Solutions

Part I – Logistic regression backpropagation with a single training example

In this part, you are using the Stochastic Gradient Optimizer to train your Logistic Regression. Consequently, the gradients leading to the parameter updates are computed on a single training example.

a) Forward propagation equations

Before getting into the details of backpropagation, let's spend a few minutes on the forward pass. For one training example $x = (x_1, x_2, ..., x_n)$ of dimension n, the forward propagation is:

$z = wx + b$

$\hat{y} = a = \sigma(z)$

$L = -(y\log(\hat{y}) + (1-y)\log(1-\hat{y}))$

b) Dimensions of the variables in the forward propagation equations

It's important to note the shapes of the quantities in the previous equations:

$x = (n,1)$, $w = (1,n)$, $b = (1,1)$, $z = (1,1)$, $a = (1,1)$, L is a scalar.

c) Backpropagation equations

Training our model means updating our weights and biases, W and b, using the gradient of the loss with respect to these parameters. At every step, we need to calculate :

$\frac{\partial L}{\partial w} \quad \frac{\partial L}{\partial b}$

To do this, we will apply the chain rule.

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial w}$$

$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial b}$$

So we need to calculate the following derivatives :

$\frac{\partial L}{\partial a} \quad \frac{\partial L}{\partial w}$

We will calculate those derivatives to get an expression of $\frac{\partial L}{\partial w}$ and $\frac{\partial L}{\partial b}$.

$$\frac{\partial L}{\partial a} = -(y\frac{\partial log(a)}{\partial a} + (1-y)\frac{\partial log(1-a)}{\partial a})$$

$$= -(y\frac{1}{a} + (1-y)\frac{1}{1-a}(-1))$$

$$\frac{\partial L}{\partial z} = -(y\frac{1}{a}a(1-a) + (1-y)\frac{1}{a-1}(-1)a(1-a))$$

$$= -(y\frac{1}{a}a(1-a) + (1-y)\frac{1}{a-1}(-1)a(1-a))$$

$$= -y(1-a) - a(1-y)$$

$$= a - y$$

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial w} = (a-y)X^T$$

Why did we choose X.T rather than X ? We can have a look at the following dimensions without forgetting that the dimensions of the derivative of a term are the same as the dimensions of the term.

$\frac{\partial L}{\partial w}$	$\frac{\partial z}{\partial w}$	$a-y$	X^T
(1, n)	(1, n)	(1, 1)	(1, n)

$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial b} = (a-y).1$$

Then :

$$w = w - \alpha(a-y)X^T$$

$$b = b - \alpha(a-y).1$$

Part II - Backpropagation for a batch of *m* training examples

In this part, you are using a Batch Gradient Optimization to train your Logistic Regression. Consequently, the gradients leading to the parameter updates are computed on the entire batch of m training examples.

a) Write down the forward propagation equations leading to J.
b) Analyze the dimensions of all the variables in your forward propagation equations.
c) Write down the backpropagation equations to compute $\frac{\partial J}{\partial w}$.

a) Forward propagation equations

Before getting into the details of backpropagation, let's study the forward pass.
For a batch of m training examples, each of dimension n, the forward propagation is:

$z = wX + b$ (1)

$a = \sigma(z)$ (2)

$J = \sum_{i=1}^{m} L^{(i)}$ where L is the binary cross entropy loss

$L^{(i)} = y^{(i)}log(a^{(i)}) + (1 - y^{(i)})log(1 - a^{(i)})$

b) Dimensions of the variables in the forward propagation equations

It's important to note the shapes of the quantities in equations (1) and (2).
$w = \Re^{1\times n}$, $X = \Re^{n\times m}$, $b = \Re^{1\times m}$, but is really of shape 1×1 and broadcasted to $1 \times m$
$z = \Re^{1\times m}$ and $a = \Re^{1\times m}$ and J is a scalar.

c) Backpropagation equations

To train our model, we need to update our weights and biases w and b, using the gradient of the loss with respect to these parameters. In other words, we need to calculate $\frac{\partial J}{\partial w}$ and $\frac{\partial J}{\partial b}$.

To do this, we will apply the chain rule.
We can write $\frac{\partial J}{\partial w}$ as $\frac{\partial J}{\partial a}\frac{\partial a}{\partial z}\frac{\partial z}{\partial w}$
The first step is to calculate $\frac{\partial J}{\partial a}\frac{\partial a}{\partial z}$.

$\frac{\partial J}{\partial a} = \sum_{i=1}^{m} \frac{\partial L^{(i)}}{\partial a^{(i)}} = -\sum_{i=1}^{m} \frac{\partial}{\partial a^{(i)}}(y^{(i)} log(a^{(i)}) + (1 - y^{(i)}) log(1 - a^{(i)})) = -\sum_{i=1}^{m} (\frac{y^{(i)}}{a^{(i)}} + (1 - y^{(i)})\frac{1}{1-a^{(i)}})$ and $\frac{\partial a^{(i)}}{\partial z^{(i)}} = a^{(i)}(1 - a^{(i)})$ which is the derivative of the sigmoid function.

Putting this together,

$\frac{\partial J}{\partial W} = \sum_{i=1}^{m} \frac{\partial J}{\partial z^{(i)}} \frac{\partial z^{(i)}}{\partial W}$

$\frac{\partial J}{\partial z^{(i)}} = -(\frac{y^{(i)}}{a^{(i)}} - (1 - y^{(i)})\frac{1}{1-a^{(i)}})a^{(i)}(1 - a^{(i)}) = -y^{(i)}(1 - a^{(i)}) + (1 - y^{(i)})a^{(i)} = a^{(i)} - y^{(i)}$

$\frac{\partial z^{(i)}}{\partial w} = \frac{\partial}{\partial w}(wX_i + b) = \frac{\partial}{\partial w} wX_i = \frac{\partial}{\partial w} \sum_{j=0}^{n-1} w_j X_{ji}$

Therefore,

$\frac{\partial J}{\partial w} = \sum_{i=1}^{m} (a^{(i)} - y^{(i)}) \frac{\partial}{\partial w} \sum_{j=0}^{n-1} w_j X_{ji}$

To evaluate this derivative, we will find the derivative with respect to each element of W.

$\frac{\partial J}{\partial w_p} = \sum_{i=1}^{m} (a^{(i)} - y^{(i)}) \frac{\partial}{\partial w_p} \sum_{j=0}^{n-1} w_j X_{ji}$

$\frac{\partial z^{(i)}}{\partial w_p} = \frac{\partial}{\partial w_p}(wX + b) = \frac{\partial}{\partial w_p} wX = \frac{\partial}{\partial w_p} \sum_{j=0}^{n-1} w_j X_{ji} = X_{pi}$ Where X_p is a row vector corresponding to the p^{th} row of the X matrix.

$\frac{\partial J}{\partial w_p} = \sum_{i=1}^{m} (a^{(i)} - y^{(i)}) X_{pi}$

To get $\frac{\partial J}{\partial w}$ we simply stack all these derivatives up, row wise.
This can efficiently be written in matrix form as:

$\frac{\partial J}{\partial w} = (A - Y)X^T$

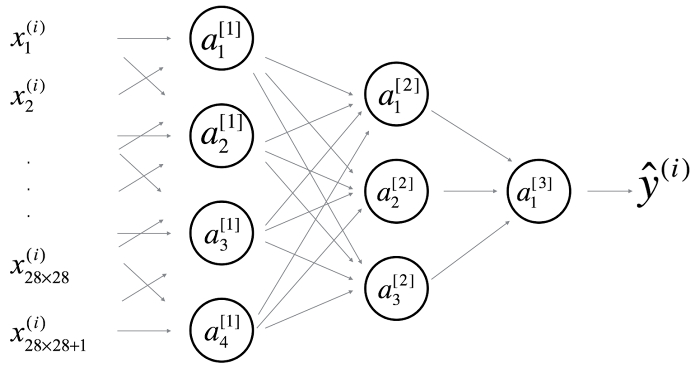
Following a very similar procedure, and noting that $\frac{\partial z^{(i)}}{\partial b} = 1$

$\frac{\partial J}{\partial w} = (A - Y).1$ Where 1 is a column vector of 1's.

Part III - Revisiting Backpropagation

There are several possible ways to obtain an optimal set of weights/parameters for a neural network. The naive approach would consist in randomly generating a new set of weights at each iteration step. An improved method would use local information of the loss function (e.g the gradient) to pick a better guess in the next iteration. Does backpropagation compute a *numerical* or *analytical* value of the gradients in a neural network? (Answer on Menti)

1. You are given the following neural network and your goal is to compute $\frac{\partial L}{\partial a_1^{[1]}}$.



a) What other derivatives do you need to compute before finding $\frac{\partial L}{\partial a_1^{[1]}}$?

b) What values do you need to cache during the forward propagation in order to compute $\frac{\partial L}{\partial a_1^{[2]}}$?

A: a) You need to compute the intermediary derivatives $\frac{\partial L}{\partial \hat{y}}, \frac{\partial \hat{y}}{\partial a_1^{[3]}}, \frac{\partial a_1^{[3]}}{\partial z_1^{[3]}}, \frac{\partial z_1^{[3]}}{\partial a_i^{[2]}}, \frac{\partial a_i^{[2]}}{\partial z_j^{[2]}}, \frac{\partial z_i^{[2]}}{\partial a_1^{[1]}}$

b)
$dz^{[L]} = da^{[L]} \odot g'(z^{[L]})$
$dW^{[L]} = dz^{[L]} \cdot a^{[L-1]}$
$db^{[L]} = dz^{[L]}$
$da^{[L-1]} = W^{[L]^T} dz^{[L]}$
$dz^{[L]} = W^{[L+1]^T} dz^{[L+1]} \odot g'(z^{[L]})$
...

2. Backpropagation example on a univariate scalar function (e.g. $f: R \rightarrow R$):

Let's suppose that you have built a model that uses the following loss function:

$$L = (\hat{y} - y)^2 \quad \text{where} \quad \hat{y} = tanh\left[\sigma(wx^2 + b)\right]$$

Assume that all the above variables are scalars. Using backpropagation, calculate $\frac{\partial L}{\partial w}$.

A: $\frac{\partial L}{\partial w} = 2(\hat{y} - y) \times \frac{\partial \hat{y}}{\partial w} = 2(\hat{y} - y) \times \left(1 - \hat{y}^2\right) \times \frac{\partial z}{\partial w} = 2(\hat{y} - y) \times \left(1 - \hat{y}^2\right) \times z(1 - z) \times x^2$
where $z = \sigma(wx^2 + b)$

3. Backpropagation example on a multivariate scalar function (e.g. $f : R^n \rightarrow R$):

Let's suppose that you have built a model that uses the following loss function:

$$L = -y\log(\hat{y}) \text{ where } \hat{y} = ReLU\,(w^T x + b)$$

a) Assume $x \in R^n$. What's the shape of w?

A: $w \in R^{n\times 1}$

b) Using backpropagation, obtain $\frac{\partial L}{\partial w}$.

A: We will derive $\frac{\partial L}{\partial w_i}$ for i=1…n:

$\frac{\partial L}{\partial w_i} = -y \times \frac{\partial \log(\hat{y})}{\partial w_i} = -y \times \frac{1}{\hat{y}}\frac{\partial \hat{y}}{\partial w_i} = -y \times \frac{1}{\hat{y}} \times f(z) \times \frac{\partial z}{\partial w_i} = -y \times \frac{1}{\hat{y}} \times f(z) \times x_i$ where $f(z) = 1$, if $z > 0$, $f(z) = 0$ otherwise (where $z = w^T x + b$.)

4. Backpropagation applied to scalar-matrix functions ($f : R^{n\times m} \rightarrow R$):

The final case that is worth exploring is:

$$L = \| \hat{y} - y \|_2^2 \text{ where } \hat{y} = \sigma(x)\cdot W$$

a) Assume that $\hat{y} \in R^{1\times m}$ and $x \in R^{1\times n}$. What is the shape of W?

A: W is an nxm matrix. (Note that the shapes of y and x differ from what you are used to in the class notations.)

b) Using backpropagation, calculate $\frac{\partial L}{\partial x}$.

A: $\frac{\partial L}{\partial x} = 2(\hat{y} - y) \times \frac{\partial \hat{y}}{\partial W} = 2\hat{y} \times W^T \odot z \odot (1 - z)$ where $z = \sigma(x)$