
Deep Learning Homework assignment

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1 Vanilla RNN vs LSTM

1.1 Vanilla RNN in pyTorch

- Question 1

With the following basic equations we will derive the partial equations w.r.t W_{ph} , W_{hh} , W_{hx} .

$$h^t = \tanh \left(W_{hx} \cdot x^t + W_{hh} \cdot h^{(t-1)} + b_h \right)$$

$$p^t = W_{ph} \cdot h^t + b_p$$

$$\mathcal{L} = - \sum_{k=1}^K y_k \log \hat{y}_k$$

$$\frac{\partial \mathcal{L}^T}{\partial W_{ph}} = \frac{\partial \mathcal{L}^T}{\partial \hat{y}^t} \frac{\partial \hat{y}^t}{\partial p^t} \frac{\partial p^t}{\partial W_{ph}}$$

$$\frac{\partial \mathcal{L}^T}{\partial \hat{y}^t} = \frac{\partial}{\partial \hat{y}} - y \log \hat{y} + -y \frac{\partial}{\partial \hat{y}} \log \hat{y}$$

$$= 0 - \frac{y}{\hat{y}}$$

$$= -\frac{y^T}{\hat{y}^T}$$

$$\frac{\partial \hat{y}^T}{\partial p^T} = \text{softmax}(p^T) \frac{\partial}{\partial p^T}$$

$$= \text{softmax}(p_i^T) (\delta_{ij} - \text{softmax}(p_j^T))$$

$$\frac{\partial p^T}{\partial W_{ph}} = \frac{\partial}{\partial W_{ph}} W_{ph} \cdot h^t + \frac{\partial}{\partial W_{ph}} b_p$$

$$= -\frac{y^T}{\hat{y}^T} \cdot \text{softmax}(p_i^T) (\delta_{ij} - \text{softmax}(p_j^T)) \cdot h^t$$

$$= -\frac{y^T}{\hat{y}^T} \hat{y}^T (\delta_{ij} - \hat{y}^T) \cdot h^T$$

$$= -y^T \cdot (\delta_{ij} - \hat{y}^T) \cdot h^T$$

$$\frac{\partial \mathcal{L}^T}{\partial W_{hh}} = \frac{\partial \mathcal{L}^T}{\partial \hat{y}^T} \frac{\partial \hat{y}^T}{\partial p^T} \frac{\partial p^T}{\partial h^T} \frac{\partial h^T}{\partial W_{hh}}$$

$$= \sum_{i=0}^T \frac{\partial \mathcal{L}^T}{\partial \hat{y}^T} \frac{\partial \hat{y}^T}{\partial p^T} \frac{\partial p^T}{\partial h^T} \frac{\partial h^T}{\partial h^i} \frac{\partial h^i}{\partial W_{hh}}$$

The gradient w.r.t to the hidden state needs to be calculated up till the initial hidden unit while that of the output layer does not. With this in mind, managing memory and gradients value can be an issue in the hidden state. There is two case for this issue, either the gradient vanishes back through the initial layer or it explodes when going through time.

- Question 2 See code implementation.
- Question 3
- Question 4
The benefit of using RMSprop or Adam rather than SGD is that the previous optimizer take the momentum into account during training, while SGD not well tuned might oscillate to find the optimal solution. Moreover SGD updates its step according through the loss value back-propagated, while the aforementioned optimizer utilize adaptive learning rates where there is a global learning rate and a targeted learning rate for each weight that changes during training depending on the sign between current gradient and velocity of that weight. Differently put, adaptive learning rate ensure that the change in signs of the weights during training will influence if the training is approaching a (global) minimum.

1.2 Long Short Term Memory (LSTM) in pyTorch

- Question 5
The forget-gate is responsible to ensure and inspect the usefulness of the information entering the cell over time, so it scales numerically the usefulness between 0 and 1 and thus behaving as switch. The input-gate also needs to evaluate the usefulness of the current input and registering it to the cell state. This gate also behaves as a switch due to the sigmoid function output. The output-gate, finally needs to evaluate the information usefulness of the system to pass to the next cell state. The output gate generates candidate with \tanh activation function according to the forget and input gate, the effect of a different activation between $-1, 1$ is either to excite or dampen the activation for the next cell state with information.
We know from the definition that there are four different weight matrices depending on the input, hidden units and biases. Thus we will require the sum of the following; for an input matrix with dimension dxn , weights of hidden units $n \times n$ and biases vectors n . This is $4 * (dxn) + 4 * (n \times n) + 4 * n$ trainable parameters that are needed for training.
- Question 6
- Question 7

2 Recurrent nets as Generative Model

- Question 1
- Question 2
- Question 3
- Question 4

3 Graph Neural network

3.1 GCN Forward Layer

- Question 1
With every node present, the layer contains informations of the nodes and their neighbours that is encoded in the adjecency matrix. As passing from one layer to another the information of the neighbours is used to traverse the graph.
- Question 2
In a graph where there is no edge between the nodes for example see Figure 2 in the assignment, with one layer it will not make it possible to pass the information from example node b to e . To resolve this issue, we should create a network with as many layer as the diameter of the graph.

- Question 3

$$\tilde{A} = \begin{pmatrix} 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 \end{pmatrix}$$

- Question 4
So, we require three updates, because there are two edges between these nodes to be traversed.

3.2 Applications of GNN

- From Shen et al. (2018) we see that the re-indentification problem in the computer vision domain an attempt to resolve it with the aid of Graph Neural Network.
- Furthermore, we see that Prates et al. (2019) uses Graph Neural network to solve an NP-Complete problem as the travelling salesman problem.

3.3 Comparing GNN and RNN

- Question 1
Using text translation with RNN would be very suitable but using the text to understand context, a GNN will likely be very suitable where perhaps every sentence or paragraph could be a node and each next sentence or paragraph could be connected with an edge. This choice of representation would make it very useful to understand the overall structure, this could act as a viable memory compared to the memory issue a regular RNN network would face if the task would be context understanding. With complex data representation where connection in the building blocks are necessary, a GNN would be very suitable and flexible to understand such data. Similarly, sequences which could have some inherently pattern as music, dance, sentences a representation with an RNN network can be very suitable.
- Question 2
As we have already learned, images are complex data structures to process in an neural network. This recent article by Liang et al. (2016) combines an LSTM with a graph network representation of an image in order to understand segmentation of an image. Each pixel as node and the spatial relation between the nodes as edges, the updates are confidence driven where the emphasis is on different semantic correlations with neighbouring nodes.

References

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- Prates, M., Avelar, P. H., Lemos, H., Lamb, L. C., and Vardi, M. Y. (2019). Learning to solve np-complete problems: A graph neural network for decision tsp. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 33, pages 4731–4738.
- Shen, Y., Li, H., Yi, S., Chen, D., and Wang, X. (2018). Person re-identification with deep similarity-guided graph neural network. In *Proceedings of the European Conference on Computer Vision (ECCV)*, pages 486–504.