros((X.shape[0], W1.shape[1])) # Initialize h
    z = np.zeros((X.shape[0], W2.shape[1])) # Initialize z

for i in range(X.shape[0]):
    h[i, :] = relu(np.dot(X[i, :], W1) + b1)
    z[i, :] = np.dot(h[i, :], W2) + b2
    return h, z
```

Note: Non-vectorized or row-wise operation

Timing the Forward Functions

```
import time
2
3 # Vectorized forward function
4 start_time = time.time()
5 h_vec, z_vec = forward(X, theta)
6 end time = time.time()
7 print(f"Vectorized time: {end_time - start_time:.5f} seconds")
8
9 # Non-vectorized forward function
  start_time = time.time()
  h_nonvec, z_nonvec = forward_nonvectorized(X, theta)
12 end_time = time.time()
print(f"Non-vectorized time: {end_time - start_time:.5f} seconds")
```

Note: Measure the time for vectorized vs. non-vectorized forward pass

Training loss

1

$$J(\boldsymbol{\theta}) := \frac{1}{N} \sum_{i=1}^{N} J_i(\boldsymbol{\theta})$$

and

$$J_i(\boldsymbol{\theta}) := L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta}), y^{(i)})$$

Backward

$$\frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{b}^{(2)}} = \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}} \iff \frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{W}^{(2)}} = g(\mathbf{h}^{(i)}) \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}^{\top}
\frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{b}^{(1)}} = (\mathbf{W}^{(2)} \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}) \odot g'(\mathbf{h}^{(i)})
\frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{W}^{(1)}} = ((\mathbf{W}^{(2)} \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}) \odot g'(\mathbf{h}^{(i)})) \mathbf{x}^{(i)\top}$$

Cross entropy

Cross entropy

$$L(\mathbf{z}, y) = -\log(\operatorname{softmax}(\mathbf{z})_y)$$

Derivative

$$\frac{\partial L}{\partial \mathbf{z}}(\mathbf{z}, y) = \underbrace{\mathbf{p}}_{\mathsf{softmax}(\mathbf{z})} - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow y\text{-th position}$$

Softmax

$$\operatorname{softmax}(\mathbf{z}^{(i)}) = \frac{1}{\sum_{j=1}^K \exp(z_j^{(i)})} \begin{bmatrix} \exp(z_1^{(i)}) \\ \vdots \\ \exp(z_K^{(i)}) \end{bmatrix} = \begin{bmatrix} \operatorname{softmax}(\mathbf{z}^{(i)})_1 \\ \vdots \\ \operatorname{softmax}(\mathbf{z}^{(i)})_K \end{bmatrix} = \begin{bmatrix} p_1 \\ \vdots \\ p_K \end{bmatrix} = \mathbf{p}$$

```
p = np.zeros((n,n_classes))
h,z = forward(X,theta)
for i in range(n):
    p[i,:] = np.exp(z[i,:])/np.sum(np.exp(z[i,:]))
```

Note: Breakout session: compute this without the for-loop

Loss derivative

$$\begin{bmatrix}
1 & 0 & 0 & \dots & 0 \\
0 & 1 & 0 & \dots & 0 \\
0 & 0 & 1 & \dots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \dots & 1
\end{bmatrix} = \begin{bmatrix}
0 \\
\vdots \\
1 \\
\vdots \\
0
\end{bmatrix}
\leftarrow y\text{-th position}$$

Identity matrix of size n_classes

```
E = np.eye(n_classes)
E[y[i], :]
```

Cross entropy

Derivative

$$\frac{\partial L}{\partial \mathbf{z}}(\mathbf{z}, y) = \underbrace{\mathbf{p}}_{\text{softmax}(\mathbf{z})} - \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \leftarrow y\text{-th position} = \mathbf{p} - \mathbf{e}^{(y)}$$

```
loss_der = np.zeros((n,n_classes))
E = np.eye(n_classes)
h,z = forward(X,theta)
for i in range(n):
    loss_der[i,:] = p[i,:] - E[y[i], :]
```

$$\frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{b}^{(2)}} = \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}} \qquad (\checkmark)$$

$$\frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{W}^{(2)}} = g(\mathbf{h}^{(i)}) \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}^{\top} \iff$$

$$\frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{b}^{(1)}} = (\mathbf{W}^{(2)} \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}) \odot g'(\mathbf{h}^{(i)})$$

$$\frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{W}^{(1)}} = ((\mathbf{W}^{(2)} \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}) \odot g'(\mathbf{h}^{(i)})) \mathbf{x}^{(i)\top}$$

Matrix multiplication

```
1 np.random.seed(42)
2 A = np.random.randint(0,9,(2,3))
3 B = np.random.randint(0,9,(3,4))
4 A@B
5 # array([[85, 70, 79, 68],
6 # [74, 72, 42, 52]])
```

Matrix multiplication

Matrix multiplication

Cross entropy

$$\frac{\partial J_i(\boldsymbol{\theta})}{\partial \mathbf{W}^{(2)}} = g(\mathbf{h}^{(i)}) \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}^{\top}$$

```
dJdW2 = np.zeros_like(W2)
# h,z = forward(X,theta) # already computed previously

for i in range(n):
    dJdW2 += np.outer(relu(h[i,:]), loss_der[i,:])

dJdW2/n
```

$$\frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{b}^{(2)}} = \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}} \qquad (\checkmark)$$

$$\frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{W}^{(2)}} = g(\mathbf{h}^{(i)}) \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}^{\top} \qquad (\checkmark)$$

$$\frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{b}^{(1)}} = (\mathbf{W}^{(2)} \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}) \odot g'(\mathbf{h}^{(i)}) \iff \frac{\partial J_{i}(\boldsymbol{\theta})}{\partial \mathbf{W}^{(1)}} = ((\mathbf{W}^{(2)} \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}) \odot g'(\mathbf{h}^{(i)})) \mathbf{x}^{(i)\top}$$

Cross Entropy

$$\frac{\partial J_i(\boldsymbol{\theta})}{\partial \mathbf{b}^{(1)}} = (\mathbf{W}^{(2)} \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}) \odot g'(\mathbf{h}^{(i)})$$

```
def relu_derivative(z):
    return 1.0*(z > 0)

dJdb1 = np.zeros_like(b1)

# h,z = forward(X,theta)
for i in range(n):
    dJdb1 += (W2@(loss_der[i,:])) * relu_derivative(h[i,:])

dJdb1 /=n
```

Cross Entropy

$$\frac{\partial J_i(\boldsymbol{\theta})}{\partial \mathbf{W}^{(1)}} = ((\mathbf{W}^{(2)} \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}) \odot g'(\mathbf{h}^{(i)})) \mathbf{x}^{(i)\top}$$

Cross Entropy

$$\frac{\partial J_i(\boldsymbol{\theta})}{\partial \mathbf{W}^{(1)}} = ((\mathbf{W}^{(2)} \frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}) \odot g'(\mathbf{h}^{(i)})) \mathbf{x}^{(i)\top}$$

How to implement the loss derivative

$$\frac{\partial L(\mathbf{z}^{(i)}, y)}{\partial \mathbf{z}}^{\top}$$

```
h,z = forward(X,theta)
p = np.exp(z[i,:])/np.sum(np.exp(z[i,:]))
loss_der = p - E[y[i], :]
dJdW1 += np.outer((W2@loss_der) * relu_derivative(h[i,:]), X[i,:]).T
dJdb1 += (W2@(loss_der)) * relu_derivative(h[i,:])
dJdW2 += np.outer(relu(h[i,:]), loss_der)
dJdb2 += loss_der
```

Stochastic gradient descent (SGD)

Let $\eta_t > 0$ be learning rates, t = 1, 2, ...Let $m \ge 1$ be an integer

- Initialize $\boldsymbol{\theta}$
- While not converged (t = iteration counter):
 - Select m samples $\{\mathbf{x}^{(1)},\dots,\mathbf{x}^{(m)}\}$ and matching labels $\{y^{(1)},\dots,y^{(m)}\}$
 - Compute gradient $\mathbf{g} \leftarrow \nabla_{\boldsymbol{\theta}} \frac{1}{m} \sum_{i=1}^{m} L(f(\mathbf{x}^{(i)}, \boldsymbol{\theta}), y^{(i)})$
 - Compute update $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} \eta_t \mathbf{g}$

Stochastic gradient descent (SGD)

Let $\eta_t > 0$ be learning rates, t = 1, 2, ...Let $m \ge 1$ be an integer

- Initialize $\boldsymbol{\theta}$
- While not converged (t = iteration counter):
 - Select 1 sample $\{\mathbf{x}^{(t)}\}$ and its label $\{y^{(t)}\}$
 - Compute gradient $\mathbf{g} \leftarrow \nabla_{\boldsymbol{\theta}} L(f(\mathbf{x}^{(t)}, \boldsymbol{\theta}), y^{(t)})$
 - Compute update $\theta \leftarrow \theta \eta_t \mathbf{g}$

References I