Tensor Networks and Deep Learning for Simulations in Quantum Mechanics

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Tensor networks and (artificial) neural networks allow us to tackle previously unsolvable problems in quantum physics and computer science

Tensor Networks

- Developed simultaneously in quantum physics and numerical mathematics
- Provide a way to decompose tensors of high order or dimensionality
- Represent tensors by contractions of many small tensors
- Inherently linear, basic arithmetic operations can be expressed
- Known to represent ground states of certain systems faithfully
- Methods to perform time evolution and much more exist

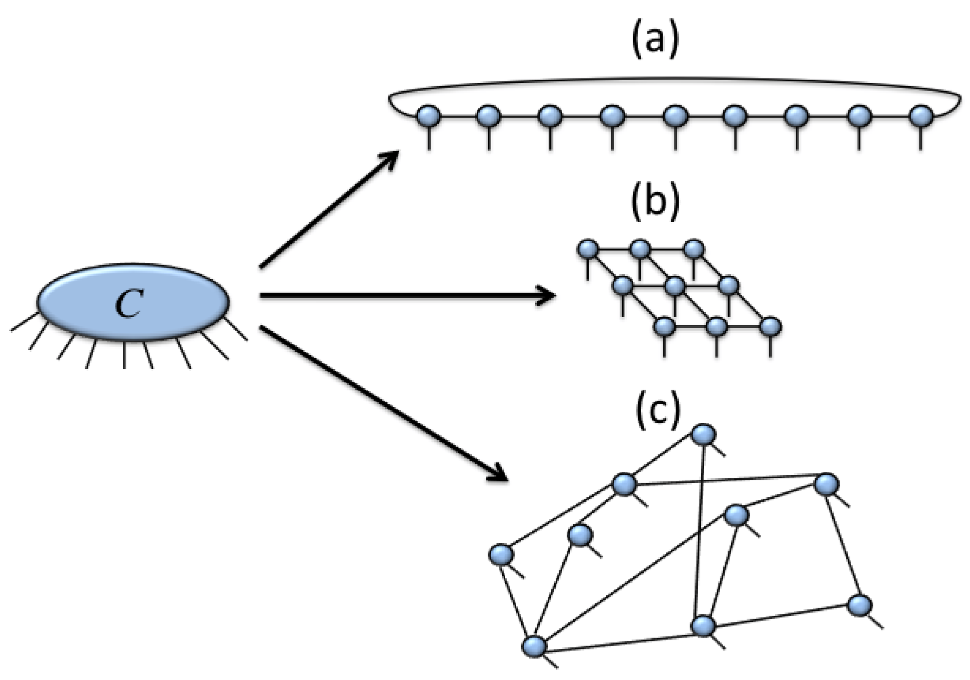


Figure taken from *A Practical Introduction to Tensor Networks: Matrix Product States and Projected Entangled Pair States* by R. Orus

Neural Networks

- Approximate function by composition and summation of simple functions
- Based on connectionist paradigm, inspired by the brain
- Topology of the networks reflects causal structure of data
- Expressive power owed to composition of simple non-linearities
- Term *Deep Learning* refers to high number of compositions
- Special kinds of networks for images, time-series data, etc.
- Can be used for regression, classification, data generation, compression ...

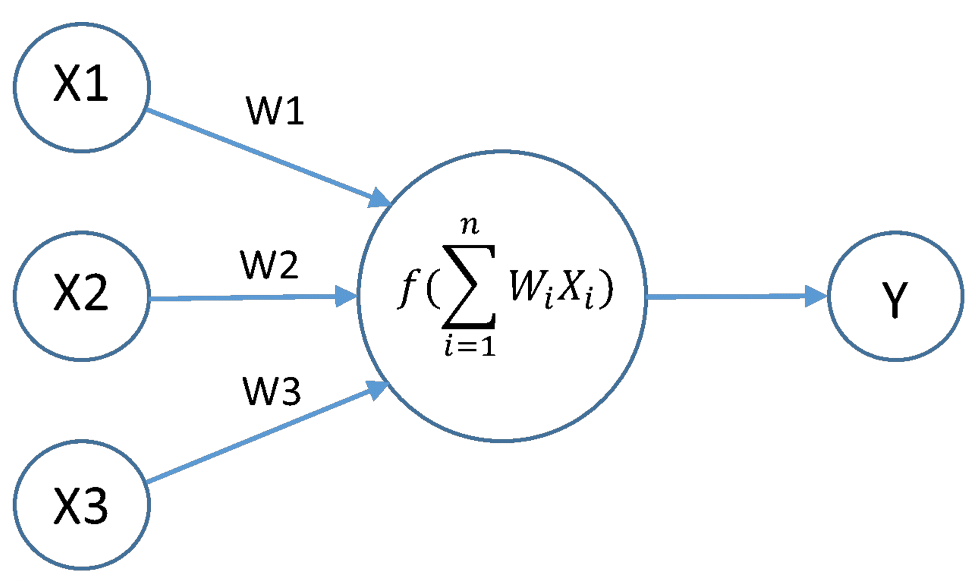


Figure taken from *2centsapiece.blogspot.de*

Our work focuses on the development of novel algorithms to solve challenging problems in quantum physics

Approximating Functionals of MPOs

Algorithm

Algorithm 1: Approximation Algorithm

Input : MPO $A[D_A] \in \mathbb{C}^{N\times N}$, Orthogonal MPO $U[D_{init}] \in \mathbb{C}^{N\times N}$, Number of Dimensions K, Maximal Bond-Dimension D_{max}, Stopping Criteria $\mathcal{S}$

$U_0 \leftarrow U$;
for $i \leftarrow 1; i \leq K$ **do**
  $U_i, T_i \leftarrow$ `orthonormalize`(A, U_{i-1}, D_{max}) ;
  $V\Lambda V^* \leftarrow$ `spectralDecomposition`(T_i) ;
  $\mathcal{G}f \leftarrow \beta_1^2 e_1^T V f(\Lambda) V^* e_1$;
  if `checkStop`$(\mathcal{G}f, \Lambda, \mathcal{S})$ **then**
    break ;
  end
end

Output: Approximation $\mathcal{G}f$ of Tr$f(A)$

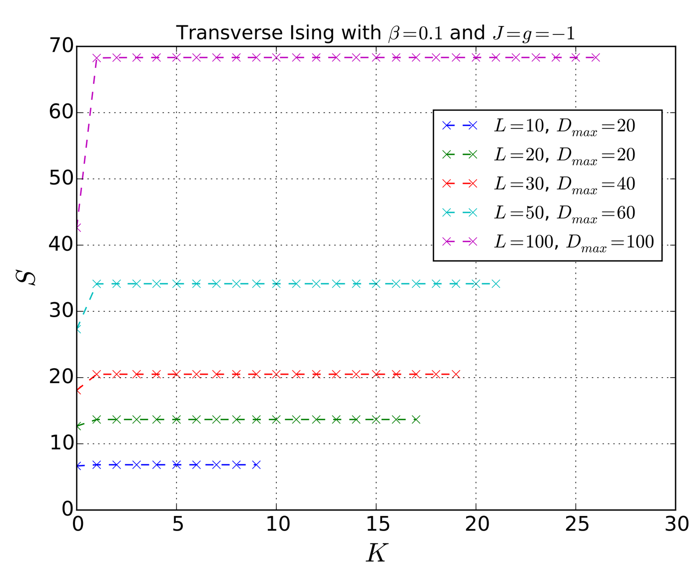
Background

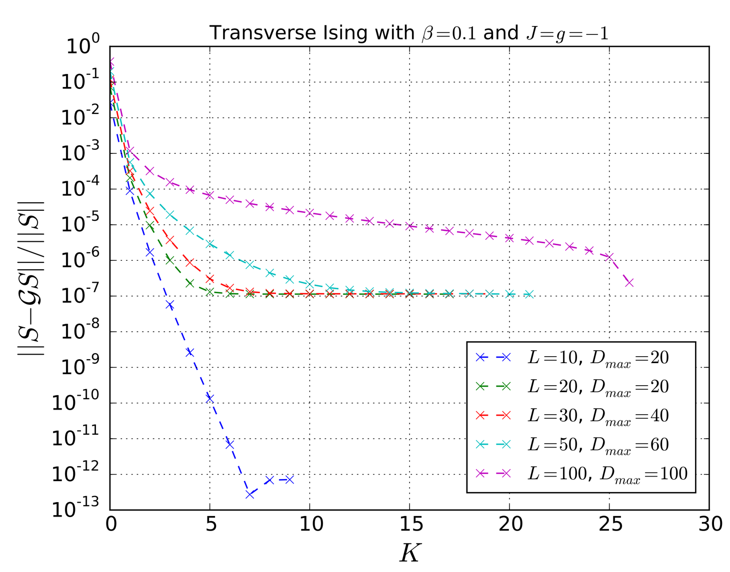
- Can we approximate functions Tr$f(A)$ like the entropy or the trace norm?
- Key idea: project MPO onto small, explicitly storable matrix
- Use Krylov basis of *MPOs* generated by $U, AU, A^2U, \cdots, A^{K-1}U$
- Starting MPO U is orthogonal and of the same dimensions as A
- Projection yields tridiagonal matrix $T_K \in \mathbb{R}^{K\times K}$ that is given by

$$T_K = \begin{bmatrix} \alpha_1 & \beta_2 & & \mathbf{0} \\ \beta_2 & \alpha_2 & \ddots & \\ & \ddots & \ddots & \beta_K \\ \mathbf{0} & & \beta_K & \alpha_K \end{bmatrix}$$

- Problem can be reformulated such that T_K is intimately related to Gauss quadrature
- We find that it holds Tr$f(A) =$ Tr$(U^* f(A) U) = \int_a^b f(\lambda)\mathrm{d}\mu(\lambda) \approx e_1^T f(T_K) e_1$

Results





Optimizing Dynamical Decoupling

Algorithm

Algorithm 2: Optimization Algorithm

Input : Number of initial models: n, Number of models to keep: k, Percentage of data: p, Set of possible topologies: $\mathcal{M}$, Size of data: d

$D \leftarrow$ `generateRandomData(`*d*`)` ;
$D, \langle\varsigma_s\rangle \leftarrow$ `keepBestData(`*D,p*`)` ;
$M \leftarrow$ `trainRandomModels(`*n, D, $\mathcal{M}$*`)` ;
$M \leftarrow$ `keepBestKModels(`*M,k*`)` ;
while $\langle\varsigma_s\rangle$ *not converged* **do**
  $M \leftarrow$ `trainBestModels(`*D*`)` ;
  $D \leftarrow$ `generateDataFromModels(`*M, d*`)` ;
  $D, \langle\varsigma_s\rangle \leftarrow$ `keepBestData(`*D,p*`)` ;
end

Output: $\langle\varsigma_s\rangle, D, M$

Background

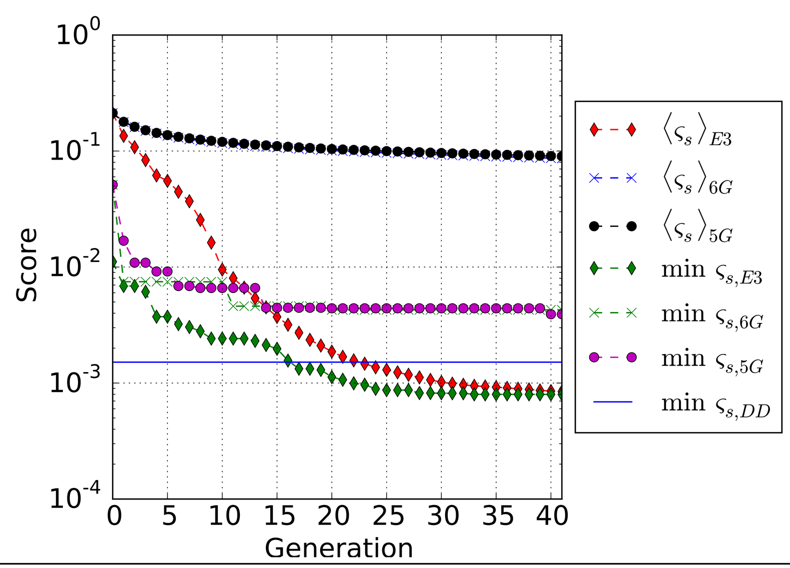
- Can we learn to generate good dynamical decoupling sequences?
- Assuming no access to fidelity measure except for effcient evaluation
- Conjecture: RNNs can learn structure of and generate good sequences
- The fidelity measure we would like to optimize is defined as

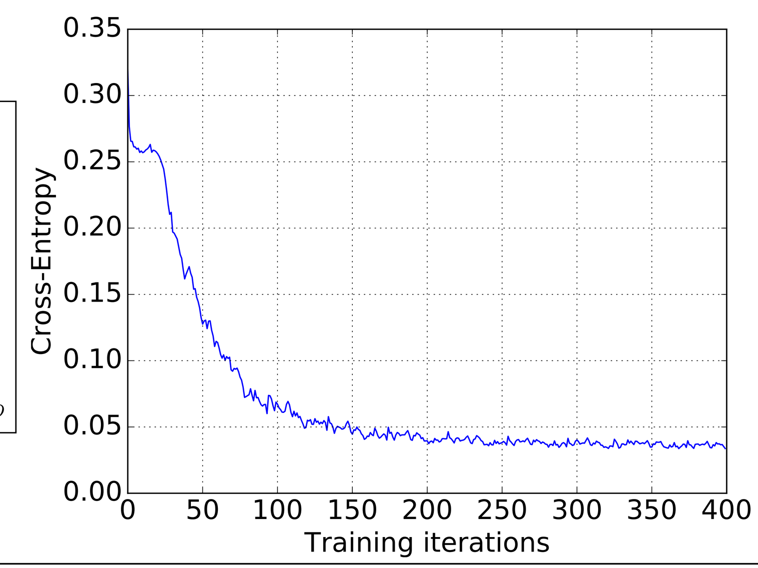
$$D(U, I) = \sqrt{1 - \frac{1}{d_S d_B} \|\mathrm{Tr}_S(U)\|_{\mathrm{Tr}}}$$

- Piecewise constant, finite strength control Hamiltonian with Pauli gates
- Ansatz: use sequence data to train RNNs, use RNNs to generate better data
- We use the *cross entropy* as error function for RNN-training

$$CE(m, \{i\}) = -\sum_t \delta_{s_t,i} \log p_{m,i}(s_{t-1}, \ldots, s_1)$$

Results





[1] M. August, M. C. Bañuls, and T. Huckle. On the approximation of functionals of very large hermitian matrices represented as matrix product operators. *arXiv preprint arXiv:1610.06086*, 2016.
[2] M. August and X. Ni. Using recurrent neural networks to optimize dynamical decoupling for quantum memory. *arXiv preprint arXiv:1604.00279*, 2016.