Neural network knowledge distillation in tensor networks

Dereck Piché

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Abstract

1   Introduction

TODO ctrl f R -¿ mathbbR TODO fix spelling TODO : TRAIN ON THE SAME SET OF EXAMPLES TODO: DO FOR DIFFERENT values of Rthe BOND DIMENSION OF THE MPS (complexity) GUILLAUME: 10, 20, 30, 80 tu peux repeter l'ensemble d'expériences environ 20 fois et regarder le standard deviation

2   Knowledge Distillation

Knowledge Distillation is a machine learning practice which involves taking a trained model and using it's parameters to train another one. The already trained model is referred to as the "teacher", and the model in which his "knowledge" is to be distilled is referred to as the "student". While this is a relatively novel technique, there are already several distinct approaches introduced by researchers. We used two of these approaches. Our inspiration for the distillation methodology was found in a a 2021 survey which resumed the emerging practice [1].

2.1   Response-Based Knowledge Distillation

The first approach we used to look exclusively at the outputs of the student and teacher. Now, we apply the logits of our functions element-wise to the

outputs and the softmax.

$$\text{softmax}(v_i) = \frac{e^{v_i}}{\sum_j e^{v_i}} \tag{1}$$

The softmax function's objective is to transform the logits into probability distributions for the different classes. We will now apply a loss function L to these two functions. Since we are trying to reduce the divergence between two distributions, we will use the Kullback-Leibler divergence loss

$$\text{KL}(P, Q) = \frac{1}{n} \sum_i^n Q \frac{\log_e(Q)}{\log_e(P)} \tag{2}$$

Here, Q is the distribution we are aiming for and P is the one we have.

2.2 Layer-based approach

The survey on Knowledge Distillation coined the term *Layer-based approach*. Deep learning models work in layers of feature maps. It is hypothesized that these different layers represent different layers of abstraction in the internal representation of their input.

3 Tensor Networks

Tensor Networks come from the study of quantum phenomena. They started being used recently as machine learning models. Tensor Networks can be thought out as two things: a visual notation system and a set of methods for tensor manipulation.

3.1 Tensors

Before explaining these two, we shall disambiguate the meaning of "tensor". In this report (and very often in the context of machine learning), we use the word "tensor" to refer to the mathematical arrays of arbitrary indices. Here, the number of indices is called the "order" of the tensor, meaning that vectors are simply tensors of order 1 and matrices tensors of order 2.

3.2 Contraction

At the heart of tensor networks is the *contraction* operation. Tensor Networks are used to compute a larger network by "contracting" several smaller

tensors over chosen indices. A "contraction" is simply an operation where we sum over indices. For example, the contraction of A_{ijk} and B_{ijk} on index j will produce the tensor $C_{ik} = \sum_j A_{ijk} B_{ijk}$. Evidently, the two indices present in a contraction must be of the same size.

3.3 Tensor Networks as a graphical system of notation

The principal motivation behind the creation of Tensor Networks to compute or approximate large tensors *contracting* several smaller tensors over chosen indices. This is all well and good until our conventional summation notation begins overclocking our primal brains. So, in order to make the manipulation of these network of tensors, mathematicians created a notational system. Tensors are represented as nodes where each vertex connected to the node represents one of the tensor's indices. If a vertex connects two nodes, it means that the indices shall be contracted in order to produce the post-contraction tensor. It should be evident that by the definitions above, no node (tensor) is completely isolated in a tensor network, as it would be completely purposeless. The shape of the post-contraction tensor can be easily visually identified, since it is found in the unconnected vertices. A simple tensor network can be found in figure 1.

3.4 Tensor Network Methods

The term *Tensor Network Methods* is used to refer to, you guessed it, the methods. There are several architectures of Tensor Networks that are frequently used, such as the *Matrix Product State (MPS)*, the *Tenso*

Figure 1: Simple tensor network illustrating the notation.
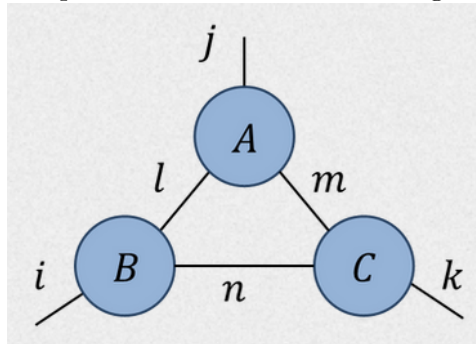
4 Single feature map functions

Before deep neural networks gained mass adoption, a common way to learn a model was to design a certain feature map of the inputs and apply a linear transformation to the output of the feature map in order to obtain the model's predictions. In this paper, we will study a model of this type. However, particular importance to our feature tensor.

4.1 Feature tensor $\Phi(x)$

Consider an input vector $x \in R^d$. Let $\phi(x) : R \mapsto R^{d_\phi}$. Then, let us take the tensor product of $\phi(x)$ applied to every element of the vector x.

$$\Phi(x) = \phi(x_1) \otimes \phi(x_2) \otimes (\dots)\phi(x_d) \tag{3}$$

We obtain a tensor $\Phi(x)$, of which the sum of it's element contain the basis of a space of products of the elements of the transformed elements of $\phi(x)$. We can take a linear map of the elements of $\Phi(x)$ and produce a function.

$$g(\Phi(x))$$

The function g can be learned.

In order to reduce the abstractness of this statement, we can take say that $\otimes$ refers to the Kronecker Product.

4.2 Multilinear feature vector

In this project, we attributed a particular importance to the local feature map

$$\phi^*(x) = \begin{bmatrix} 1 \\ x \end{bmatrix} \tag{4}$$

With, this particular transformation, the Kronecker Product gives us a global feature map $\Phi(x)$ which is a tensor where each element is a basis of the space of multilinear functions on the elements of the vector x. Here, the order or shape of the tensor is superfluous and gives no theoretical advantage.

4.3 Linear Combinations

Now, the question is how do we use $\Phi(x)$, how does it become useful? Well, it becomes useful when we take a linear map of it's elements. Let our $\Phi(x)$

be an arbitrarily shaped tensor of d_Φ dimensions. The final form of our function $f(x)$ will be

$$f(x) = \sum_i^{d_\Phi} \theta_i [\Phi(x)]_i \tag{5}$$

Now, we have a function that can, under some choice of transformation ϕ, become extremely expressive. For our particular local feature map ϕ^*, it can represent any multililinear function of the input vector x. We shall represent linear combinations of $\Phi(x)$ by $T\Phi(x)$.

5 Using The Matrix Product State Tensor Network

In this project, we used the *Matrix Product State* (MPS) tensor network to approximate the function $T\Phi(x)$. Here, this function is computed by contracting a Tensor Network. Before the contraction, some of the elements of the tensors in the tensor network are set by applying the mapping $\phi^*(x)$.

5.1 Building the model using a single MPS

As proposed in the paper [3], we are going to use a particular Tensor Network Method in order to reproduce a model of the form 5. Before going over the use of MPS, let's think of a way to use tensors and contraction to learn a model of a function $f : R_d \mapsto R_q$. First, we create a tensor of the form $T^{o_1 o_2 (\dots) o_d i}$, where, each o is of dimension 2 and i is of dimension q (the dimension of the output of f). Then, if we apply a contraction between every o_i and it's corresponding vector $\begin{bmatrix} 1 \\ x_i \end{bmatrix}$, we obtain a function $m : R_d \mapsto R_q$. Our model m can learn f by adjusting the parameters of the tensor T by supervised learning.

The problem is that as of now, the tensor T has 2^d elements. In order to reduce the size of T, we can approximate it by using a decomposition called the *Matrix Product State*.

$$T^{o_1 o_2 (\dots) o_d} \approx T_{MPS} = \sum_{\{b_1, b_2, (\dots), b_d\}} t^{o_1}_{b_1} t^{o_2}_{b_1, b_2} t^{o_3}_{b_2 b_3} \cdots t^{o_d}_{b_{d-1}} \tag{6}$$

Here, the complexity of the MPS is determined by the *bond dimension* of it's tensors. The *bond dimension* of T_{MPS} is the dimension of the contracted

indices of the network. In equation 6, it would be the dimension of the b indices.

Now, our goal is rather to use the MPS to perform a certain computation, not compress tensors.

In order to do this, we will contract every index of the tensor B. TODO: add number of parameters of MPS and how it grows with respect to size

5.2 Composition of MPS

As mentionned before, taking a linear map of tensor product of the local feature map $\begin{bmatrix} 1 \\ x \end{bmatrix}$ amounts to producing a multilinear function of x.

Since our MPS model can only approximate this function, it means that it's expressivity will be somewhat limited. For example, it could never express the function $f(X) = x_1 x_2^2$.

A pretty obvious solution for this problem is to add another layer by feeding to ouputs of our MPS model into a second one.

Instead of looking at the expressivity of this composition directly, we will analyse the expressivity of the functions that the MPS models are trying to approximate. This will give us a good idea of how expressive this composition can be. Also, from now on, this composition will be refered to as *2-MPS*.

The 2-MPS model approximates a function of the form.

$$g' \circ f \circ g \circ f(x)$$

In the following subsection, we will prove that this composed function can express any multivariate polynomial function of degree z.

5.2.1 Proof of expressivity

Definition 5.1 (A ψ function). A multilinear polynomial is a function $f : R^n \mapsto R$ of the form A ψ function is a function of the form

$$g' \circ f \circ g \circ f(x)$$

, where f is a function that returns a basis of a multililinear function and g' and g are arbitrary linear maps.

Definition 5.2 (Multilinear polynomial). A multilinear polynomial is a function $f : R^n \mapsto R$ of the form

$$f(x) = T \cdot \left(\begin{bmatrix} 1 \\ x_1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ x_2 \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} 1 \\ x_d \end{bmatrix} \right) \tag{7}$$

Where $T \in R^{p \times R^n}$. In other words, a multilinear polynomial is a polynomial that is linear if $\forall x_i$ then the polynomial is linear if we fix every variable except x_i.

Definition 5.3 (v_i-variate). Function of the variables of the vector v. (Each element of v is considered as a variable).

Theorem 5.1. Any polynomial function $\Gamma : R^d \mapsto R$ of degree z can be expressed as a $\mathtt{psi}$ function by choosing particular g' and g maps.

Proof. Let the function g in a ψ function be defined such that

$$g(f(x)) = \begin{bmatrix} repeated\ z\ times \begin{cases} x_1 \\ (\dots) \\ x_1 \end{cases} \\ repeated\ z\ times \begin{cases} x_2 \\ (\dots) \\ x_2 \end{cases} \\ (\dots) \\ repeated\ z\ times \begin{cases} x_n \\ (\dots) \\ x_n \end{cases} \end{bmatrix} \tag{8}$$

We can rewrite this vector as

$$g(f(x)) = \begin{bmatrix} \varepsilon_{1,1} \\ (\dots) \\ \varepsilon_{1,z} \\ \varepsilon_{2,1} \\ (\dots) \\ \varepsilon_{2,z} \\ (\dots) \\ \varepsilon_{d,z} \end{bmatrix} = \lambda \tag{9}$$

Let Z be the space of x_i-variate polynomial functions of degree $\leq z$. By definition, every monomial of $\zeta \in Z$ is of the form

$$x_1^{k_1} x_2^{k_2} (\dots) x_d^{k_d} \tag{10}$$

, where $\sum k_i \leq z$.
However, for every set $\{k_1, k_2, (\dots), k_d\}$ meeting this condition, we can rewrite

the monomial as

$$\left(\prod_{i_1=1}^{k_1} \varepsilon_{1,i_1}\right) \left(\prod_{i_2=1}^{k_2} \varepsilon_{2,i_2}\right) (\dots) \left(\prod_{i_d=1}^{k_d} \varepsilon_{d,i_d}\right) \tag{11}$$

by using the elements of λ from equation (9).

However, we can clearly see that this term is a multilinear monomial of the variables in λ. This implies that $f(\lambda *)$ returns a basis-vector of x_i-variate polynomial function of degree $\leq z$.

In other words,

$$\xi(x, \Theta) = M\left(f\left(M\left(f(x), \Theta^*\right)\right), \Theta\right) \tag{12}$$

can express any x_i-variate polynomial function of degree $\leq z$ under fixed Θ.

This process can be visualised as

$$X \in R^d \xrightarrow{f} Y_1 \in R^{2^d} \xrightarrow{g} Y_2 \in R^{zd} \xrightarrow{f} Y_3 \in R^{2^{zd}} \xrightarrow{g'} Y_4 \in R \tag{13}$$

$$\square$$

5.3 Patching of MPS (experimental)

6 Methodology

The experiments done for the projet were programmed using Python. Now, evidently, using Python alone was not possible. The big deep learning library we used was Pytorch, as is common in machine learning today. However, it does not provide many tools to train and build Tensor Networks. We thus used TorchMPS [2], a library built using Pytorch for the creation and training of learning Matrix Product State tensor networks.

TODO: mention custom feature map in forked code

Learning rate
We used the very standard learning rate of $1e-4$. This is the proposed learning rate in the code of [2].

Model size

Approach to the results As a matter of scientific integrity, we have chosen to show the results even if they are heavily disappointing. Not doing so can result in certain statistical biases which can be avoided.

Learning rate for neural network: 0.01 Learning rate for MPS: 1e-3 = 0.001 Nb of normal epochs: 25 Nb of gaussian epochs: 5

7 Results

7.1 Training the single MPS

Bond Dimensions	MPS	NN to MPS	2-MPS	NN to 2-MPS
10	None	None	None	None
20	None	None	None	None
40	None	None	None	None
80	None	None	None	None

8 Conclusion

8.1 Further Exploration

TODO talk about capturing locality in the mappings TODO talk about capturing locality in general with tensors

References

[1] Jianping Gou et al. "Knowledge Distillation: A Survey". In: *International Journal of Computer Vision* 129.6 (Mar. 2021), pp. 1789–1819. DOI: 10.1007/s11263-021-01453-z. URL: https://doi.org/10.1007%2Fs11263-021-01453-z.

[2] Jacob Miller. *TorchMPS*. https://github.com/jemisjoky/torchmps. 2019.

[3] E. Miles Stoudenmire and David J. Schwab. *Supervised Learning with Quantum-Inspired Tensor Networks*. 2017. arXiv: 1605.05775 [stat.ML].