AI and TN - a love affair

Bram Vanhecke

University of Vienna

28 Nov 2023

Collaborators





Overview

[1] https://arxiv.org/abs/2208.08713
[2] https://arxiv.org/abs/2311.11894

Overview

- Using MPS for active inference planning[1]
    - What is Active inference
    - How MPS can help

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- Using MPS for active inference planning[1]
  - What is Active inference
  - How MPS can help
- AD for PEPS optimization[2]
  - What is PEPS
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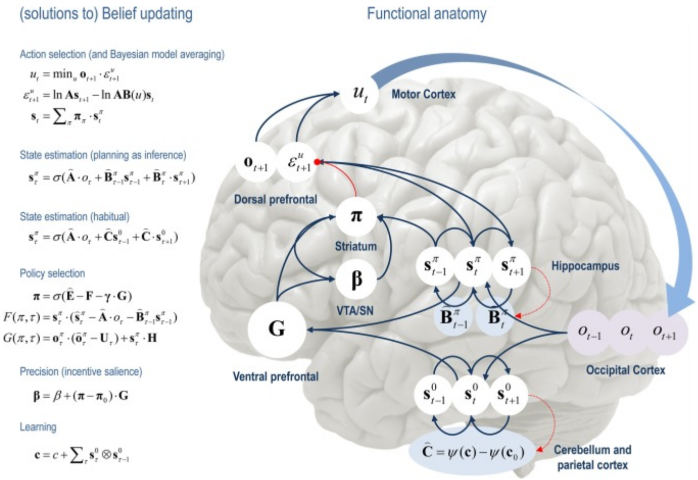
Active Inference



3

[3] https://doi.org/10.1016/j.neubiorev.2016.06.022

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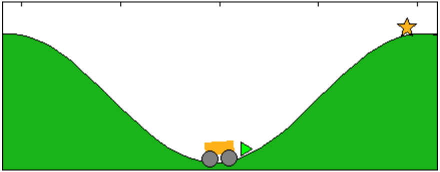
  - the model may also be represented by a TN

Active Inference - Example - Mountain Car



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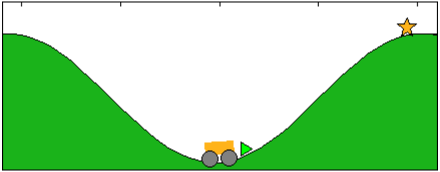

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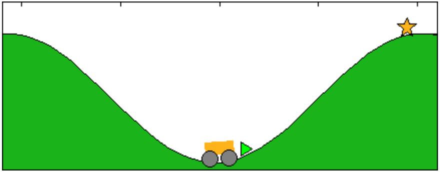

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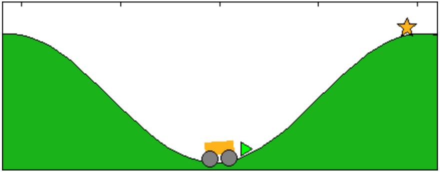

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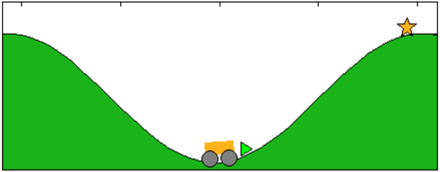

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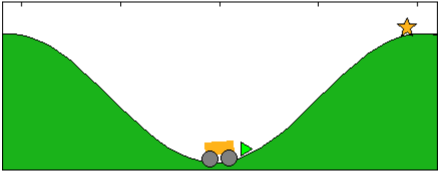

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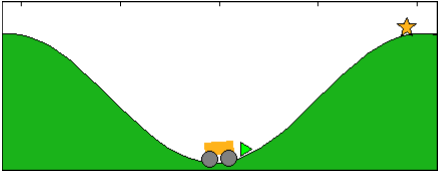

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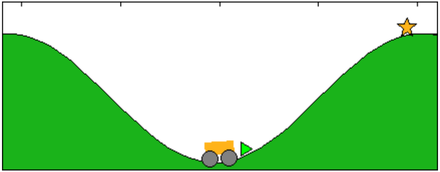

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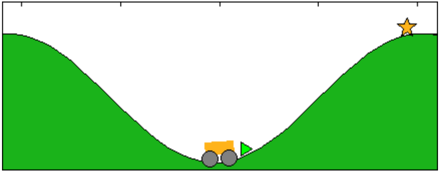

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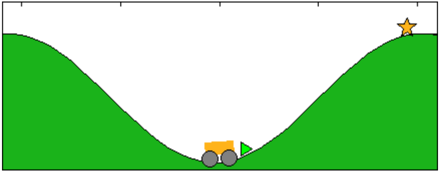

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TN preeliminaries

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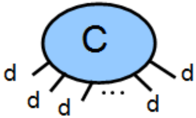
Big tensor $C_{i_1,..i_N}$

Arbitrary tensor
($|i_k\rangle$ – local $\mathcal{H}$ space of dim d):

$$|\Psi\rangle = \sum_{i_1,\dots,i_N} C_{i_1,i_2,\dots,i_N} |i_1 i_2 \dots i_N\rangle$$



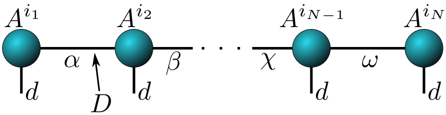
d^N parameters $C_{i_1,\dots,i_N}$

exp(N)

Network of tensors

Matrix product state:

$$\sum_{i_1,\dots,i_N} \sum_{\{\alpha\beta\dots\omega\}} A^{i_1}_{\alpha} A^{i_2}_{\alpha\beta} \dots A^{i_{N-1}}_{\chi\omega} A^{i_N}_{\omega} |i_1 i_2 \dots i_N\rangle$$



$\mathcal{O}(ND^2d)$ par. (D – dim of bond index)

poly(N)

T-maze

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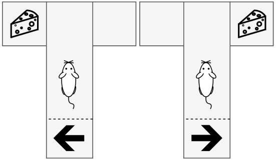

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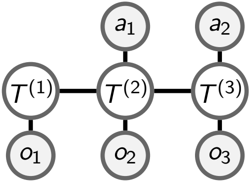

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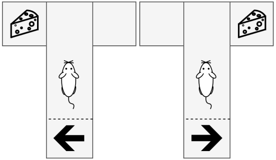
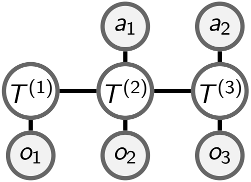


$$\Psi(\tilde{a}, \tilde{o}) =$$ 

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- Generate data set of consistent actions and observations

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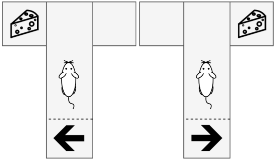

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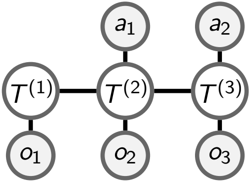

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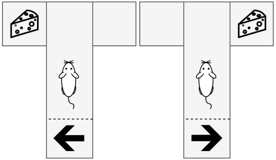

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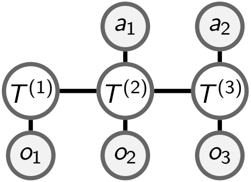

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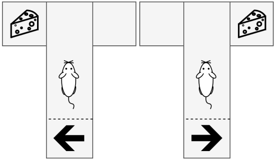

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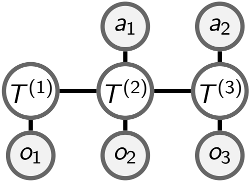

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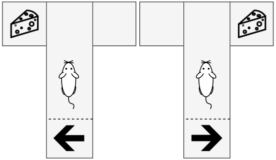
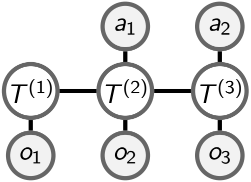


$\Psi(\tilde{a}, \tilde{o}) =$ 

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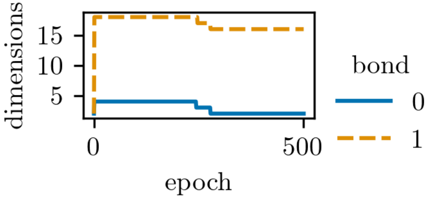

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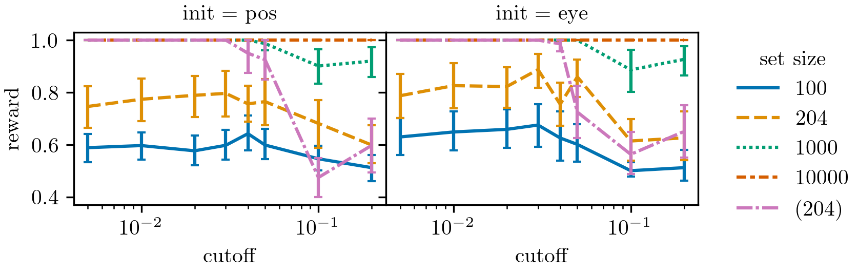

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PEPS

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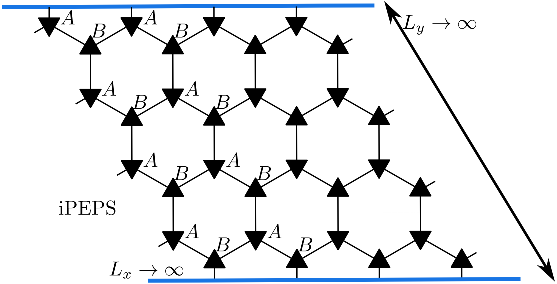

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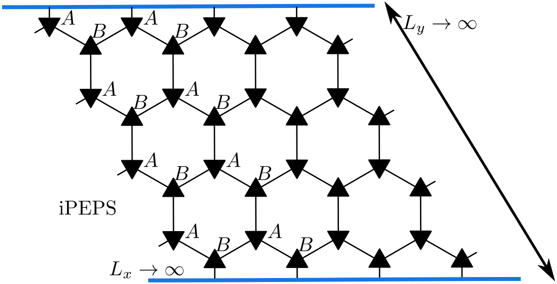

- Natural generalization of MPS to 2D

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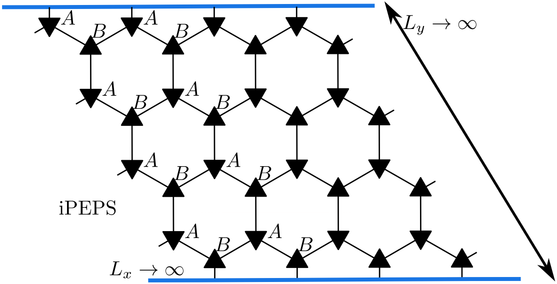

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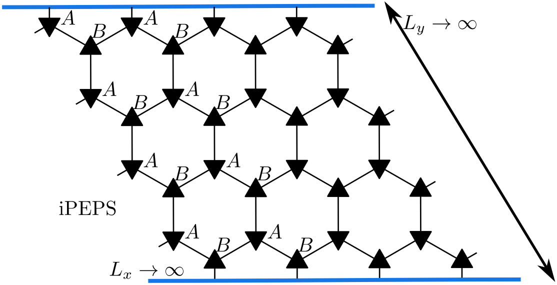

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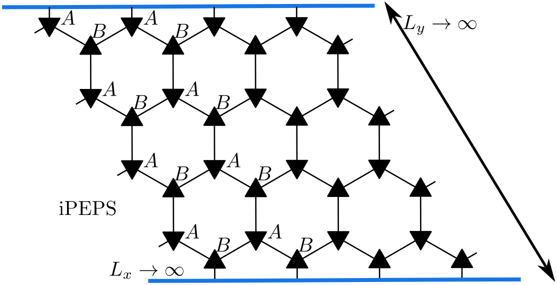

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Gapped $\mathbb{Z}_2$ vs gapless $U(1)$ SL in S=1/2 Kagome AF? H.J.Liao et al. PRL 118 (2017)

Contracting PEPS: Corner Transfer Matrix[4]

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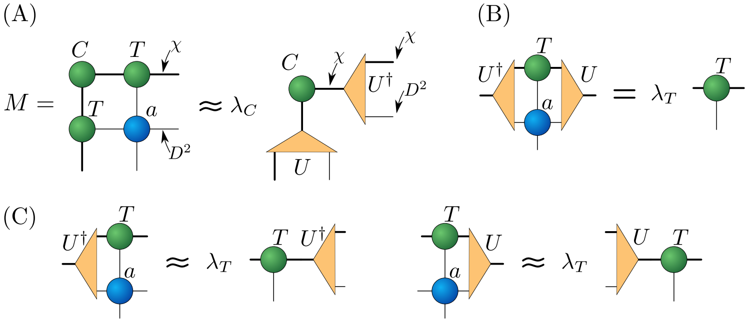
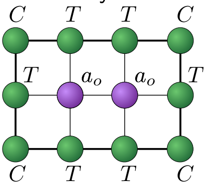


- Enables calculation with infinite TN
- Random initialization and iterated to convergence

Energy calculated approximately with CTM:

$$E \approx \tilde{E} = F(C, T, A, H) =$$



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    expensive, erroneous
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    approximate, expensive for 'larger' Hamiltonians
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- Analytical gradients: Automatic/Algorithmic differentiation
  memory expensive, can be problematic if treated as black box
  H-J. Liao, J-G. Liu, L. Wang, and T, Xiang, PRX 9, 031041 (2019)
  J. Hasik, D. Poilblanc, F. Becca, SciPost Phys. 10, 012 (2021)

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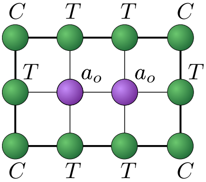

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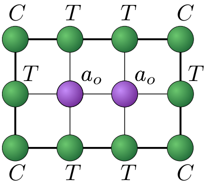

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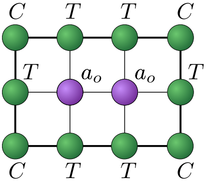

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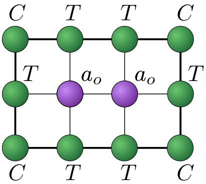

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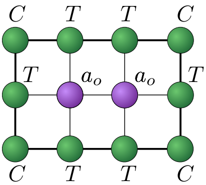

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1. costly in memory, need for many iterations

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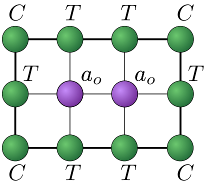

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$$\begin{aligned} d\tilde{E} &= \frac{\partial F}{\partial A} dA + \frac{\partial F}{\partial x_n} dx_n, \\ dx_n &= \frac{\partial f}{\partial A} dA + \frac{\partial f}{\partial x_{n-1}} \left(\frac{\partial f}{\partial A} dA + \frac{\partial f}{\partial x_{n-2}} (\ldots)) \right), \end{aligned}$$

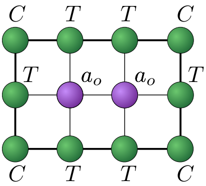
Problems:

1. costly in memory, need for many iterations
2. gradient of EIG (SVD) poorly conditioned in case of degenerate spectra

Energy gradient

Energy calculated approximately with CTM:

$$E \approx \tilde{E} = F(C_n, T_n, A, H) =$$



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3. currently only approximate!

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With $PP^\dagger + P_\perp P_\perp^\dagger = \mathbb{I}$, leading to Sylvester equation for dP:

$$(\mathbb{I} - PP^\dagger)dMP = dPC - \underline{(\mathbb{I} - PP^\dagger)MdP}$$

Problem: divergencies in the gradient of EIG(SVD)

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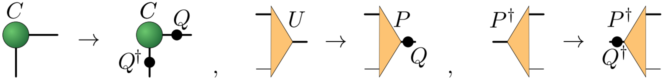
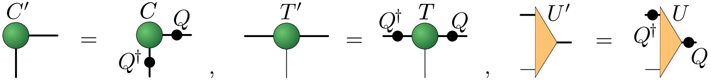
Solution: Q-deformed CTM with $Q = \mathbb{I}$

(A) Q-deformation step



(B) Gauge transformation



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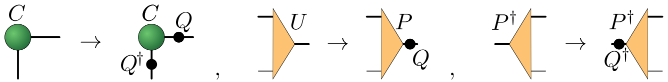

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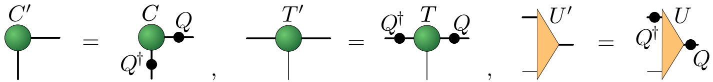

regular CTM:

$$\begin{aligned} dC &= \mathbb{I} \circ (P^\dagger dMP) \\ P^\dagger dP &= F \circ (P^\dagger dMP), \quad F_{ij} = 1/(c_j - c_i) \end{aligned}$$

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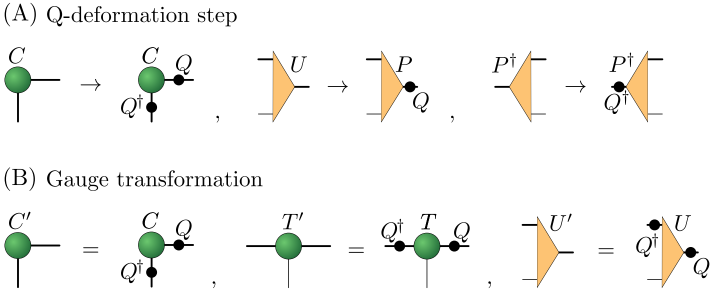

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$\rightarrow$

Q-deformed CTM:

$$
\begin{aligned}
dC &= P^\dagger dMP \\
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$$UCU^\dagger = \big(U\sigma\big) C \big(\sigma^\dagger U^\dagger\big) \;\Rightarrow\; \hat{T} \xrightarrow{\text{f}} \sigma^\dagger \hat{T} \sigma = T.$$

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Hamiltonian: $H = J_1 \sum_{i,j \in NN,\alpha} f(\alpha) S_i^\alpha S_j^\alpha + J_2 \sum_{i,j \in NNN} \overrightarrow{S}_i \cdot \overrightarrow{S}_j$

with $SU(2)$ symmetry breaking anisotropy $f([x, y, z]) = [-1, 1 + \beta, -1 + \beta]$

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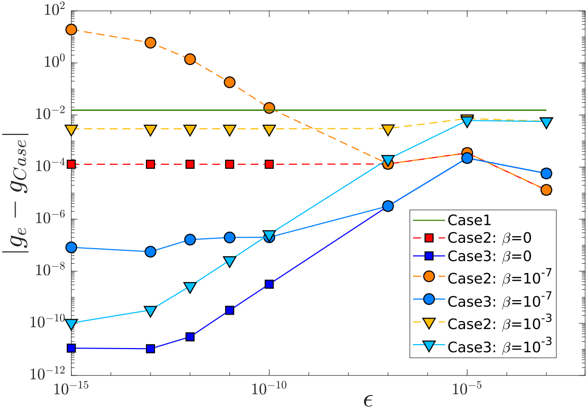

$F_{ij} \to \frac{c_j - c_i}{(c_j - c_i)^2 + \epsilon}$

- our gradient g_e
- Case 1: $dP = 0$
- Case 2: current AD
- Case 3: using Sylvester equation for dP

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- allows for more efficient algorithms
- may allow to reach higher bond dimensions D, χ and hence higher correlation lengths ξ, tackle challenging problems with bigger accuracy

Thank You