

1 Background

We want to determine gradients of a Loss function to adjust parameters of the model: $\{w, b\}$. To do this, I have to use the chain rule, for:

$$a_j^{(L)} = \sigma(z_j^{(L)}) = \sigma(w_{ji}^{(L)} a_i^{(L-1)} + b_j^{(L)}) \quad (1)$$

$$C = \frac{1}{2}[f(x) - a_j^{(L)}]^2 \quad (2)$$

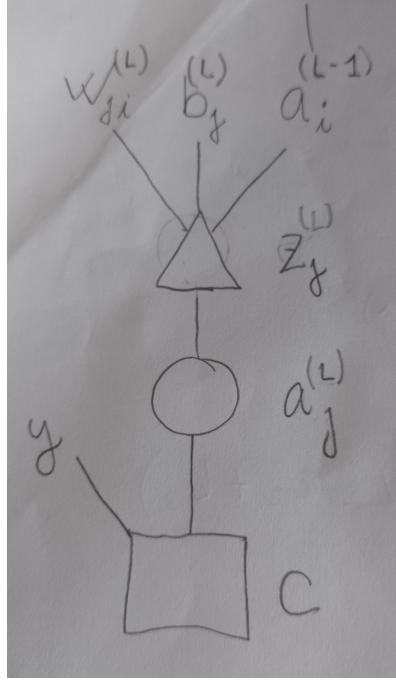


Figure 1: The proposed NN.

$$\frac{\partial C}{\partial w_{ji}^{(L)}} = \frac{\partial C}{\partial a_j^{(L)}} \frac{\partial a_j^{(L)}}{\partial z_j^{(L)}} \frac{\partial z_j^{(L)}}{\partial w_{ji}^{(L)}} \quad (3)$$

$$\frac{\partial C}{\partial b_j^{(L)}} = \frac{\partial C}{\partial a_j^{(L)}} \frac{\partial a_j^{(L)}}{\partial z_j^{(L)}} \frac{\partial z_j^{(L)}}{\partial b_j^{(L)}}, \quad (4)$$

$$\frac{\partial C}{\partial w_{ji}^{(L-1)}} = \frac{\partial C}{\partial a_j^{(L)}} \frac{\partial a_j^{(L)}}{\partial z_j^{(L)}} \frac{\partial z_j^{(L)}}{\partial a_i^{(L-1)}} \frac{\partial a_i^{(L-1)}}{\partial z_i^{(L-1)}} \frac{\partial z_i^{(L-1)}}{\partial w_{ik}^{(L-1)}} \quad (5)$$

resulting in

$$\frac{\partial C}{\partial w_{ji}^{(L)}} = [a_j^{(L)} - f(x)] \times \sigma'(z_j^{(L)}) \times a_i^{(L-1)} \quad (6)$$

$$\frac{\partial C}{\partial b_j^{(L)}} = [a_j^{(L)} - f(x)] \times \sigma'(z_j^{(L)}) \quad (7)$$

$$\frac{\partial C}{\partial w_{ji}^{(L-1)}} = [a_j^{(L)} - f(x)] \times \sigma'(z_j^{(L)}) \times w_{ji}^{(L)} \times w_{ik}^{(L-1)} \times a_k^{(L-2)}. \quad (8)$$

2 1-3-1 architecture

We will try to reproduce a function $f(x)$, such as quadratic, cubic, etc..

Training set: Choose a large number N of pairs $x, f(x)$.

Activation: a sigmoid will only fit curves inside $f(x) = [0, 1]$; the ReLU only positive $f(x)$. So, it should be useful not to use a linear activation for the last layer: $\sigma = x$.

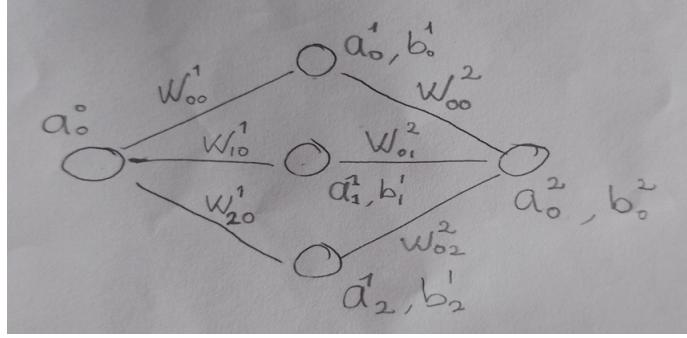


Figure 2: The proposed NN.

3 Equations

$$a_0^{(2)} = \sigma(z_0^{(2)}) = \sigma(w_{00}^{(2)} a_0^{(1)} + w_{01}^{(2)} a_1^{(1)} + w_{02}^{(2)} a_2^{(1)} + b_0^{(2)}) \quad (9)$$

$$a_0^{(1)} = \sigma(z_0^{(1)}) = \sigma(w_{00}^{(1)} a_0^{(0)} + b_0^{(1)}) \quad (10)$$

$$a_1^{(1)} = \sigma(z_1^{(1)}) = \sigma(w_{10}^{(1)} a_0^{(0)} + b_1^{(1)}) \quad (11)$$

$$a_2^{(1)} = \sigma(z_2^{(1)}) = \sigma(w_{20}^{(1)} a_0^{(0)} + b_2^{(1)}) \quad (12)$$

Loss function (stochastic GD):

$$C = \frac{1}{m} \sum_{x=0}^{m-1} \sum_{i=0}^0 \frac{1}{2} [f(x) - a_i^{(2)}]^2 = \frac{1}{m} \sum_{x=0}^{m-1} C_x, \quad (13)$$

with $C_x = \frac{1}{2} [a_0^{(2)} - f(x)]^2$. The number m is the subgroup of points to apply the stochastic GD method (mini-batch).

4 Back-propagation equations

Model parameters: $\{w_{00}^{(2)}, w_{01}^{(2)}, w_{02}^{(2)}, w_{00}^{(1)}, w_{10}^{(1)}, w_{20}^{(1)}, b_0^{(2)}, b_0^{(1)}, b_1^{(1)}, b_2^{(1)}\}$.

$$\frac{\partial C_x}{\partial w_{00}^{(2)}} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)})a_0^{(1)} \quad (14)$$

$$\frac{\partial C_x}{\partial w_{01}^{(2)}} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)})a_1^{(1)} \quad (15)$$

$$\frac{\partial C_x}{\partial w_{02}^{(2)}} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)})a_2^{(1)} \quad (16)$$

$$\frac{\partial C_x}{\partial w_{00}^{(1)}} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)})w_{00}^{(2)}\sigma'(z_0^{(1)})a_0^{(0)} \quad (17)$$

$$\frac{\partial C_x}{\partial w_{10}^{(1)}} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)})w_{01}^{(2)}\sigma'(z_1^{(1)})a_0^{(0)} \quad (18)$$

$$\frac{\partial C_x}{\partial w_{20}^{(1)}} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)})w_{02}^{(2)}\sigma'(z_2^{(1)})a_0^{(0)} \quad (19)$$

$$\frac{\partial C_x}{\partial b_0^{(2)}} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)}) \quad (20)$$

$$\frac{\partial C_x}{\partial b_0^{(1)}} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)})w_{00}^{(2)}\sigma'(z_0^{(1)}) \quad (21)$$

$$\frac{\partial C_x}{\partial b_1^{(1)}} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)})w_{01}^{(2)}\sigma'(z_1^{(1)}) \quad (22)$$

$$\frac{\partial C_x}{\partial b_2^{(1)}} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)})w_{02}^{(2)}\sigma'(z_2^{(1)}) \quad (23)$$

4.1 Using error notation

We see a lot of repetition of (now called error) $\delta_0^{(2)} = \frac{\partial C_x}{\partial z_0^{(2)}} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)})$ and $\frac{\partial C_x}{\partial z_i^{(1)}}$:

$$\delta_0^{(1)} = \frac{\partial C_x}{\partial z_0^{(1)}} = \delta_0^{(2)} w_{00}^{(2)} \sigma'(z_0^{(1)}) \quad (24)$$

$$\delta_1^{(1)} = \frac{\partial C_x}{\partial z_1^{(1)}} = \delta_0^{(2)} w_{01}^{(2)} \sigma'(z_1^{(1)}) \quad (25)$$

$$\delta_2^{(1)} = \frac{\partial C_x}{\partial z_2^{(1)}} = \delta_0^{(2)} w_{02}^{(2)} \sigma'(z_2^{(1)}) \quad (26)$$

The back-propagation equations read

$$\frac{\partial C_x}{\partial w_{00}^{(2)}} = \delta_0^{(2)} a_0^{(1)} \quad (27)$$

$$\frac{\partial C_x}{\partial w_{01}^{(2)}} = \delta_0^{(2)} a_1^{(1)} \quad (28)$$

$$\frac{\partial C_x}{\partial w_{02}^{(2)}} = \delta_0^{(2)} a_2^{(1)} \quad (29)$$

$$\frac{\partial C_x}{\partial w_{00}^{(1)}} = \delta_0^{(1)} a_0^{(0)} \quad (30)$$

$$\frac{\partial C_x}{\partial w_{10}^{(1)}} = \delta_1^{(1)} a_0^{(0)} \quad (31)$$

$$\frac{\partial C_x}{\partial w_{20}^{(1)}} = \delta_2^{(1)} a_0^{(0)} \quad (32)$$

$$\frac{\partial C_x}{\partial b_0^{(2)}} = \delta_0^{(2)} \quad (33)$$

$$\frac{\partial C_x}{\partial b_0^{(1)}} = \delta_0^{(1)} \quad (34)$$

$$\frac{\partial C_x}{\partial b_1^{(1)}} = \delta_1^{(1)} \quad (35)$$

$$\frac{\partial C_x}{\partial b_2^{(1)}} = \delta_2^{(1)} \quad (36)$$

which in compact form for layer 2 is:

$$\frac{\partial C_x}{\partial w_{0i}^{(2)}} = \delta^{(2)} a_i^{(1)} \quad (\text{for } i = 0, 1, 2) \quad (37)$$

$$\frac{\partial C_x}{\partial b_0^{(2)}} = \delta^{(2)} \quad (38)$$

and for layer 1 is:

$$\frac{\partial C_x}{\partial w_{i0}^{(1)}} = \delta_i^{(1)} a_0^{(0)} \quad (\text{for } i = 0, 1, 2) \quad (39)$$

$$\frac{\partial C_x}{\partial b_i^{(1)}} = \delta_i^{(1)} \quad (\text{for } i = 0, 1, 2) \quad (40)$$

supplemented by

$$\delta_0^{(2)} = [a_0^{(2)} - f(x)]\sigma'(z_0^{(2)}) \quad (41)$$

$$\delta_i^{(1)} = \delta_0^{(2)} w_{0i}^{(2)} \sigma'(z_i^{(1)}) \quad (42)$$

were the activation functions are different for each layer. 1) layer 1 (hidden): ReLu; 2) layer 2 (output): linear, just z . These choices will prevent the output to be bound to 1 (case 1) and speed up learning (case 2).

I note that $a_0^{(0)} = x$ and $a_0^{(2)} = f(x)$.

4.2 Pseudocode

```

N = 100 // size of training set
x_interval = (0, 1)
// input: a function f(x) and an interval
// generate_Nps() returns an N-long array of pairs {x, f(x)}:
// the training set
N_pair_set = generate_Nps(f(x), x_interval, N)
// using sql, generate_sql_Ndb() creates the training database
training_Ndb = generate_sql_Ndb(N_pair_set)
// choose arbitrarily a set of weights and biases using normal
// distr around norm_mean
wb = initialize_w_and_b(norm_mean, norm_deviation)
delta = 0.01 // threshold for C
eta = 0.01 // learning rate

mini_batch_size = 10
epoch_number = 100

FOR epoch IN 0..epoch_number - 1:
    // shuffle_Ndb() shuffles and separates into mini-batches
    // of size m
    training_Ndb_shuffled = shuffle_Ndb(training_Ndb, m)
    C[epoch] = 0
    FOR mini_batch IN training_Ndb_shuffled:
        C_mb = 0
        gradC_mb = 0
        FOR x IN mini_batch:
            // calculate vector of a's with eqs. 1-4
            a_0^0 = x

```

```

a = forward_pass(wb, x)
// calculate Loss function;
// f(x) extracted from mini_batch
C_x = calc_Cx(a, f(x))
C_mb = C_mb + C_x
// calculate gradient with eqs. 6-15;
// f(x) extracted from mini_batch
grad_C_x = grad(a, f(x), wb)
gradC_mb = gradC_mb + grad_C_x
C_mb = C_mb / m // this is C in the latex notes
gradC_mb = gradC_mb / m
// new weights and biases
wb = wb { eta * gradC_mb
// --- accumulating C for all mini-batches
C[epoch] = C[epoch] + C_mb
// C[epoch] is average over the entire epoch (N points)
C[epoch] = C[epoch] / (N/m)
IF epoch % 5 = 0 AND C[epoch] < delta : BREAK
IF epoch > 0:
    IF Abs( 2*(C[epoch-1] - C[epoch])/(C[epoch-1] + C[epoch]) ) < 0.01 : \eta = 0.8 * \eta

```

FUNCTIONS

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// generate_Nps() returns an N-long array of pairs {x, f(x)}:
// the training set
generate_Nps(f(x), x_interval, N)
// using sql, generate_sql_Ndb() creates the training database
training_Ndb = generate_sql_Ndb(N_pair_set, m)
// calculate Loss function for a single x point
calc_Cx(a, training_Ndb_shuffled)
// calculate gradient with eqs. 6-15
grad(a, training_Ndb_shuffled, wb)

```