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# Tensor, Tensor Networks, Quantum Tensor Networks in Machine Learning: An Hourglass Architecture

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## Abstract

1 Quantum tensor networks in machine learning (QTNML) are envisioned to have  
2 great potential to advance AI technologies. Recent works show that (quantum)  
3 tensor networks provide powerful simulations of quantum machine learning al-  
4 gorithms on classical computers. We observe that tensor, tensor networks and  
5 quantum tensor networks in machine learning exhibit a layered architecture that  
6 resembles an hourglass. In this paper, we describe a seven-layer architecture to  
7 characterize the role of tensor, tensor networks and quantum tensor networks in  
8 machine learning, point out current challenges and discuss recent innovations. As  
9 a cornerstone data structure, tensor and tensor networks lie at the waist of the  
10 hourglass-shaped architecture, while the lower and upper layers tend to see fre-  
11 quent innovations. We expect tensor, tensor networks and quantum tensor networks  
12 continue to serve as an *amplifier* for computational intelligence, a *transformer* for  
13 machine learning innovations, and a *propeller* for AI industrialization.

## 14 1 Introduction

15 *Why do conventional machine learning algorithms use vectors and matrices, while deep learning*  
16 *algorithms and neural networks mostly rely on tensors? A simple and direct answer is that deep*  
17 *learning usually involves hundreds, if not thousands, of features.*

18 Quantum tensor networks [6] in machine learning (QTNML) are envisioned to have great potential to  
19 advance AI technologies. Quantum machine learning [7] promises quantum advantages (potentially  
20 exponential speedups in training, quadratic speedup in convergence, etc.) over classical machine  
21 learning, while (quantum) tensor networks provide powerful simulations of quantum machine learning  
22 algorithms on classical computers. QTNML is now a rapidly growing interdisciplinary area.

23 (Quantum) Tensor networks<sup>1</sup>, a contracted network of factor tensors, have arisen independently  
24 in several areas of science and engineering. Such networks appear in the description of physical  
25 processes and an accompanying collection of numerical techniques have elevated the use of quantum  
26 tensor networks into a variational model of machine learning. Underlying these algorithms is  
27 the compression of high-dimensional data needed to represent quantum states of matter. These  
28 compression techniques have recently proven ripe to apply to many traditional problems faced in deep  
29 learning. (Quantum) Tensor networks have shown significant power in compactly representing deep  
30 neural networks [55], and efficient training and theoretical understanding of deep neural networks.  
31 More potential tensor network technologies are rapidly emerging, such as approximating probability

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<sup>1</sup>A major difference of quantum tensor networks from tensor networks would be the contractions are required to be unitary transforms.

functions and probabilistic graphical models [67, 22]. A merger of (quantum) tensor network algorithms with state-of-the-art approaches in deep learning is now taking place.

Quantum algorithms are typically described by quantum circuits (quantum computational networks). These networks are indeed a class of tensor networks, creating an evident interplay between classical tensor network contraction algorithms and executing tensor contractions on quantum processors. The modern field of quantum enhanced machine learning has started to utilize several tools from tensor network theory to create new quantum models of machine learning and to better understand existing ones.

The interplay between tensor networks, machine learning and quantum algorithms is rich. Indeed, this interplay is based not just on numerical methods but on the equivalence of tensor networks to various quantum circuits, rapidly developing algorithms from the mathematics and physics communities for optimizing and transforming tensor networks, and connections to low-rank methods for learning. A merger of tensor network algorithms with state-of-the-art approaches in deep learning is now taking place. A new community on quantum tensor networks in machine learning (QTNML) is forming, which this workshop aims to foster.

The three wagons (driving forces) for the success of machine learning are as follows

- **Big data** (represented as data structures of tensor and tensor networks): the past decade witnesses an exponential explosion of sensory data due to the great advances in sensor manufacturing, leading to the debate of “*More is less?*” or “*More is more!*” [5]. As a cornerstone data structure, tensor and tensor networks are powerful in representing unstructured, multi-modal data and are envisioned to have great potentials to promote the development and deployment of machine learning technologies.
- **Machine learning algorithms and models**: Treating datasets as past experiences, algorithms instruct machines on what they should do. Machine learning algorithms and models allow computers to learn on their own. On the other hand, deep reinforcement learning algorithms train themselves through interactions with an unknown environment.
- **Intelligent computing**. Faster computers can process more data and play a critical role in future AI advancements. Deep learning [39] are computational models with multiple processing layers that learn representations of data with multiple levels of abstraction. In the post Moore’s law era [69], the rise of deep learning [39] can be largely credited to a new paradigm *Intelligent computing for computational intelligence!* E.g., Google has designed and built TPU (Tensor Processing Units) specifically for machine learning and claims to be  $15\times$  faster than a GPU (graphics processing units), while IBM and Google are both developing quantum computing systems.

We observe that tensor, tensor networks and quantum tensor networks in machine learning exhibit a layered architecture that resembles an hourglass. Such an observation is analogy to the hourglass structure [4] of the Internet protocol stack (known as TCP/IP) that successfully provides end-to-end data communication by specifying how data should be packetized, addressed, transmitted, routed, and received.

In this paper, we attempt to initiate a layered architecture for tensor and tensor networks, which will benefit the development of machine learning theory, AI chip manufacturing, and AI applications. This seven-layer architecture resembles an hourglass, namely, tensor, tensor networks and quantum tensor networks lie at the waist while the lower and upper layers tend to see frequent innovations. The bottom layer is the hardware, the highest layer is the AI applications and products. We point out current challenges and discuss recent innovations.

We advocate intelligent computing of quantum tensor networks to achieve computational intelligence. Quantum tensor networks provide a unified full-stack architecture to explore and fulfill the potential of quantum machine learning and general artificial intelligence (AI) on both classical computer and quantum computing platforms, which is envisioned to advance one-step ahead of the current deep learning driven AI. Actually, there is plenty of room at the bottom [19], in the middle, and at the top [40]. In the past, we have already saw  $30\times \sim 100\times$  speedups in basic operations and  $300\times \sim 1,000\times$  speedups in multiple AI tasks, such as image and video processing/recognition, autonomous driving, Internet of Things, gene data analysis, quantitative finance, etc.

Such an hourglass-shaped layer architecture enjoys disciplinary advantages, including layer-wise standardization, intra-layer modularity and inter-layer separability. The *layer-wise standardization* encourages an eco-system for machine learning research and industrialization. With the *intra-layer modularity*, one can update a functional module without interfering other modules. The *inter-layer separability* means that the lower layer is transparent to the upper layer that calls the APIs provided by the lower layer. We expect tensor and tensor networks continue to serve as an *amplifier* for computational intelligence, a *transformer* for machine learning innovations, and a *propeller* for AI industrialization.

We aim to promote discussions (by a series of workshops and academic events) among researchers investigating innovative tensor network technologies from perspectives of fundamental theory and algorithms, novel approaches in machine learning and deep neural networks, and various applications in computer vision, biomedical image processing, natural language processing, and many other related fields. In this survey, we also provide pointers to key references, hardware, software for beginners.

The remainder of this paper is organized as follows. Section 2 describes the proposed hourglass architecture. Section 3 discussed key challenges, recent innovations and broad impacts. We conclude this paper in Section 4.

## 2 The Proposed Hourglass Architecture

We propose a seven-layer architecture for tensor, tensor networks and quantum tensor networks, which resembles an hourglass. Quantum tensor networks provides a unified framework where both classical and quantum computing share the same theoretical and algorithmic developments, and the same model can be trained classically then transferred to a quantum processor. A take-home message would be: there is plenty of room at the bottom [19], in the middle, and at the top [40].

### 2.1 Layer 1: X Processing Unit

In the post Moor’s law era [69], the rise of deep learning [39] can be largely credited to a new paradigm *Intelligent computing for computational intelligence!* The impetus to AI computation is made-for-AI processors, such as GPUs, FPGAs, ASICs (NPU), quantum circuits/processors, etc. We call them *XPU*s.

There is an emergence of dedicated AI accelerator using the ASIC (Application Specific Integrated Circuit) technology, called *NPU* (neural processing unit). Of particular interest are tensor-based NPUs, including Google TPU (tensor processing unit) [29], tensor cores in NVIDIA Volta/Turing Architecture, Intel Nervana neural network processors (NNP), Tensor Computing Processor BM1684, Alibaba Ali-NPU, Knupath Hermosa, Baidu XPU [57], the Huawei Ascend 910 using 32 DaVinci AI cores [44], etc.

The computing power of quantum circuits/processors lies in an optimistic believe of “quantum supremacy” [23], which is a key milestone when certain computational tasks might be executed exponentially faster on a quantum computer than on a classical computer. A recent breakthrough would be Google’s Sycamore processor with 53 qubits. Interested readers may refer to [2] for principles of quantum computing and [1] for discussions of its limits.

Note that quantum circuits can be directly expressed as quantum tensor networks [53].

### 2.2 Layer 2: BLAS and Automatic Tensor Differentiation

To fully utilize the computing power of XPU in Layer 1, *BLAS* (Basic Linear Algebra Subprograms, or Basic Tensor Algebra Subroutines *BTAS*) and *AutoDiff* (Automatic differentiation) [58] are “a knife and fork” to support effective implementation of machine learning models at the top.

Such BLAS standards are implemented and optimized in different programming languages. For example, numpy in Python, cuBLAS in CUDA.

- BLAS level 1 (1969): “vector-vector”;
- BLAS level 2 (1972): “matrix-vector”;

- BLAS level 3 (1980): “matrix-matrix”;
- BLAS level 4 (Now?), “tensor-tensor”: tensor operations include tensor (Kronecker) product, Khatri-Rao product, Hadamard product, tensor contraction, t-product [33] or  $\mathcal{L}$ -product [47], etc.

Automatic differentiation is a technique to numerically evaluate the derivative of a function, which is believed to be very powerful when combining the back-propagation algorithm. Interested readers may refer to AutoDiff [58] and DDSP (differentiable digital signal processing) [16], etc.

Of particular interest is the automatic differentiation for tensors [38] and (quantum) tensor networks [43]. Experimental results [38] show a speedup of up to two orders of magnitude over state-of-the-art frameworks when evaluating higher order derivatives on CPUs and a speedup of about three orders of magnitude on GPUs. H.-J. Liao *et al* [43] advocates that differential programming of tensor networks open the door to many innovations and applications.

### 2.3 Layer 3: Tensor Data Structure

Tensor is the most popular data structure in machine learning, especially in deep learning. For instance, a) input data: color image set, video sequence, MRI/fMRI, EEG, gene expression, traffic data, social network data, knowledge graph; b) High-order statistical information, high-order moment, covariance, cumulant, etc.; c) model parameters: fully connected layer, convolutional layer, multi-task weight parameters, multi-modal feature fusion, and etc.; and d) function: probability mass function of multiple discrete variables.

In the past, a unified notation set for tensors [34], tensor networks [10] and quantum tensor networks [7][6] successfully helps the adoption of tensor tools and the development of tensor network libraries in machine learning.

From a machine learning perspective, an  $N$ -th order<sup>2</sup> *tensor* is a container that can house  $N$ -dimensional data and associates with linear/multi-linear operations. A scalar is 0-dimensional, a vector has a single dimension (1D), a matrix has two dimensions (2D), and a higher-order tensor has more than two dimensions.

From a spectral (or transform) perspective, tubal-scalars [33][32][47] are vectors with the multiplication operation defined according to the convolution theorem. Considering a graph transform, one can have graph-tensors [52] or connected matrices [68], and graph tensor neural networks [49].

### 2.4 Layer 4: Tensor Decompositions, Tensor Networks and Quantum Tensor Networks

Many practically useful and efficient tensor models are built upon tensor decompositions, tensor networks and quantum tensor networks.

**Tensor Decompositions:** Canonical Polyadic (CP) tensor decomposition, Tucker tensor decomposition, TT [56] or TR [76] tensor decomposition, HT, tSVD, reshuffling TD. Sparse tensor decomposition and nonnegative tensor decompositions are also developed as extensions of CP, Tucker, TT, TR and HT.

The uniqueness of CP tensor decompositions [11] indicates that multilinear algebra may have theoretical advantages over bilinear and linear algebra.

Other important applications includes tensor completion [66, 45], tensor time series [62, 50], spectral learning on matrix/tensor [26], and data privacy [35, 20, 18].

**Tensor Networks and quantum tensor networks:** TNs show advantages mostly in space complexity reduction and computation efficiency. Tensor Networks have been employed to a) large-scale optimization problems, large-scale eigenvalue problem, large-scale SVD, large-scale matrix pseudo-inverse; b) model compression in DNN, including fully connected layer and convolutional layer; c) expressive power analysis of DNN,

<sup>2</sup>In quantum physics, *rank* corresponds to *order*, while *bond dimension* corresponds to *rank*.

## 2.5 Layer 5: Tensor Libraries and Programming IDEs

Widely used tensor IDEs are TensorFlow [3], PyTorch [59], TensorRT [70], Theano, Keras, Apache MXNet, Caffe2, CNTK, PaddlePaddle, MindSpore, MegEngine, etc.

Other libraries include TensorLayer [15], TensorLy [37]; Tensor decomposition in TensorFlow [54], sparse tensor computing [60], and differentiating tensor networks library [43]

For quantum physics, iTensor (Intelligent Tensor)<sup>3</sup> provides a collection of optimized tensor network algorithms. TensorTrace [17] is an application designed to facilitate the implementation of tensor network algorithms and provides a drag-and-drop interface for building tensor networks.

Google’s TensorNetwork [61] is a library for both physics and machine learning, which is wrapper for TensorFlow, JAX, PyTorch, and Numpy.

## 2.6 Layer 6: Machine Learning Algorithms and Models

There are active research on designing tensor-based machine learning models. We describe a few approaches in the following.

TensorFace [71][72] presents facial image ensembles, where the relevant factors include different faces, expressions, viewpoints, and illuminations. TensorMask [9] is proposed for dense object segmentation.

Tensor regression [36] extends the conventional regression models to tensor representation, while tensor mixture model [64] proposed a probabilistic graphic model in tensor form.

AutoEncoder can be extended to tensor form, such as tensor sparse coding [28].

The generative adversarial network framework is extended to tensor GAN [48] with application to real-time indoor localization for smartphones.

In the model-based direction, tensor neural networks are proposed by unfolding tensor algorithms into deep neural networks, e.g., [51][21] design fast decoders for snapshot compressive imaging cameras, [49] considered recovery of nodes’ data matrices, and [75] investigated the video synthesis problem.

Many complicated TN models including DMRG, TTN, MERA, MERA 2D, PEPS, and etc, which have widely applied to machine learning but may have potential advantages in particular problems.

## 2.7 Layer 7: Applications and Products

Many products embracing AI is enjoying a booming market, penetrating our daily lives: from smartphones to self-driving cars and robotics, search engines, typing assistants (auto-completion), to healthcare services.

Compressing and optimizing neural networks for inference at mobile devices: (i) TVM (tensor virtual machine) [8]; (ii) the Tensor Algebra Compiler (taco) is a C++ library that computes tensor algebra expressions on sparse and dense tensors. It uses novel compiler techniques to get performance competitive with hand-optimized kernels in widely used libraries for both sparse tensor algebra and sparse linear algebra.

**AutoML and neural architecture search (NAS)** are promising, where the training and inference are performed at cloud servers. Many applications are now successfully deployed, including speech recognition, visual object recognition, object detection; others: drug discovery and genomics. Note that health-care is one of the hottest trends, while agriculture applications may have broad social impacts, including automatic quality check, mineral delivery optimization in hydroponics. Disaster recovery is also a critical application.

Big data analysis [65] for image, video; sensory data processing; EEG brain data; finance, genetics, etc.

AI is now being applied massively in entertainment industry, such as chess and poker, medias (e.g. Netflix), music industry (IBM Watson), and online games, etc.

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<sup>3</sup>iTensor: <https://itensor.org/index.html>

224 Other AI products that benefits tensor network algorithms are listed as follows:

- 225 • reCAPTCHA is a CAPTCHA-like system designed to establish that a computer user is  
226 human.
- 227 • SIRI is one of many voice assistants available today.
- 228 • Gmail recently introduced autocomplet tools.
- 229 • Plagiarism checking by searching for matches in billions of documents.
- 230 • FaceID is a feature recently introduced by Apple for authentication on iPhone.
- 231 • Recommendation systems in Amazon and Alibaba Taobao that suggests users other products  
232 based on their preferences and click history.
- 233 • Facebook face detection and tagging is a services of Facebook which automatically detects  
234 faces in images and tags people from the user friendship set.

### 235 3 Challenges, Innovations and Broad Impacts

#### 236 3.1 Challenges

237 The “4V+P” challenge of big data: IBM data scientists break big data into four dimensions [14]:  
238 volume for scale of data, variety for different forms of data, velocity for analysis streaming data, and  
239 veracity for uncertainty of data. We would like to advocate the privacy-preserving requirement as a  
240 plus aspect of tensor learning algorithms. Furthermore, the data acquisition process is expensive in  
241 terms of either time or budget.

242 The  $C^3$ -challenges of machine learning algorithms are the intertwined computing, caching and  
243 communication:

- 244 • *Computing*: Training a model requires substantial amount of time, which in turn slows down  
245 the development. How do we speed up machine learning by  $100\times$ ? Real-time operations  
246 requires fast inference, e.g., cuTensor in NVIDIA CUDA.
- 247 • *Caching*: How to support Billion/Trillion-scale tensor computing? How to compress neural  
248 network for mobile platforms?
- 249 • *Communication*: the bandwidth between CPU and GPU, the link capacity of data centers,  
250 the communication between cloud and edge servers.

251 **Quantitatively characterizing the efficiency-accuracy tradeoff**: how to select tensor network  
252 models for different neural networks? How to tune the hyperparameters in the tensor network model?

253 **Trustworthy AI**: Explainability, interpretability, and understandable. Interpretability is about the  
254 extent to which a cause and effect can be observed within a system. Explainability (for decision  
255 making), meanwhile, is the extent to which the internal mechanics of a machine or deep learning  
256 system can be explained in human terms.

257 **Understanding neural-intelligence**: a two-layer feedforward network [27] is analyzed using CP  
258 tensor decomposition and such a network is believed to learn a mapping between data distribution  
259 priors and labels. On the other hand, an elementary function of neural net’s intelligence is to recognize  
260 symmetry structures in the data [63]: *The glove for the left hand is able to fit the right hand if we*  
261 *turn it inside out like placing an imaginary mirror near the opening. Analogously, neural networks*  
262 *play a similar role as a glove when dealing with inputs of symmetry structures.* The classic Kruskal  
263 uniqueness theorem is exploited to provide a sufficient condition for the situations where such a  
264 generalization capability will hold.

265 Tensor networks provide a rigorous approach to investigate *Why deep is good?* Nadav [12] considered  
266 sum-product networks and CNN with ReLU activation functions [13]. Khrulkov [31][30] took a  
267 similar approach to analyze RNNs.

268 **Robustness of Machine Learning Models**: deep adversarial learning; The notion of differential  
269 privacy is believed to be very power to construct ensemble methods that fuse sub-networks into a  
270 more robust one [42].

## 3.2 Innovations

One recent trend regarding both AI software and hardware is to consider inference and training as two separate different phases with different computational approaches. It is becoming standard to develop specific chips for training and specific chips for inference.

**Cross-layer Codesign.** High performance tensor learning operations by exploiting the massive parallelisms are important for both training and inference: 1). Tensor decompositions on GPUs/FPGA such as cuTensor library [74][46][24][25] and swTensor [77]; 2). Tensor completion [73].

**Federated learning** [35] or **Privacy-preserving tensor algorithms**; homomorphic encryption methods for tensor decompositions.

**Quantum Machine Learning** [7]: tensor networks provide powerful simulations of quantum machine learning algorithms on classical computers, which may promise quantum advantages, such as potentially exponential speedups in training, quadratic speedup in convergence, etc. [41]

**Tensor network learning vs deep learning:** TN has the power to express functions, will tensor network learning be used as a general machine learning model like deep learning?

## 4 Conclusion

Tensor, tensor networks and quantum tensor networks are envisioned to have great potentials to promote the development and deployment of machine learning technologies. In this paper, we have proposed a seven-layer architecture to characterize the role of tensor and tensor networks in machine learning, point out current challenges and discuss the development trends. Such a layered architecture resembles an hourglass. As a cornerstone data structure, tensor and tensor networks lie at the waist of the hourglass, while the lower and upper layers tend to see frequent innovations. We expect tensor and tensor networks continue to serve as a *transformer* for machine learning innovations, an *amplifier* for computational intelligence, and a *propeller* for AI industrialization.

The interplay between tensor networks and machine learning algorithms is rich. Indeed, this interplay is based not just on numerical methods but on the equivalence of tensor networks to various arithmetic circuits, rapidly developing algorithms from the mathematics and physics communities for optimizing and transforming tensor networks, and connections to low-rank methods for learning. A merger of tensor network algorithms with state-of-the-art approaches in deep learning is now taking place. A new community is forming, which this workshop aims to foster.

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