Data 188 Introduction to Deep Learning
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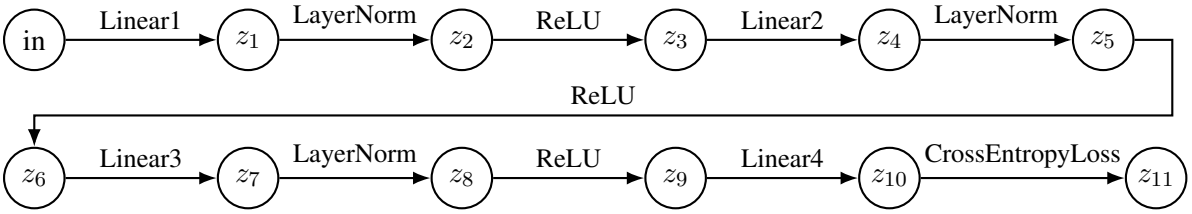
Discussion 04

This discussion will cover normalization and regularization.

1. Model Size

Consider the following classification model architecture:



Suppose we know some of the dimensions of the model parameters as follows:

- `in.shape = [batchsize=4, in_feats=52]`
- `Linear1(in_feats=52, out_feats=_____)`
- `Linear2(in_feats=128, out_feats=256)`
- `Linear3(in_feats=_____, out_feats=20)`
- `Linear4(in_feats=_____, out_feats=_____)`
- `num_classes=1000`

(a) Fill in the missing dimensions above. Additionally, label the diagram above with the dimensions of the intermediate activations (z_1 through z_{10}) and output (z_{11}).

Solution:

- `Linear1(in_feats=52, out_feats=128)`
- `Linear3(in_feats=256, out_feats=20)`
- `Linear4(in_feats=20, out_feats=1000)`
- z_1, z_2, z_3 `shape = [4, 128]`
- z_4, z_5, z_6 `shape = [4, 256]`
- z_7, z_8, z_9 `shape = [4, 20]`
- z_{10} `shape = [4, 1000]`
- z_{11} `shape = [4, 1]`

(b) Which term is called the "logits"? How do we transform logits to class probabilities?

Solution: z_{10} is the logits. We use softmax normalization to convert logits to probabilities.

(c) Let `batchsize=n` and let K be the total size of all intermediate activations. What is the total number of elements in all intermediate activations?

Solution: $n * K$. You can compute the total number of elements in all intermediate activations Z as follows where $\hat{z_i}$ denotes the number of elements at z_i:

$$
\begin{aligned}
Z &= \hat{z_1} + \hat{z_2} + \cdots + \hat{z_{10}} \\
&= 3 * n * 128 && \text{Output of Linear1, LayerNorm, ReLU} \\
&+ 3 * n * 256 && \text{Output of Linear2, LayerNorm, ReLU} \\
&+ 3 * n * 20 && \text{Output of Linear3, LayerNorm, ReLU} \\
&+ n * 1000 && \text{Output of Linear4} \\
&= (3 * 4 * 128) + (3 * 4 * 256) + (3 * 4 * 20) + (4 * 1000) \\
&= 8848
\end{aligned}
$$

As you can see, Z is a multiple of n.

(d) Let C be the total number of model parameters. How would you compute this? (You don't need to do the arithmetic, but you should understand how to compute C on an exam.)

Solution: To compute C, you would need to sum:

- The total number of parameters for each `Linear` layer, where each layer has its weights (`in_feats * out_feats`) and biases (`out_feats`).
- The total number of parameters for each `LayerNorm` layer. Recall each of these layers has γ and β learnable parameters, each of shape `[dim_feat]` which matches the `[out_feats]` of the preceding `Linear` layer.

For reference, here is the full math for this specific model architecture:

$$
\begin{aligned}
C &= (52 * 128) + 128 && \text{Linear1 weights and biases} \\
&+ 128 + 128 && \text{LayerNorm gamma and beta parameters} \\
&+ (128 * 256) + 256 && \text{Linear2 weights and biases} \\
&+ 256 + 256 && \text{LayerNorm gamma and beta parameters} \\
&+ (256 * 20) + 20 && \text{Linear3 weights and biases} \\
&+ 20 + 20 && \text{LayerNorm gamma and beta parameters} \\
&+ (20 * 1000) + 1000 && \text{Linear4 weights and biases} \\
&= 66,756
\end{aligned}
$$

(e) Recall that GPU memory is a limited resource, and assume that all `ndarrays` (e.g. activations/parameters) are stored in GPU memory. When training (or inferencing) with large `batchsizes`, do activations or parameters take up more memory?

Solution: It depends! Most of the time (e.g. if your model parameters aren't extremely large, e.g. trillions), activation size is larger than model parameter size. But, you can imagine constructing a model architecture where the $C \geq n * K$ for some `batchsize` n. Still, in the limit, as `batchsize` increases, eventually $n * K$ will surpass C - assuming you have enough GPU memory to increase the `batchsize` enough!

2. Layer Normalization

Recall that *layer normalization* (LayerNorm) is a normalization technique that normalizes across the feature dimension (e.g. the rows) of its input X, where X has shape `[batchsize, dim_feat]`:

$$\text{LayerNorm}(X) = \frac{X - \mu}{\sqrt{\sigma^2 + \epsilon}} \odot \gamma + \beta$$

where μ and σ^2 are the mean and variance of each **row** of X (shape `[batchsize, dim_feat]`), ϵ is a small constant to prevent division by zero, γ and β (both shape `[dim_feat]`) are learnable parameters that scale and shift the normalized output, and $\odot$ denotes element-wise multiplication.

(a) Perform LayerNorm(X) given the following (assume $\epsilon = 0$ for simplicity):

$$X = \begin{bmatrix} 4 & 4 & 8 & 8 \\ 0 & 2 & 2 & 8 \\ 1 & 1 & 1 & 5 \end{bmatrix}, \quad \gamma = [1, 2, 3, 4], \quad \beta = [0, -1, 1, 0]$$

Solution: First, we compute the mean and variance of each row of X:

$$\begin{aligned} \mu_1 &= 6, \quad \sigma_1^2 = 4 \\ \mu_2 &= 3, \quad \sigma_2^2 = 9 \\ \mu_3 &= 2, \quad \sigma_3^2 = 3 \end{aligned}$$

Next, we normalize each row of X:

$$\begin{aligned} \hat{X}_1 &= \frac{X_1 - \mu_1}{\sqrt{\sigma_1^2 + \epsilon}} = \frac{[4, 4, 8, 8] - 6}{\sqrt{4 + \epsilon}} = \frac{[-2, -2, 2, 2]}{2} = [-1, -1, 1, 1] \\ \hat{X}_2 &= \frac{X_2 - \mu_2}{\sqrt{\sigma_2^2 + \epsilon}} = \frac{[0, 2, 2, 8] - 3}{\sqrt{9 + \epsilon}} = \frac{[-3, -1, -1, 5]}{3} \approx [-1, -0.33, -0.33, 1.67] \\ \hat{X}_3 &= \frac{X_3 - \mu_3}{\sqrt{\sigma_3^2 + \epsilon}} = \frac{[1, 1, 1, 5] - 2}{\sqrt{3 + \epsilon}} \approx \frac{[-1, -1, -1, 3]}{1.73} \approx [-0.58, -0.58, -0.58, 1.73] \end{aligned}$$

Finally, we scale and shift the normalized output:

$$\begin{aligned} \text{LayerNorm}(X)_1 &= \hat{X}_1 \odot \gamma + \beta \\ &= [-1, -1, 1, 1] \odot [1, 2, 3, 4] + [0, -1, 1, 0] \\ &= [-1, -2, 3, 4] + [0, -1, 1, 0] \\ &= [-1, -3, 4, 4] \\ \text{LayerNorm}(X)_2 &= \hat{X}_2 \odot \gamma + \beta \\ &\approx [-1, -0.33, -0.33, 1.67] \odot [1, 2, 3, 4] + [0, -1, 1, 0] \\ &\approx [-1, -0.66, -0.99, 6.68] + [0, -1, 1, 0] \\ &\approx [-1, -1.66, 0.01, 6.68] \\ \text{LayerNorm}(X)_3 &= \hat{X}_3 \odot \gamma + \beta \end{aligned}$$

$$\approx [-0.58, -0.58, -0.58, 1.73] \odot [1, 2, 3, 4] + [0, -1, 1, 0]$$
$$\approx [-0.58, -1.16, -1.74, 6.92] + [0, -1, 1, 0]$$
$$\approx [-0.58, -2.16, -0.74, 6.92]$$

Therefore, the output of LayerNorm(X) is:

$$\text{LayerNorm}(X) = \begin{bmatrix} -1 & -3 & 4 & 4 \\ -1 & -1.66 & 0.01 & 6.68 \\ -0.58 & -2.16 & -0.74 & 6.92 \end{bmatrix}$$

(b) Notice that in the previous subpart, `batchsize = 3`. If we instead had `batchsize = 1`, can we still take the LayerNorm? Why or why not?

Solution: Yes, because LayerNorm normalizes across the feature dimension (e.g. the rows) of its input X, so it is not dependent on the batch size.

3. Batch Normalization

Recall that *batch normalization* (BatchNorm) is a normalization technique that normalizes across the batch dimension (e.g. the columns) of its input X, where X has shape `[batchsize, dim_feat]`:

$$\text{BatchNorm}(X) = \frac{X - \mu}{\sqrt{\sigma^2 + \epsilon}} \odot \gamma + \beta$$

where μ and σ^2 are the mean and variance of each **column** of X (shape `[batchsize, dim_feat]`), ϵ is a small constant to prevent division by zero, γ and β (both shape `[dim_feat]`) are learnable parameters that scale and shift the normalized output, and $\odot$ denotes element-wise multiplication.

Note that both the element-wise multiplication and sum with β broadcasts across the batch dimension.

(a) Perform BatchNorm(X) given the following (assume $\epsilon = 0$ for simplicity):

$$X = \begin{bmatrix} 2 & 2 & 1 & 1 \\ 2 & 5 & 4 & 1 \\ 5 & 5 & 10 & 10 \end{bmatrix}, \quad \gamma = [1, 2, 3, 4], \quad \beta = [0, -1, 1, 0]$$

Solution: First, we compute the mean and variance of each column of X:

$$\mu_1 = 3, \quad \sigma_1^2 = 2$$
$$\mu_2 = 4, \quad \sigma_2^2 = 2$$
$$\mu_3 = 5, \quad \sigma_3^2 = 14$$
$$\mu_4 = 4, \quad \sigma_4^2 = 18$$

Next, we normalize each column of X:

$$\hat{X}_1 = \frac{X_1 - \mu_1}{\sqrt{\sigma_1^2 + \epsilon}} = \frac{[2, 2, 5] - 3}{\sqrt{2 + \epsilon}} \approx [-0.71, -0.71, 1.41]$$

$$\hat{X}_2 = \frac{X_2 - \mu_2}{\sqrt{\sigma_2^2 + \epsilon}} = \frac{[2,5,5] - 4}{\sqrt{2+\epsilon}} \approx [-1.41, 0.71, 0.71]$$
$$\hat{X}_3 = \frac{X_3 - \mu_3}{\sqrt{\sigma_3^2 + \epsilon}} = \frac{[1,4,10] - 5}{\sqrt{14+\epsilon}} \approx [-1.07, -0.27, 1.34]$$
$$\hat{X}_4 = \frac{X_4 - \mu_4}{\sqrt{\sigma_4^2 + \epsilon}} = \frac{[1,1,10] - 4}{\sqrt{18+\epsilon}} \approx [-0.71, -0.71, 1.41]$$

Finally, we scale and shift the normalized output. Recall that the element-wise multiplication and sum with β are broadcasted across the batch dimension, e.g.:

$$\text{BatchNorm}(X) = \hat{X} \odot \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix} + \begin{bmatrix} 0 & -1 & 1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 1 & 0 \end{bmatrix}$$

Here is the equivalent computation for each column since we're computing by hand for this exercise:

$$\text{BatchNorm}(X)_1 = \hat{X}_1 \odot \gamma + \beta \approx [-0.71, -0.71, 1.41] \odot [1,1,1] + [0,0,0] = [-0.71, -0.71, 1.41]$$
$$\text{BatchNorm}(X)_2 = \hat{X}_2 \odot \gamma + \beta \approx [-1.41, 0.71, 0.71] \odot [2,2,2] + [-1,-1,-1] = [-3.82, 0.42, 0.42]$$
$$\text{BatchNorm}(X)_3 = \hat{X}_3 \odot \gamma + \beta \approx [-1.07, -0.27, 1.34] \odot [3,3,3] + [1,1,1] = [-2.21, 0.19, 5.02]$$
$$\text{BatchNorm}(X)_4 = \hat{X}_4 \odot \gamma + \beta \approx [-0.71, -0.71, 1.41] \odot [4,4,4] + [0,0,0] = [-2.84, -2.84, 5.64]$$

Therefore, the output of BatchNorm(X) is:

$$\text{BatchNorm}(X) = \begin{bmatrix} -0.71 & -3.82 & -2.21 & -2.84 \\ -0.71 & 0.42 & 0.19 & -2.84 \\ 1.41 & 0.42 & 5.02 & 5.64 \end{bmatrix}$$

(b) Notice that in the previous subpart, `batchsize = 3`. If we instead had `batchsize = 1`, can we still take the BatchNorm? Why or why not?

Solution: No, because BatchNorm normalizes across the batch dimension (e.g. the columns) of its input X, so it is dependent on the batch size. If there is only one element in the batch, we cannot compute a meaningful mean and variance.

4. Dropout

Recall that *dropout* is a regularization technique that randomly sets a fraction p of its input units to zero during training to prevent overfitting. There is also a variant of dropout called *dropout with correction* where we scale up the units that aren't zeroed out by $\frac{1}{1-p}$.

In this problem, we'll perform dropout on a toy example. Suppose we have an input vector $x = [2,6,4,4,5,3,4,4]$, weight vector $w = [1,1,1,1,1,1,1,1]$, output $y = w \cdot x$ (dot product), and dropout probability $p = 0.75$. Additionally, assume that dropout results in the first 6 values being dropped (set to 0).

(a) Compute y_{drop}, the output of regular dropout (without correction).

Solution:

$$\begin{aligned} y_{\text{drop}} &= w \cdot x_{\text{drop}} \\ &= 1*0+1*0+1*0+1*0+1*0+1*0+1*4+1*4 \\ &= 0+0+0+0+0+0+4+4 \\ &= 8 \end{aligned}$$

(b) Compute y_{corr}, the output of dropout with correction.

Solution:

$$\begin{aligned} y_{\text{corr}} &= w \cdot x_{\text{corr}} \\ &= 1*0+1*0+1*0+1*0+1*0+1*0+1*4*(\frac{1}{1-0.75})+1*4*(\frac{1}{1-0.75}) \\ &= 0+0+0+0+0+0+1*4*4+1*4*4 \\ &= 16+16 \\ &= 32 \end{aligned}$$

(c) Compute y_{orig}, the output without any dropout (i.e. the original output).

Solution:

$$\begin{aligned} y_{\text{orig}} &= w \cdot x \\ &= 1*2+1*6+1*4+1*4+1*5+1*3+1*4+1*4 \\ &= 2+6+4+4+5+3+4+4 \\ &= 32 \end{aligned}$$

(d) Observe that $\|y_{\text{corr}}\|$ more closely matches $\|y_{\text{orig}}\|$ than $\|y_{\text{drop}}\|$ does. Why is this desirable?

Solution: Simply zeroing out units like in y_{drop} would change the expected value of the output during training compared to test time when we disable dropout (this is called "domain shift"), which would decrease test-time task performance. By scaling up the units that aren't zeroed out by $\frac{1}{1-p}$, dropout with correction maintains the expected value of the output during training, resulting in better performance. (Note that it is not guaranteed that y_{corr} will always be closer to y_{orig} than y_{drop} is, but in expectation, it will be.)

(e) Dropout is an example of a layer that has different behavior at train vs. test time. What other layer also has different behavior for train vs. test time?

Solution: BatchNorm. During training, BatchNorm normalizes using the mean and variance of the current batch, while during test time, it normalizes using running estimates of the mean and variance computed during training.

5. ℓ_2 Regularization

Recall that ℓ_2 regularization is a technique used to prevent overfitting by adding a penalty term to the loss function that encourages the model parameters to be small. The ℓ_2 regularization term is defined as:

$$\ell_2(\theta) = \lambda \cdot \|\theta\|_2^2$$

where θ represents the model parameters, $\|\theta\|_2^2$ is the squared ℓ_2 norm of θ (i.e. the sum of the squares of the parameters), and λ is a hyperparameter that controls the strength of the regularization.

Consider the following optimization problem with ℓ_2 regularization where θ is the model parameters, ℓ_{ce} is cross-entropy loss, h is the hypothesis function (e.g. output logits of a neural network), X is the input data, and y is the true labels:

$$\arg\min_{\theta} \ell_{ce}(h(X), y) + \lambda \cdot \|\theta\|_2^2$$

(a) When λ is very large, which of the following θ values are likely to be the result of the above optimization?

(a) $\theta = 0$
(b) $\theta = 1$
(c) $\theta = 1000000$
(d) $\theta = \theta^*$, where θ^* is the result of solving: $\arg\min_\theta \ell_{ce}(h(X), y)$

Solution: (a) $\theta = 0$. With a large λ, the optimization will ignore the ℓ_{ce} term, and focus on minimizing $\|\theta\|_2^2$, which is to set $\theta = 0$.

(b) When λ is very small (e.g. $\lambda = 0.0000001$), which of the following θ values are likely to be the result of the above optimization?

(a) $\theta = 0$
(b) $\theta = 1$
(c) $\theta = 1000000$
(d) $\theta = \theta^*$, where θ^* is the result of solving: $\arg\min_\theta \ell_{ce}(h(X), y)$

Solution: (d) $\theta = \theta^*$. With a small λ, the optimization will ignore the regularization term, and focus on minimizing $\ell_{ce}(h(X), y)$, which is to set $\theta = \theta^*$.

(c) Suppose we solve $\theta^* = \arg\min_\theta \ell_{ce}(h(X), y)$. Suppose we then add an ℓ_2 regularization term with a "moderate" value of λ such that $\theta = \arg\min_\theta \ell_{ce}(h(X), y) + \lambda \cdot \|\theta\|_2^2$.

i. How would you expect $\|\theta\|_2$ to compare against $\|\theta^*\|_2$?

Solution: We would expect $\|\theta\|_2 < \|\theta^*\|_2$. This is because the regularization term encourages smaller parameter values, so the optimization will find a θ that has a smaller ℓ_2 norm than θ^*, which only minimizes the ℓ_{ce} term.

ii. How would you expect θ to compare against θ^* when comparing **training** dataset metrics (e.g. **classification accuracy**)?

Solution: We'd expect θ to behave a little worse on training dataset metrics than θ^*. This is because the presence of the regularization term introduces a tradeoff between "do well on the training dataset" and "satisfy the regularization penalty".

iii. How would you expect θ to compare against θ^* when comparing **test** dataset metrics (e.g. **generalizability**)?

Solution: We'd hope that θ generalizes better to unseen data than θ^* due to the presence of the added regularization term. This is the motivation for why we do regularization in the first place: to train models that don't overfit on the training data, and generalize better to unseen data.

