Deep learning HW 1

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1.1 two layer neural networks

1.1.1 Regression task

(a) (1pt) Name and mathematically describe the 5 programming steps you would take to train this model with PyTorch using SGD on a single batch of data

- pass the input x_i through the model F to produce our prediction $\tilde{y}^{(i)} = F(x_i)$
- compute the loss $L(\tilde{y}^{(i)}, y^{(i)})$ between our prediction $\tilde{y}^{(i)}$ and the true value $y^{(i)}$
- compute the gradient of our loss function accumulated over all parameters $\nabla_\theta = \sum_{\theta_i} \frac{\partial L}{\partial \theta_i}$
- update our model parameters $\theta \leftarrow \theta - \eta \nabla_\theta L(\tilde{y}^{(i)}, y^{(i)})$
- zero our gradient $\nabla_\theta L(\tilde{y}^{(i)}, y^{(i)}) \leftarrow 0$

(b) (4pt)For a single data point(x,y),write down all inputs and outputs for forward pass of each layer. You can only use variable $x, y, W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)}$ in your answer. (note that $Linear_i(x) = W^{(i)}x + b^{(i)}$).

- our input x^i is passed to our first linear layer to produce $s^1 = W^{(1)}x^i + b^{(1)}$
- $s^{(1)}$ is then passed to our first activation function f to produce $a^{(1)} = f(s^{(1)}) = 5reLU(s^1)$
- $a^{(1)}$ is then passed to our second linear layer to produce $s^{(2)} = W^{(2)}a^{(1)} + b^{(2)}$
- $s^{(2)}$ is then passed to our second activation function g to produce our final prediction $\tilde{y}^{(i)} = I(s^{(2)}) = s^{(2)}$
- our prediction $\tilde{y}^{(i)}$ is finally compared against the true value of example i $y^{(i)}$ to produce our loss $L(\tilde{y}^{(i)}, y^{(i)}) = ||\tilde{y}^{(i)} - y^{(i)}||_2$

- and those our the steps of this networks forward pass.

(c) write down the gradients from the backwards pass.

- first we want to find $\frac{\partial C}{\partial \mathbf{W^2}} = \frac{\partial C}{\partial \tilde{\mathbf{y}}} \frac{\partial \tilde{\mathbf{y}}}{\partial \mathbf{s^2}} \frac{\partial \mathbf{s^2}}{\partial \mathbf{W}^2} = a^{2^t} 2(\tilde{y} - y) \in \mathbb{R}^{d \times k}$ where $W^2 \in \mathbb{R}^{k \times d}$
- next we want $\frac{\partial C}{\partial \mathbf{W^2}} = \frac{\partial C}{\partial \tilde{\mathbf{y}}} \frac{\partial \tilde{\mathbf{y}}}{\partial \mathbf{s^2}} \frac{\partial \mathbf{s^2}}{\partial \mathbf{b}^2} = 2(\tilde{y} - y) * 1 = 2(\tilde{y} - y)^t \in \mathbb{R}^{1 \times k}$
- then we want $\frac{\partial c}{\partial \mathbf{b^1}} = \frac{\partial C}{\partial \tilde{\mathbf{y}}} \frac{\partial \tilde{\mathbf{y}}}{\partial \mathbf{s^2}} \frac{\partial \mathbf{s^2}}{\partial \mathbf{a}^1} \frac{\partial \mathbf{a^1}}{\partial \mathbf{z}^1} \frac{\partial \mathbf{z^1}}{\partial \mathbf{b}^1} = 2(\tilde{y} - y) W^2 \frac{\partial \mathbf{z^1}}{\partial \mathbf{a^1}}$
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- then we want $\frac{\partial c}{\partial \mathbf{W^1}} = \frac{\partial C}{\partial \tilde{\mathbf{y}}} \frac{\partial \tilde{\mathbf{y}}}{\partial \mathbf{s^2}} \frac{\partial \mathbf{s^2}}{\partial \mathbf{a}^1} \frac{\partial \mathbf{a^1}}{\partial \mathbf{z}^1} \frac{\partial \mathbf{z^1}}{\partial \mathbf{a}^1} = 2(\tilde{y} - y) W^2 \frac{\partial \mathbf{z^1}}{\partial \mathbf{a^1}} x$

(d) show the elements of $\frac{\partial a_1}{s_1}, \frac{\tilde{y}}{s_2}, \frac{\partial C}{\partial \tilde{y}}$

- $\frac{\partial \mathbf{a^1}}{\partial \mathbf{s^1}}_i = \begin{cases} 5 & \text{if } s_i^1 > 0 \\ 0 & \text{if } s_i^1 < 0 \text{else} \end{cases} \in \mathbb{R}^D$
- now suppose that we know that $\tilde{y} \in \mathbb{R}^K$ and $s_2 \in \mathbb{R}^K$ then we can see that $\frac{\partial \tilde{y}}{s_2} \in \mathbb{R}^K$ and $\frac{\partial \tilde{y}}{\partial s_2} = \frac{\partial s^2}{s^2} = I \in \mathbb{R}^K$ thus we can see that $\frac{\partial \tilde{y}}{s_2}_{i,j} = 1 \in \mathbb{R}^k$
- finally we can see that $C \in \mathbb{R}$ and $\tilde{y} \in \mathbb{R}^k$ thus $\frac{\partial C}{\partial \tilde{\mathbf{y}}} \in \mathbb{R}^{1 \times K}$ and $\frac{\partial C}{\tilde{\mathbf{y}}} = \frac{\partial}{\partial \tilde{\mathbf{y}}} ||y - \tilde{y}||_2 = \frac{\partial}{\partial \tilde{y}} (y - \tilde{y})^t (y - \tilde{y}) = -2(y - \tilde{y})^t$ thus we can see that $\frac{\partial C}{\partial \tilde{\mathbf{y}}}_i = -2(y - \tilde{y})_i$

1.1.2 Classification task

(a) If you want to train this network, what do you need to change in the equations of (b), (c) and (d), assuming we are using the same squared Euclidean distance loss function

- we need to change our forward pass in the following ways.
  - set our first layer activation function to be $f(s^1) = tanh(s^1)$
  - set our second layer activation function to be $\sigma(s^2) = \frac{1}{1+e^{-s^2}}$
- we also need to change our backward pass in the following ways.
  - change $\frac{\partial a^1}{\partial s^1} = \frac{\partial f}{\partial s^1} = \frac{\partial}{\partial s^1} tanh(s^1) = \frac{\partial}{\partial s^1} \frac{sinh(s^1)}{cosh s^1} = 1 - tanh^2(s^1)$
  - also change $\frac{\partial \tilde{y}}{\partial s^2} = \frac{\partial}{\partial s^2}(\sigma(s^2)) = \frac{\partial}{\partial s^2}(\frac{1}{1+e^{-s^2}}) = \frac{e^{-s^2}}{((1+e^{-s^2})^2)} = \sigma(s^2)(1 - \sigma(s^2))$
- the following things change in the elements of our gradients
  - we have $a^1 \in \mathbb{R}^D, s^1 \in \mathbb{R}^d \frac{\partial \mathbf{a^1}}{\partial \mathbf{s^1}} \in \mathbb{R}^d$ where $\frac{\partial a^1}{\partial s^1}_i = \Big\{ 1 - tanh^2(s_i^1)$

- similarly we have $\tilde{y} \in \mathbb{R}^k, s^2 \in \mathbb{R}^k$ meaning that $\frac{\partial \tilde{\mathbf{y}}}{\partial \mathbf{s^2}} \in \mathbb{R}^k$ and $\frac{\partial \tilde{y}}{\partial s^2}_i = \Big\{ \sigma(s_i^2)(1-\sigma(s_i^2))$

(b) Now you think you can do a better job by using a Bi- nary Cross Entropy (BCE) loss function $\ell(y, \tilde{y}) = \frac{1}{K}\sum_{i=1}^{k} -[y_i log(\tilde{y}_i) + (1-y_i)log(1-\tilde{y}_i)]$What do you need to change in the equations of (b), (c) and (d)?

- in our forward pass we need to make the following change
  - set $C(y, \tilde{y}) = \frac{1}{K}\sum_{i=1}^{k} -[y_i log(\tilde{y}_i) + (1-y_i)log(1-\tilde{y}_i)]$
- in the backwards pass we need to make the following change
  - set $\frac{\partial C}{\partial \tilde{y}} = \frac{\partial}{\partial \tilde{y}} \frac{1}{K}\sum_{i=1}^{k} -[y_i log(\tilde{y}_i) + (1-y_i)log(1-\tilde{y}_i)] = -\frac{1}{k}(N_1 \sum_{y_i=1} \frac{1}{\tilde{y}} - (K-N_1)\sum_{y_i \neq 1} \frac{1}{1-\tilde{y}})$ where N_1 is the number of samples of class one.
  - this can also be expressed as $\frac{\partial c}{\partial \mathbf{y}} = -(\frac{y}{\tilde{y}} - \frac{1-y}{1-\tilde{y}})$
  - the rest of our computation does not change from the last part as long as we update the above variable
- finally the elements of our gradients can be changed as
  - $C \in \mathbb{R}, \tilde{y} \in \mathbb{R}^K$, $\frac{\partial \tilde{y}}{\partial \tilde{y}} \in \mathbb{R}^{1 \times K}$ and we also have $\frac{\partial C}{\partial \tilde{y}}_i = \begin{cases} -\frac{1}{k}\frac{N_1}{\tilde{y}_i} & \text{if } y_i = 1 \\ \frac{1}{k}\frac{K-N_1}{1-\tilde{y}_i} & \text{if } y_i \neq 1 \end{cases} = -(\frac{y}{\tilde{y}} - \frac{1-y}{(1-\tilde{y})})$
  - $\frac{\partial \tilde{y}}{\partial s^2} = \frac{e^{-s^2}}{(1-e^{s^2})^2}$
  - $\frac{\partial a^1}{\partial s^1} = 1 - tanh(s^1)^2$

(c) (1pt) Things are getting better. You realize that not all intermediate hidden activations need to be binary (or soft version of binary). You decide to use $f(*) = (*)^+$ but keep g as σ. Explain why this choice of f can be beneficial for training a (deeper) network.

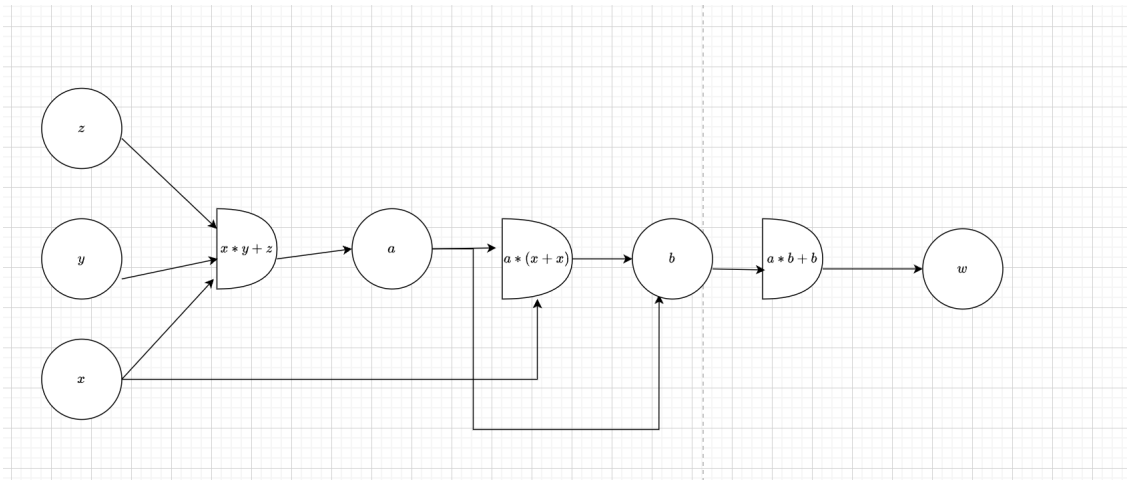
- suppose we have a deep neural network, and two examples x_i, x_j such that we are quite confidante (say we know it 100%) in the Classification of x_i and only fairly confidante in the Classification of x_j say we are only %75 sure, in a binary or soft binary activation function these two examples will have a similar output that is $s^1(x_j) \approx s^1(x_i)$, then these s^1 values are passed onto the second layer of the network with little to no information about how confidante our previous layer was. You can intuitively understand how over many layers this could lead our networks activations to become distorted

1.2 Conceptual Questions

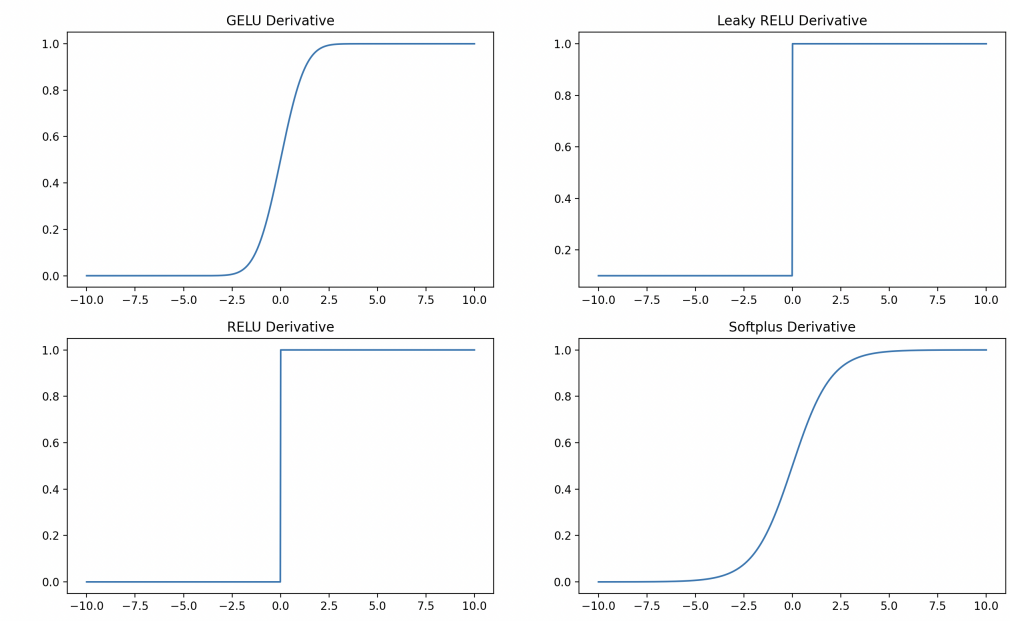
(a) why is the softmax function really softmaxarg function

- the soft max function is defined as $\sigma(x_i) = \frac{e^{x_i}}{\sum_i e^{x^i}}$ so intuitively what this function is doing is normalizing our our network outputs be all positive and sum to one. in this way we can think of them as probabilities.
- thus if we are using the softmax in a Classification we will predict the class with the highest probability ie (assuming index class labels) $\tilde{y} = argmax_i \sigma(x_i)$

(b) draw the computation graph

- 

(c) draw the graphs



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(d) given the functions $f(x) = W^1x, g(x) = W^2x: \quad W^1 \in \mathbb{R}^{b\times a}, W^2 \in \mathbb{R}^{b\times A}$

(a) what are the gradients of f and g with respect to x?

- we can see that $\frac{\partial f}{\partial x} = W^1 \in \mathbb{R}^{b\times a}$ and $\frac{\partial g}{\partial x} = W^2 \in \mathbb{R}^{b\times A}$
- thus our jacobians are $\nabla_f(x) = W^1, \nabla_g(x) = W^2$

(b) what is the gradient of $h(x) = f(x) + g(x)$

- we know that differentiation is a linear operation thus $\frac{\partial h}{\partial x} = \frac{\partial}{\partial x}(f(x) + g(x)) = \frac{\partial}{\partial x}(f(x)) + \frac{\partial}{\partial x}(g(x)) = W^1 + W^2$
- thus our jacobian is $\nabla_h(x) = W^1 + W^2$

(c) what is the gradient of $h(x) = f(x) + g(x)$ when $W^1 = W^2$

- using what we showed above we know $\frac{\partial h}{\partial x} = W^1 + W^2 = 2W^1 = 2W^2$
- thus our jacobian is $\nabla_h(x) = 2W^1 = 2W^2$

(e) given the functions $f(x) = W^1x, g(x) = W^2x: \quad W^1 \in \mathbb{R}^{b\times a}, W^2 \in \mathbb{R}^{c\times b}$

(a) what are the gradients of f and g with respect to x?

- we can see that $\frac{\partial f}{\partial x} = W^1 \in \mathbb{R}^{b\times a}$ and $\frac{\partial g}{\partial x} = W^2 \in \mathbb{R}^{b\times A}$
- thus our jacobians are $\nabla_f(x) = W^1, \nabla_g(x) = W^2$

(b) what is the gradient of $h(x) = g(f(x))$

- by the chain rule we know that $\frac{\partial h}{\partial x} = \frac{\partial g}{\partial f}\frac{\partial f}{\partial x}$

- we know that $f(x) = W^1 x \in \mathbb{R}^b$ is a vector so using what we showed above we can see $\frac{\partial g}{\partial f} = \frac{\partial}{\partial f} W^2 f = W^2$
- and also from what we showed above we have $\frac{\partial f}{\partial x} = W^1$
- so finally we can see that our jacobian matrix $\nabla_h(x) = W^2 W^1$ meaning that $\nabla_h(x)_{i,j} = W_i^{2^t} W_j^1$

(c) what is the gradient of $h(x) = g(f(x))$ if $W^1 = W^2$

- using what we showed above we know $\frac{\partial h}{\partial x} = W^1 W^2 = W^1 W^2 = W^2 W^2$
- thus our jacobian is $\nabla_h(x) = W^1 W^1 = W^2 W^2$

1.3 Deriving Loss Functions

Derive the loss function for the following algorithms based on their common update rule $w_i \leftarrow w_i + \eta(y_i - \tilde{y}_i)x_i$Showthestepsofthederivationgiventhefollowing inference rules (simply stating the final loss function will receive no points).

1. Perceptron: $\tilde{y} = sign(b + \sum_{i=1}^{d} w_i x_i)$

   - from a geometric perspective we can see that the perceptron is trying to find a hyperplane that separates the data. our function makes a binary prediction of either 1 or -1 (corresponding to sides of the hyperplane).
   - out update rule keeps our weight vector the same if the $\tilde{y} = y$, and if $y = 1 \wedge \tilde{y} = -1$ moves w_i in the direction of x_i and if $y = -1 \wedge \tilde{y} = 1$ moves w_i in the direction of $-x_i$
   - though our activation function $sign(*)$ is binary we would still like our predictions to be as confidant as possible. this confdince is reflected in the linear activation $b + \Sigma_{i=1}^{d} w_i x_i$ thus we can see that our loss function should be a function of the distance between our prediction and the true value.
   - so we would like a loss function that respects these facts as well as our learning rule $w_i \leftarrow w_i + \eta(y_i - \tilde{y}_i)x_i$ meaning that for gradient descent to work we want $\nabla_c(w_i) = (y - \tilde{y})x_i$
   - all of these conditions can most simply be achieved with $C(y, \tilde{y}) = -(y - \tilde{y}) \sum_{i=1}^{d} x_i w_i$ which is the loss function we ultimately use for the perceptron.
   - note however that this does not have to result in a unique hyperplane, any hyperplane which devides all of the points correctly result in a zero loss

2. Adeline: $\tilde{y} = b + \sum_{i=1}^{d} x_i w_i$

   - the Adeline is a Regression problem with an identity activation function.

- this is effectively linear Regression that is we can think of our weight vector w (and bias b) as the best linear function mapping x_i to y
- we can Conceptualize best in this case as meaning the minium Euclidean distance between our prediction and the true value.
- thus our cost function can be thought of as $\frac{1}{2}C(y, \tilde{y}) = ||y - \tilde{y}||_2$ or $\frac{1}{2}(y-\tilde{y})^2$ (or as a loss function $L(x_i, w_i, y) = \frac{1}{2}(y-(b+\sum_{i=1}^{d} x_i w_i))^2)$
- here we are adding the $\frac{1}{2}$ so the gradient of our cost function is the same as our update rule that is $-(y - \tilde{y})x_i$
- this will result in a unique solution for our weight vector w and bias b

3. Logistic Regression: $\tilde{y} = tanh(\sum_{i=1}^{d} w_i x_i)$
   - the tanh activation function (which is a shifted version of the sigmoid $tanh(x) = 2\sigma(2x) - 1$) scales our output to be between -1 and 1
   - so we want a cost function that is 0 when $y = \tilde{y}$ and increases as y and $\tilde{y}$ diverge, and also respects our weight update rule $w_i \leftarrow w_i + \eta(y - \tilde{y})x_i$.
   - this loss function is given by $\ell(x_i, y, w_i) = -2log(1+e^{-y*w_i^t x_i})$. checking this is more or less just calculus at this point
   - note that this loss function is convex and thus has a unique solution for our weight vector w
   - also note that this loss function is the same as the binary cross entropy loss function we derived in the previous section
   - $\frac{\partial \tilde{y}}{\partial \mathbf{w}_i} = 1 - tanh^2(w^t x + b)x$
   - $\frac{\partial \ell}{\partial \tilde{y}} = \frac{(\tilde{y}-y)}{1-tanh^2(w^t x+b)}$
   - then we can finally see that $L = \int \frac{\partial L}{\partial \tilde{y}} dy = \frac{\tilde{y}^2 - y\tilde{y}}{2-2tanh(b+w^t x)}$