THE DEEP LEARNING DUMP

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Contents

Part 1. Deep Neural Networks

- 1. Cross Entropy Loss
- 2. Gaussian Processes

Part 2. Recurrent Neural Networks

3. Long Short Term Memory, LSTM

Part 3. Transformer Networks

4. Transformers

References

ABSTRACT. Everything Deep Learning, Deep Neural Networks

Part 1. Deep Neural Networks

1. Cross Entropy Loss

See Pytorch "CrossEntropyLoss".

Consider the classification problem such that $y \in S$ where S is some finite set, i.e. $S \in \mathbf{FiniteSet}$. Let $C \equiv \text{total number of "classes" or elements in this set <math>S$.

For what Pytorch calls minibatch in the documentation for "CrossEntropyLoss", let minibatch $\equiv N$ for our notation (the reason is we can say we have N samples in our batch).

 d_1, \ldots, d_k with $K \ge 1$ for the K-dimensional case, with K being the number of additional "features" for a single data point x. We've seen K be denoted D in other literature.

The Pytorch literature says that the input into torch.nn.CrossEntropyLoss is a "Tensor" of size (C) for unbatched input, (minibatch, C) or (minibatch, $C, d_1, d_2, \ldots d_K$). The documentation says the last "being useful for higher dimension inputs". I interpret this as being for a single data point with multiple features.

Consider these 2 examples: for a classification problem with C=3 such as cat, dog, or mouse, if there are no additional features, we could imagine that for training data point X,

$$X \mapsto h \in \mathbb{R}^C \mapsto y, y \in S \text{ s.t. } |S| = C$$

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where $h \in \mathbb{R}^C$ are the so-called "logits" generated by the "forward pass" (the linear transformations and nonlinear element wise mappings of the model) which then result into a prediction for a $y \in S$. The input is of size (N, C) as there are no further additional features to consider.

Consider a grayscale image (i.e. each pixel has a single value for brightness, 0 to 255). Generalize this to each pixel having a value in $\{0, \dots P_b - 1\}$. If the image has "dimensions" $H \times W = 28 \times 28$ for example, then $d_1 = H$ and $d_2 = W$ and K = 2. So in this case the input dimensions are $(N, C, d_1 = H, d_2 = W)$.

2. Gaussian Processes

Yang (2021) for Tensor Programs I[1]

Part 2. Recurrent Neural Networks

3. Long Short Term Memory, LSTM

The NVIDIA CUDNN Documentation, in 7.1.2.8. cudnnRNNMode_t says these following equations apply for the 4-gate Long Short-Term Memory (LSTM) network with no peephole connections, and for the default mode of CUDNN_RNN_DOUBLE_BIAS:

$$i_{t} = \sigma(W_{i}x_{t} + R_{i}h_{t-1} + b_{Wi} + b_{Ri}) = \sigma(W_{i}x_{t} + b_{Wi} + R_{i}h_{t-1} + b_{Ri})$$

$$f_{t} = \sigma(W_{f}x_{t} + R_{f}h_{t-1} + b_{Wf} + b_{Rf}) = \sigma(W_{f}x_{t} + b_{Wf} + R_{f}h_{t-1} + b_{Rf})$$

$$o_{t} = \sigma(W_{o}x_{t} + R_{o}h_{t-1} + b_{Wo} + b_{Ro}) = \sigma(W_{o}x_{t} + b_{Wo} + R_{o}h_{t-1} + b_{Ro})$$

$$c'_{t} = \tanh(W_{c}x_{t} + R_{c}h_{t-1} + b_{Wc} + b_{Rc}) = \tanh(W_{c}x_{t} + b_{Wc} + R_{c}h_{t-1} + b_{Rc})$$

$$c_{t} = f_{c} \circ c_{t-1} + i_{t} \circ c'_{t}$$

$$h_{t} = o_{t} \circ \tanh(c_{t})$$

where \circ denotes an element-wise operation.

Compare this with the expression given in PyTorch, LSTM and they are similar, but $c'_t \equiv g_t$ and \odot denotes the element-wise operation. In Eq. 1,

 x_t is input at time t,

 i_t is the so-called input gate,

 f_t is the so-called forget gate,

 g_t is the so-called cell gate,

1

 o_t is the so-called output gate.

and

(3)

(2)
$$\sigma \equiv \text{ sigmoid operator, s.t. } \sigma(x) = \frac{1}{1 + \exp(-1)}$$

is the sigmoid function.

Also, output hidden (state of each) layer h_t can be multiplied by a learnable projection matrix $h_t = W_{hr}h_t$. Let us write Eq. 1 in the following manner:

$$(x_{t}, h_{t-1}) \xrightarrow{\sigma \odot (W_{i}, b_{Wi})(R_{i}, b_{Ri})} i_{t}$$

$$(x_{t}, h_{t-1}) \xrightarrow{\sigma \odot (W_{f}, b_{Wf})(R_{f}, b_{Rf})} f_{t}$$

$$(x_{t}, h_{t-1}) \xrightarrow{\sigma \odot (W_{o}, b_{Wo})(R_{o}, b_{Ro})} o_{t}$$

$$(x_{t}, h_{t-1}) \xrightarrow{\sigma \odot (W_{c}, b_{Wc})(R_{c}, b_{Rc})} c'_{t} \equiv g_{t}$$

$$(f_t, c_{t-1}, i_t, c'_t) \longrightarrow c_t$$

$$(o_t, c_t) \longrightarrow h_t$$

From this we can clearly see that $\forall t \in \{0, 1, ..., T-1 \text{ where } T \text{ is the } sequence length \text{ (Pytorch denotes this as } L = \text{sequence length in the Pytorch LSTM documentation)}$ the inputs in are (x_t, h_{t-1}) and the output is h_t and that c_t is also effectively an output for the next time step t+1.

EY: 20230903 It is not clear however, what form does c_{-1} takes that'd be necessary for the computation of c_0 for t = 0. While one could maybe make some guess or ansatz about what h_{-1} to use initially and compute i_0, f_0, o_0 to use for some initialized values for the operators W, R, and biases b's, does one have to make a guess or ansatz about c_{-1} as well?

Part 3. Transformer Networks

Including Attention

4. Transformers

4.1. **Input.** See Turner (2023) [2].

Let input data s.t. sequence of N $\mathbf{x}_n^{(0)}$ of dim. D, n = 0, 1, ..., N - 1, $\mathbf{x}_n^{(0)} \in F^D$, where F is some field (i.e. some data type such as float, double, etc.).

Let matrix $X^{(0)} \in F^{D \times N}$ or $\mathrm{Mat}_F(D, N)$, a sequence of N arrays of dim. D collected into a matrix.

Let
$$M \in \{0, 1, \dots \text{ i.e. } M \in \mathbb{Z}^+.$$

The goal is to map $X^{(0)}$ to $X^{(M)} \in \operatorname{Mat}_F(D, N)$ i.e. $X^{(M)}$ of size $D \times M$ s.t. since $x_n = X_{;n}^{(M)}$ is a vector of features representing the sequence at location of n in the sequence.

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4.2. Attention $A^{(m)}$. Consider output vector at location n, $\mathbf{y}_n^{(m)}$, where

(4)
$$\mathbf{y}_{n}^{(m)} = \mathbf{x}_{n'}^{(m-1)} A_{n'n}^{(m)}, \quad n' = 0, 1, \dots N - 1$$

(Eq. (1) of Turner (2023) [2]), where $A_{n'n}^{(m)} = A^{(m)}$ is called the attention matrix, $A^{(m)} \in \operatorname{Mat}_F(N, N)$ and normalizes over its columns:

(5)
$$\sum_{n'=1}^{N} A_{n'n}^{(m)} = 1$$

4.3. Projection of Q, K, V, queries, keys, and values. Recall an input $\mathbf{x}_n = X_{;n}^{(M)} \in F^D$. Recall the linear transform resulting so-called queries or query vectors:

$$\mathbf{q}_{h,n}^{(m)} = U_{q,h}^{(m)} \mathbf{x}_n^{(m-1)} \in F^K, \quad U_{q,h}^{(m)} \in \text{Mat}_F(K, D)$$

where h = 0, 1, ... H - 1 with H heads in Turner's notation (Turner (2023)[2]). Compare this with NVIDIA's notation, [3], i = 0, 1, ... nHeads -1, so that $H \equiv$ nHeads.

Generalize K in dimensiosn $k \times D$ of $U_{q,h}^{(m)}$ to $qSize \equiv D_q$, i.e.

$$\mathbf{q} \equiv \mathbf{q}_{h;n}^{(m)} = U_{q;h}^{(m)} \mathbf{x}_n^{(m-1)} \in F^{D_q}, \quad U_{q;h}^{(m)} \in \text{Mat}_F(D_q, D)$$

See 7.2.45. cudnnSetAttnDescriptor

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