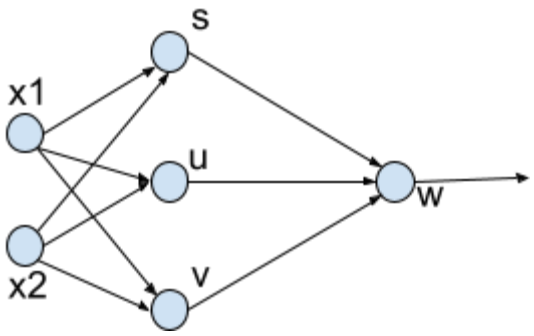
In this document we will study how to train a convolutional neural network. First, we see how to train a single layer neural network shown below.



The loss is given by $f = ((w_1, w_2, w_3)^T(\sigma(s^T x), \sigma(u^T x), \sigma(v^T x)) - y)^2$ where $\boldsymbol{\sigma}$(x) is an activation function such as sigmoid or relu. In this document we let $\boldsymbol{\sigma}$(x) be the sigmoid activation: $\sigma(x) = 1/(1 + e^{-x})$.

We optimize the loss with gradient descent by initializing all weights to random. We then update each weight w with $w = w - \eta df/dw$ until the loss converges. This is the same as moving the weight vector in the direction of the negative gradient which gives the optimal direction to decrease the objective.

We call $\boldsymbol{\eta}$ the learning rate. This is usually a small value such as 0.1 when the search starts and we change it to a smaller value as the number of epochs proceed. In other words, we want to take smaller step sizes as we approach the local minima.

Thus we need only first derivatives to optimize neural network parameters to reach a local minimum.

In order to calculate the update equations let $z_1 = \sigma(s^T x) = \sigma(s_1 x_1 + s_2 x_2)$. This means I can write f as $f = ((w_1, w_2, w_3)^T(z_1, z_2, z_3) - y)^2$. Then

$df/dw_1 = 2\sqrt{(f)} z_1$ => same as $df/dw_1 = 2((w_1, w_2, w_3)^T(z_1, z_2, z_3) - y)\, z_1$

Thus we can write df/dw as

$df/dw = (2((w_1, w_2, w_3)^T(z_1, z_2, z_3) - y))(z_1, z_2, z_3)$

Now we calculate df/ds by doing the first coordinate df/ds1.

$df/ds_1 = (df/dz_1)(dz_1/ds_1)$

where $df/dz_1 = 2\sqrt{(f)} w_1$ and $dz_1/ds_1 = d\sigma/ds_1 = \sigma(s^T x)(1 - \sigma(s^T x))x_1$

since $d\sigma/df(x) = \sigma(f(x))(1 - \sigma(f(x))df/dx$

$df/ds_2 = (df/dz_1)(dz_1/ds_2)$

where
$df/dz_1 = 2\sqrt{(f)}w_1$ and

$dz_1/ds_2 = \sigma(s^T x)(1 - \sigma(s^T x))x_2$ since $d\sigma/df(x) = \sigma(f(x))(1 - \sigma(f(x))df/dx$

This means $df/ds = (df/ds_1, df/ds_2) = (2\sqrt{(f)}, w_1\sigma(s^T x)(1 - \sigma(s^T x))x_1, 2\sqrt{(f)}w_1\sigma(s^T x)(1 - \sigma(s^T x))x_2)$

We can simplify into

$df/ds = (df/ds_1, df/ds_2) = 2\sqrt{(f)}w_1(\sigma(s^T x)(1 - \sigma(s^T x))x_1, \sigma(s^T x)(1 - \sigma(s^T x))x_2) = 2\sqrt{(f)}w_1\sigma(s^T x)(1 - \sigma(s^T x))(x_1, x_2)$

In the same way, we calculate the updated weights for the other parameters u_1, u_2, v_1, v_2.

What are df/du and df/dv (TODO for homework)?

The regularized objective would be to add the squared length of the hidden and final layer parameters.

$f = ((w_1, w_2, w_3)^T(z_1, z_2, z_3) - y)^2 + \lambda(||w||^2 + ||s||^2 + ||u||^2 + ||v||^2)$

which can be expanded into

$f = ((w_1, w_2, w_3)^T(z_1, z_2, z_3) - y)^2 + \lambda(w_1^2 + w_2^2 + w_3^2 + s_1^2 + s_2^2 + u_1^2 + u_2^2 + v_1^2 + v_2^2)$

Runtimes

Assume the input data has n rows and m columns.

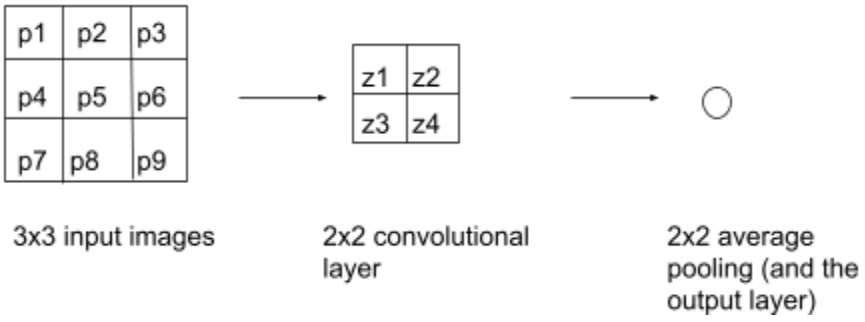
Q1. What is the runtime of one iteration of our gradient descent algorithm for the above network?

To answer this question we need to get the runtime of updating w and s, u, and v. We also need the runtime to calculate the objective.

Q2. What is the runtime of one iteration of our gradient descent algorithm for the above network with k hidden nodes? Now your answer depends upon m, n, and k.

Answer: O(mnk) time to update hidden layer and O(nk) time to update the final layer - Can you derive it?

Now consider a simple convolutional neural network shown below. In this network our input images are 3x3 and we have one 2x2 convolutional layer with average pooling



We define the loss as the squared difference between the final layer and the desired output:

$$f = ((z_1 + z_2 + z_3 + z_4)/4 - y)^2$$

We optimize this in the same way as we do a single layer network. We start with random weights and update each with the gradient (first derivatives). Let our convolutional filter be

c1	c2
c3	c4

Then $z_1 = \sigma(c_1 p_1 + c_2 p_2 + c_3 p_4 + c_4 p_5)$ where $\boldsymbol{\sigma}$(x) is the sigmoid activation. We also have $z_2 = \sigma(c_1 p_2 + c_2 p_3 + c_3 p_5 + c_4 p_6)$.

Note that f is actually a function of c1,c2,c3, and c4. Therefore I can write f as

$$f = ((\sigma(c_1 p_1 + c_2 p_2 + c_3 p_4 + c_4 p_5) + \sigma(c_1 p_2 + c_2 p_3 + c_3 p_5 + c_4 p_6) + \sigma(c_1 p_4 + c_2 p_5 + c_3 p_7 + c_4 p_8) + \sigma(c_1 p_5 + c_2 p_6 + c_3 p_8 + c_4 p_9))/4 - y)^2$$

We then have

$$df/dc_1 = 1/2 * \sqrt{f} * (dz_1/dc_1 + dz_2/dc_1 + dz_3/dc_1 + dz_4/dc_1)$$

where

$$dz_1/dc_1 = (dz_1/d_\sigma)(d_\sigma/dc_1) = \sigma(c_1 p_1 + c_2 p_2 + c_3 p_4 + c_4 p_5)(1 - \sigma(c_1 p_1 + c_2 p_2 + c_3 p_4 + c_4 p_5))p_1$$

$$dz_2/dc_1 = \sigma(c_1p_2 + c_2p_3 + c_3p_5 + c_4p_6)(1 - \sigma(c_1p_2 + c_2p_3 + c_3p_5 + c_4p_6))p_2$$

$$dz_3/dc_1 = \sigma(c_1p_4 + c_2p_5 + c_3p_7 + c_4p_8)(1 - \sigma(c_1p_4 + c_2p_5 + c_3p_7 + c_4p_8))p_4$$

$$dz_4/dc_1 = \sigma(c_1p_5 + c_2p_6 + c_3p_8 + c_4p_9)(1 - \sigma(c_1p_5 + c_2p_6 + c_3p_8 + c_4p_9))p_5$$

Similarly, we calculate the gradient updates for parameters c_2, c_3, c_4.

$$df/dc_2 = (1/2) * \sqrt{f} * (dz_1/dc_2 + dz_2/dc_2 + dz_3/dc_2 + dz_4/dc_2)$$

where

$$dz_1/dc_2 = \sigma(c_1p_1 + c_2p_2 + c_3p_4 + c_4p_5)(1 - \sigma(c_1p_1 + c_2p_2 + c_3p_4 + c_4p_5))p_2$$

$$dz_2/dc_2 = \sigma(c_1p_2 + c_2p_3 + c_3p_5 + c_4p_6)(1 - \sigma(c_1p_2 + c_2p_3 + c_3p_5 + c_4p_6))p_3$$

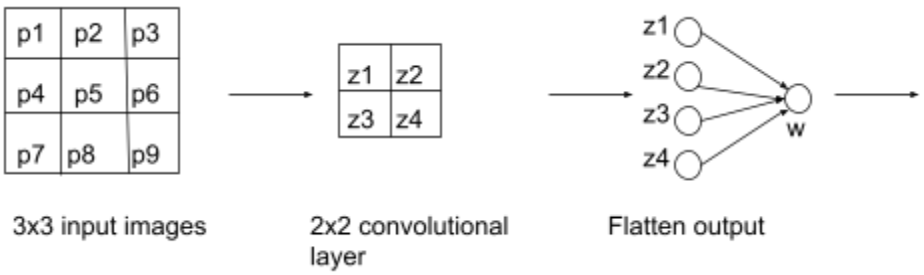
$$dz_3/dc_2 = \sigma(c_1p_4 + c_2p_5 + c_3p_7 + c_4p_8)(1 - \sigma(c_1p_4 + c_2p_5 + c_3p_7 + c_4p_8))p_5$$

$$dz_4/dc_2 = \sigma(c_1p_5 + c_2p_6 + c_3p_8 + c_4p_9)(1 - \sigma(c_1p_5 + c_2p_6 + c_3p_8 + c_4p_9))p_6$$

For $c_3$we have (complete below on your own)

Exercises:

1. Calculate the gradient update equations for the network below. Instead of average pooling we flatten the output of the convolution and give it to a linear classifier w. First, write the loss function and then calculate the first derivatives. Here w=(w1,w2,w3,w4) is a four-dimensional vector.



What is the loss function?
Solution:

We start with the loss for the simpler network where we average the outputs:

$$f = ((\sigma(c_1 p_1 + c_2 p_2 + c_3 p_4 + c_4 p_5) + \sigma(c_1 p_2 + c_2 p_3 + c_3 p_5 + c_4 p_6) + \sigma(c_1 p_4 + c_2 p_5 + c_3 p_7 + c_4 p_8) + \sigma(c_1 p_5 + c_2 p_6 + c_3 p_8 + c_4 p_9))/4 - y)^2$$

We modify this for the new network in this exercise

$$f = ((z_1, z_2, z_3, z_4)^T (w_1, w_2, w_3, w_4) - y)^2$$

Now we need update equations. Writing out the loss in terms of the variables we see

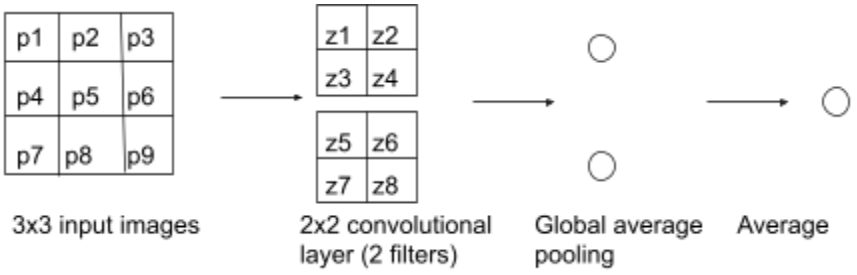
$$f = (\sigma(c_1 p_1 + c_2 p_2 + c_3 p_4 + c_4 p_5) w_1 + \sigma(c_1 p_2 + c_2 p_3 + c_3 p_5 + c_4 p_6) w_2 + \sigma(c_1 p_4 + c_2 p_5 + c_3 p_7 + c_4 p_8) w_3 + \sigma(c_1 p_5 + c_2 p_6 + c_3 p_8 + c_4 p_9) w_4 - y)^2$$

$$df/dc_1 = 2\sqrt{f}(w_1 \sigma(c_1 p_1 + c_2 p_2 + c_3 p_4 + c_4 p_5)(1 - \sigma(c_1 p_1 + c_2 p_2 + c_3 p_4 + c_4 p_5)) p_1 + w_2 \sigma(c_1 p_2 + c_2 p_3 + c_3 p_5 + c_4 p_6)(1 - \sigma(c_1 p_2 + c_2 p_3 + c_3 p_5 + c_4 p_6)) p_2 + w_3 \sigma(c_1 p_4 + c_2 p_5 + c_3 p_7 + c_4 p_8)(1 - \sigma(c_1 p_4 + c_2 p_5 + c_3 p_7 + c_4 p_8)) p_4 + w_4 \sigma(c_1 p_5 + c_2 p_6 + c_3 p_8 + c_4 p_9)(1 - \sigma(c_1 p_5 + c_2 p_6 + c_3 p_8 + c_4 p_9)) p_5)$$

$$df/dw_1 = 2\sqrt{f}\sigma(c_1 p_1 + c_2 p_2 + c_3 p_4 + c_4 p_5)$$

Similarly, we can calculate the updates for the other variables.

2. Calculate the gradient update equations if the network has two 2x2 convolutional filters as shown below. The output of each filter is averaged and then averaged again.



Suppose our convolutional kernels are:

c1	c2
c3	c4

c5	c6
c7	c8

Below is the objective for one convolution.

$$f = ((\sigma(c_1p_1 + c_2p_2 + c_3p_4 + c_4p_5) + \sigma(c_1p_2 + c_2p_3 + c_3p_5 + c_4p_6) + \sigma(c_1p_4 + c_2p_5 + c_3p_7 + c_4p_8) + \sigma(c_1p_5 + c_2p_6 + c_3p_8 + c_4p_9))/4 - y)^2$$

We can modify this to do two convolutions.

$$f = (((\sigma(c_1p_1 + c_2p_2 + c_3p_4 + c_4p_5) + \sigma(c_1p_2 + c_2p_3 + c_3p_5 + c_4p_6) + \sigma(c_1p_4 + c_2p_5 + c_3p_7 + c_4p_8) + \sigma(c_1p_5 + c_2p_6 + c_3p_8 + c_4p_9))/4 + (\sigma(c_5p_1 + c_6p_2 + c_7p_4 + c_8p_5) + \sigma(c_5p_2 + c_6p_3 + c_7p_5 + c_8p_6) + \sigma(c_5p_4 + c_6p_5 + c_7p_7 + c_8p_8) + \sigma(c_5p_5 + c_6p_6 + c_7p_8 + c_8p_9))/4)/2 - y)^2$$

$$df/dc_1 = \sqrt{f}/4(dz_1/dc_1 + dz_2/dc_1 + dz_3/dc_1 + dz_4/dc_1)$$

where

$$dz_1/dc_1 = \sigma(c_1p_1 + c_2p_2 + c_3p_4 + c_4p_5)(1 - \sigma(c_1p_1 + c_2p_2 + c_3p_4 + c_4p_5))p_1$$

$$dz_2/dc_1 = \sigma(c_1p_2 + c_2p_3 + c_3p_5 + c_4p_6)(1 - \sigma(c_1p_2 + c_2p_3 + c_3p_5 + c_4p_6))p_2$$

$$dz_3/dc_1 = \sigma(c_1p_4 + c_2p_5 + c_3p_7 + c_4p_8)(1 - \sigma(c_1p_4 + c_2p_5 + c_3p_7 + c_4p_8))p_4$$

$$dz_4/dc_1 = \sigma(c_1p_5 + c_2p_6 + c_3p_8 + c_4p_9)(1 - \sigma(c_1p_5 + c_2p_6 + c_3p_8 + c_4p_9))p_5$$

Similarly, we can do the update for the other parameters. What is the update for c5? We define z5, z6, z7, and z8 as we did z1, z2, z3, and z4. Then we have

$$df/dc_5 = \sqrt{f}/4(dz_5/dc_5 + dz_6/dc_5 + dz_7/dc_5 + dz_8/dc_5)$$

where

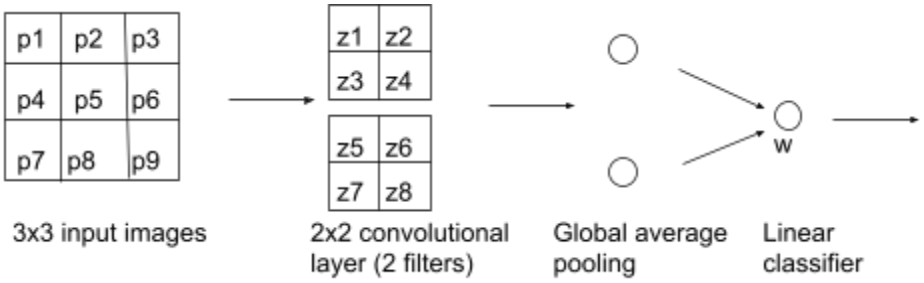
$$dz_5/dc_5 = \sigma(c_5p_1 + c_6p_2 + c_7p_4 + c_8p_5)(1 - \sigma(c_5p_1 + c_6p_2 + c_7p_4 + c_8p_5))p_1$$

$$dz_6/dc_5 = \sigma(c_5p_2 + c_6p_3 + c_7p_5 + c_8p_6)(1 - \sigma(c_5p_2 + c_6p_3 + c_7p_5 + c_8p_6))p_2$$

$$dz_7/dc_5 = \sigma(c_5p_4 + c_6p_5 + c_7p_7 + c_8p_8)(1 - \sigma(c_5p_4 + c_6p_5 + c_7p_7 + c_8p_8))p_4$$

$$dz_8/dc_5 = \sigma(c_5p_5 + c_6p_6 + c_7p_8 + c_8p_9)(1 - \sigma(c_5p_5 + c_6p_6 + c_7p_8 + c_8p_9))p_5$$

3. Calculate the gradient update equations if the network has two 2x2 convolutional filters as shown below. The output of each filter is averaged and given to a linear classifier w=(w1,w2). As we did the optimization for (2) above, can you derive the updates for the network in this problem?



4. What is the objective of the network below? Instead of average pooling we just flatten the output from the convolutional filters.