Tensor Network for Supervised Learning at Finite Temperature

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workshop on Tensor Network representation on Machine Learning,
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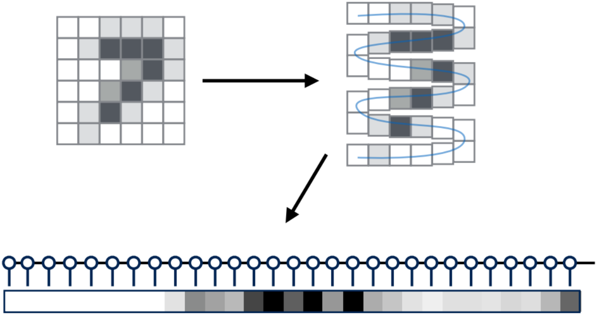
Matrix Product State (MPS) classifier

Map image to the feature map through zigzag order.



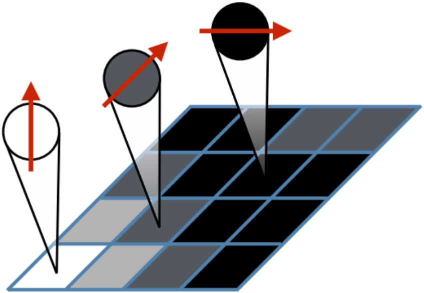
Feature map is the Kronecker product of local feature maps[1].

$$\mathbf{\Psi}(\boldsymbol{X}) = \mathbf{\Psi}^{S_1 S_2 \dots S_N}(\boldsymbol{p}) = \psi^{S_1}(p_1) \otimes \psi^{S_2}(p_2) \otimes \dots \psi^{S_N}(p_N)$$

[1] Edwin Stoudenmire and David J Schwab. Supervised learning with tensor networks. In Advances in Neural Information Processing Systems, pages 4799–4807, 2016.

Matrix Product State (MPS) classifier

Transform grayscale value $x \in [0, 1]$ into a local feature vector ψ.

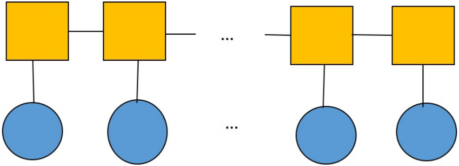


Example mapping:

$$\psi(x) = [\cos(\frac{\pi}{2}x), \sin(\frac{\pi}{2}x)]; \qquad \psi(x) = [x, 1 - x]$$

Matrix Product State (MPS) classifier

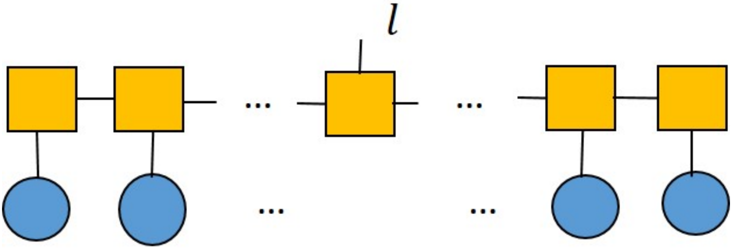
Yellow Cubic: the Matrix Product State (MPS)



Blue circle: the feature map.

Matrix Product State (MPS) classifier

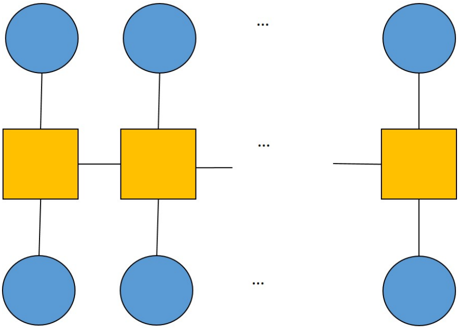
Yellow Cubic: the Matrix Product State (MPS)



Blue circle: the feature map.
For classification task, add an extra label tensor.

Minimally Entangled Typical Quantum States (METTS)

Yellow Cubic: the Matrix Product State (MPS), observable A in physics.



Blue circle: the feature map, wavefunction ψ in physics.
The contraction of it gives the observable $\langle\psi|A|\psi\rangle$.

Minimally Entangled Typical Quantum States (METTS)

If we consider the temperature effect[2]:

$$\langle A \rangle = \frac{1}{Z} \sum_i |\langle i e^{-\beta H/2} A e^{-\beta H/2} | i \rangle$$

In machine learning task,
Treat $|i\rangle$ as image
Treat A (MPS) as energy (H)

[2] EM Stoudenmire and Steven R White. Minimally entangled typical thermal state algorithms. New Journal of Physics, 12(5):055026, 2010.

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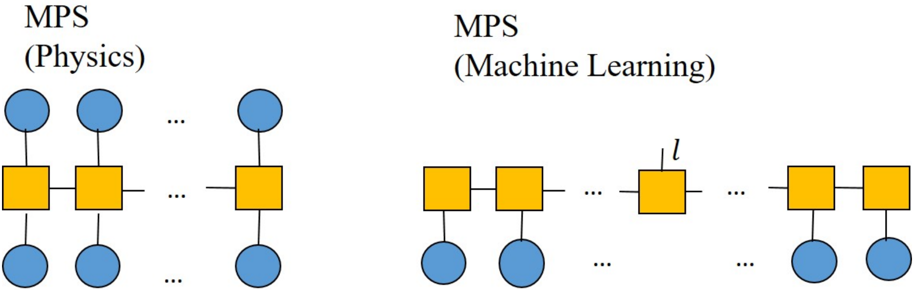
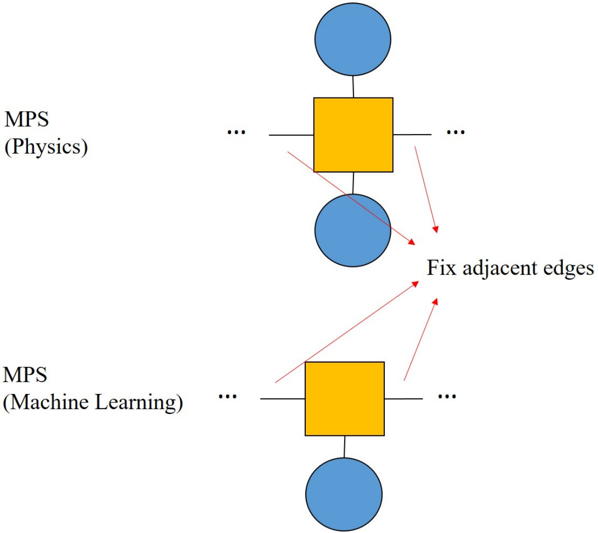
Machine Learning to Physics



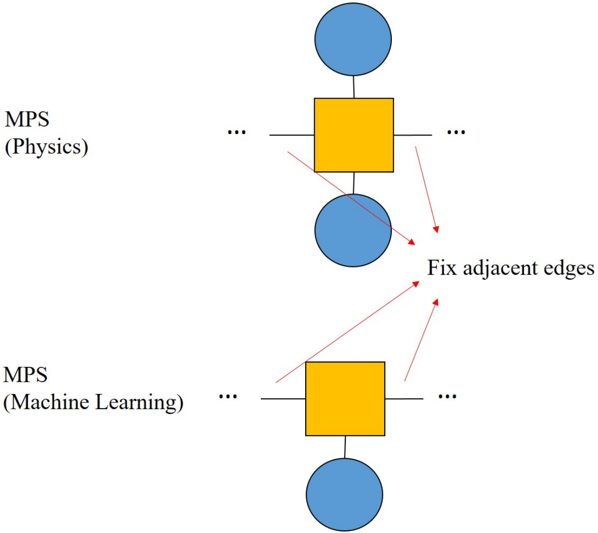
Machine Learning to Physics



$$A'[:,i,j,:] = \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{bmatrix}$$

$$A[:,i,:] = [A_1 \quad \ldots \quad A_n]$$

Machine Learning to Physics

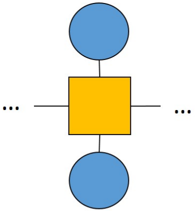


$$A'[:, i, j, :] = \begin{bmatrix} A_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & A_n \end{bmatrix}$$

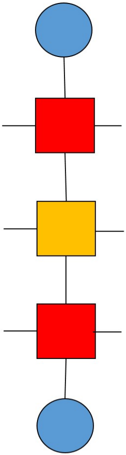
diagonal element

$$A[:, i, :] = [A_1 \quad \ldots \quad A_n]$$

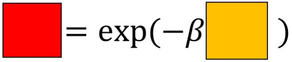
Insertion of Temperature Layer



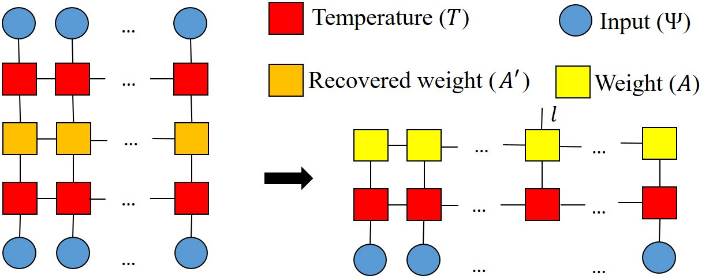
MPS
without temperature



MPS
With temperature



Insertion of Temperature Layer



Until now the Finite Temperature Tensor Network (FTTN) has constructed.

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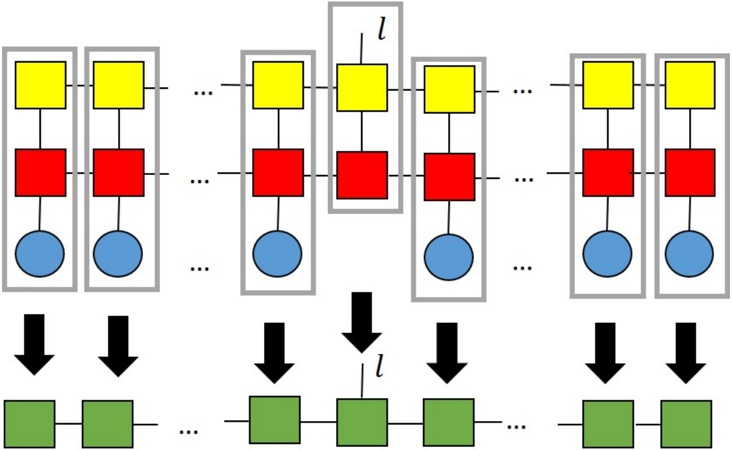
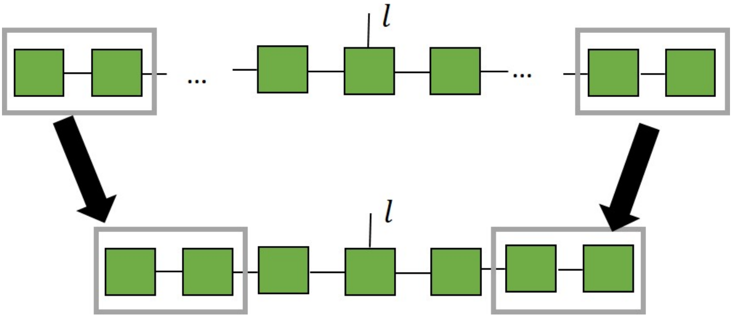
Parallel Contraction Algorithm

Step 1:



Parallel Contraction Algorithm

Step 2: Contract in pairs.



Step 3: repeat step 2 until converge.

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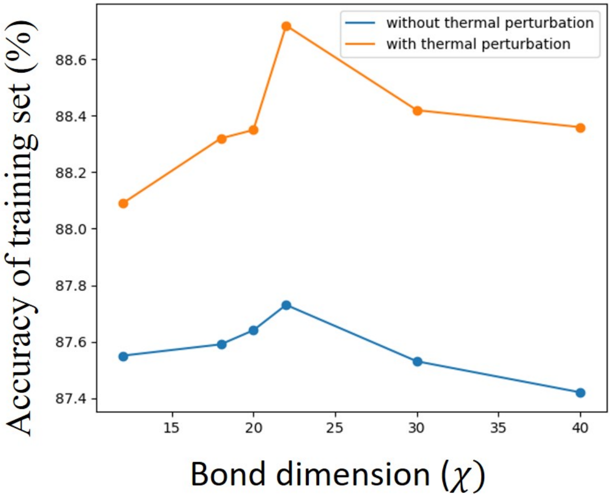
Same setup as [3]

Dataset: Fashion-MNIST

- Optimizer: Adam
- Learning Rate: 1e-4
- Batch Size: 50
- Image Size: 28×28
- Local Feature Map: $\psi(x) = [x, 1 - x]^T$
- Loss function: multi-class cross-entropy $\text{Loss} = \frac{1}{2} \sum_{n=1}^{N_T} \sum_l (f^l(\boldsymbol{x}_n) - \boldsymbol{y}_n^l)$

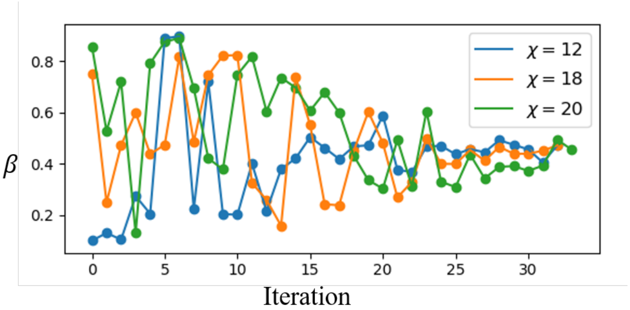
[3] Stavros Efthymiou, Jack Hidary, and Stefan Leichenauer. Tensornetwork for machine learning. arXiv preprint arXiv:1906.06329, 2019.

Experiment results



Interesting Discovery

We tried to optimize temperature-like parameter β by simulated annealing algorithm.



This parameter is nearly independent of bond dimension χ.

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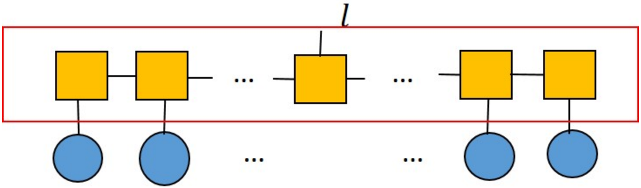
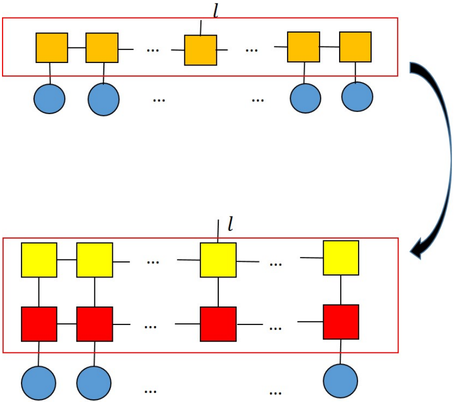
Physical Interpretation



MPS can also represent a feature map $|\rho\rangle$.
Contraction gives inner product, the result comes from the largest one.

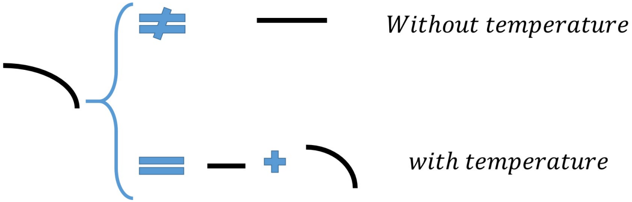
Physical Interpretation



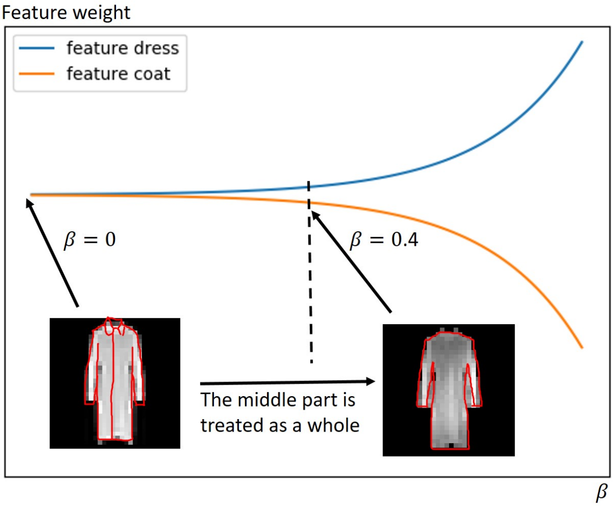
$|\rho\rangle.$

$e^{-\beta H}|\rho\rangle.$

Physical Interpretation



Physical Interpretation

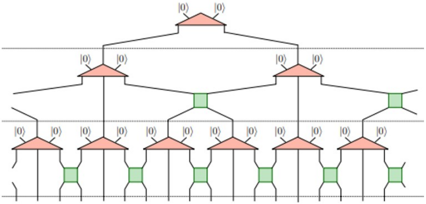


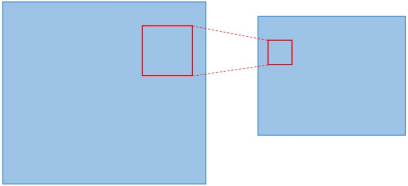
Outlook

Multi-scale Entangled Renormalization Ansatz (MERA)

Similar structure

Convolutional Neural Network





References

[1] **MPS classifier:** Edwin Stoudenmire and David J Schwab. Supervised learning with tensor networks. In Advances in Neural Information Processing Systems, pages 4799–4807, 2016.

[2] **METTS algorithm:** EM Stoudenmire and Steven R White. Minimally entangled typical thermal state algorithms. New Journal of Physics, 12(5):055026, 2010.

Thanks for listening