Approximating local observables on MPS / PEPS tensor networks with translation-invariant properties

Yupan Liu

College of Computer Science and Technology
Zhejiang University

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Joint work with Itai Arad (Technion)

Local Hamiltonian Problem

Given k-local Hamiltonian $H = \sum_{i=1}^{m} H_i$ on n-qudits with m local terms. Promise that the ground energy $\lambda_0(H) = \langle\Omega|H|\Omega\rangle$ satisfies $\lambda_0(H) \leq \alpha$ or $\lambda_0(H) \geq \beta$ with $\beta - \alpha \geq \frac{1}{poly(n)}$. The output is YES if $\lambda_0(H) \leq \alpha$ otherwise NO if $\lambda_0(H) \geq \beta$.

- *k*-local Hamiltonian satisfies $H = \sum_i H_i \in \mathcal{L}(\mathbb{C}^{d\otimes n})$;
- Each interaction $H_i \in \mathcal{L}(\mathbb{C}^k)$ involving at most *k* particles.
- Here we focus on *gapped* local Hamiltonian in *2D*.

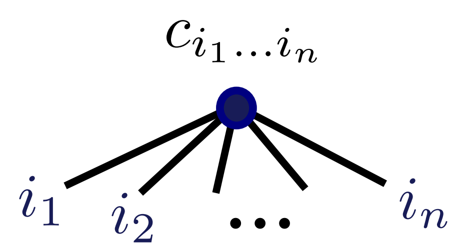
- In general, k-LHP is even hard for a quantum computer, since it is QMA-complete(QMA=$quantum$ NP).
- But we knew that there exist some special cases are easier, such as the *gapped* or the *commute*.

? Given *local observables B* and a *ground state* $|\Omega\rangle$, how to calculate its *expectation value* $\langle\Omega|B|\Omega\rangle$ efficiently?

Tensor networks: *efficient* representation of $|\Omega\rangle$

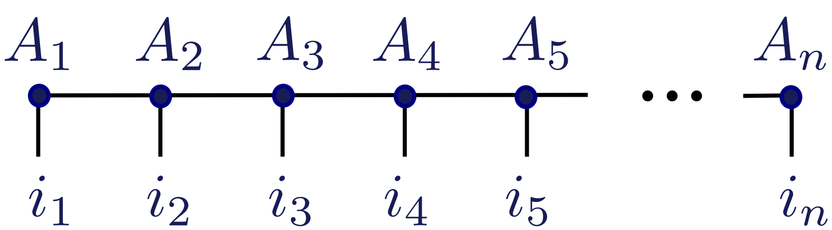
- Using only *poly(n)* parameters instead of the exponantial size;
- Corollary of area law(*conjecture*), only with proofs in *1D*;
- Related local Hamiltonian problem is inside NP (*conjecture*);
- MPS / PEPS(*conjecture*) tensor networks serve as the witness.

$$|\psi\rangle = \sum_{i_1,\ldots,i_n} c_{i_1\ldots i_n} |i_1 \ldots i_n\rangle$$

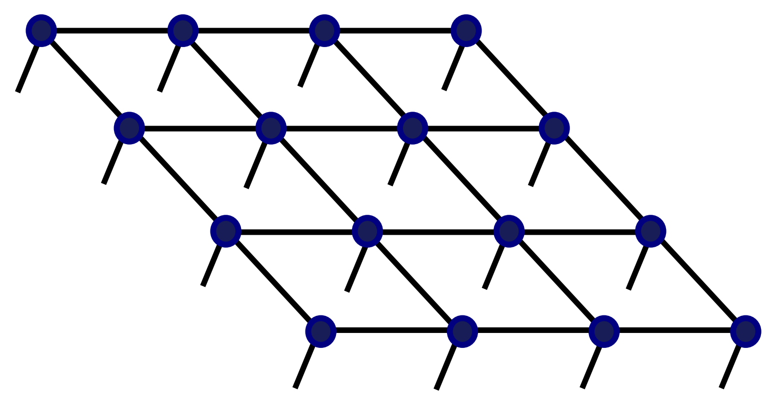


rank-*n* tensor

- Matrix Product State (MPS)



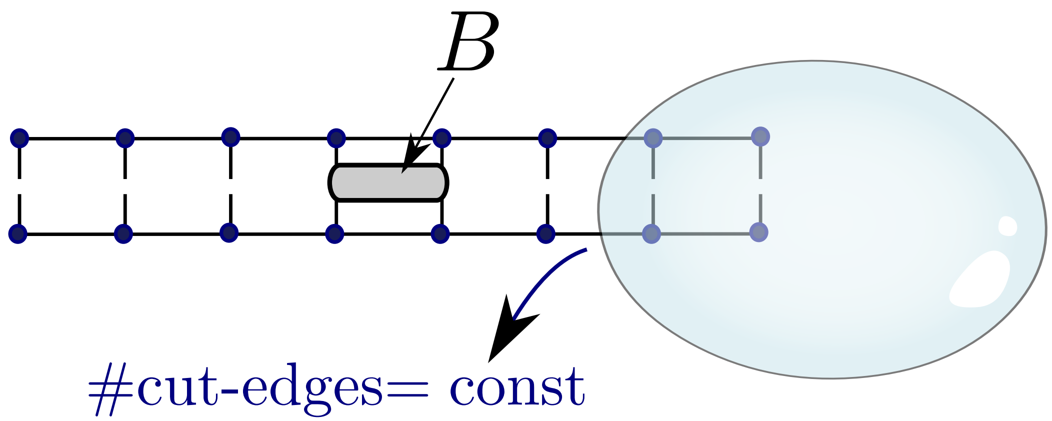
- Projected Entangled-Pair State (PEPS)



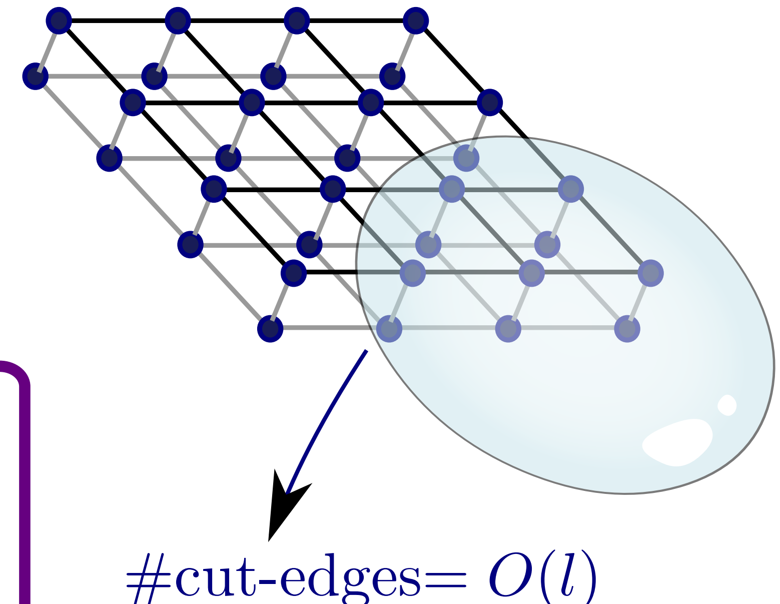
- Network structure corresponds to entanglement structure;
- Allows variational algorithms.

Contracting the tensor network of $\langle\Omega|B|\Omega\rangle$

- *1D*: Matrix Product State (MPS)



- *2D*: Projected Entangled-Pair State (PEPS)



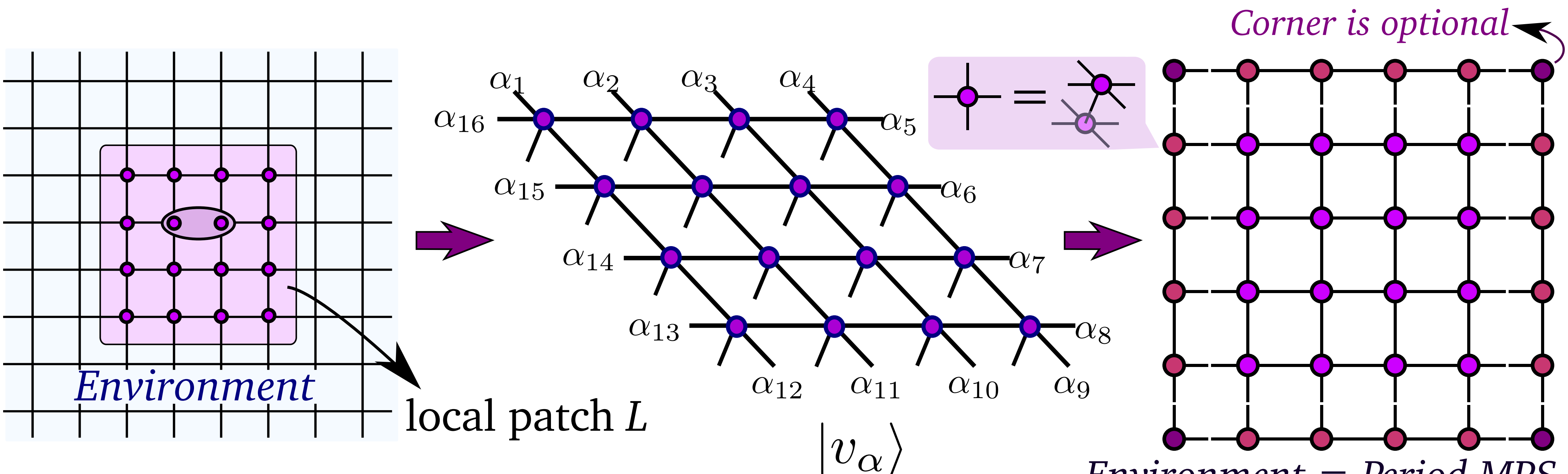
- Using the swalling bubbles;
- Contracting a general PEPS is #P-hard, which is as least harder than NP-hard.
- Approximations must be used, such as boundary MPS, CTM etc.

? Can we approximate $\langle\Omega|B|\Omega\rangle$ using only a local patch of the tensor network, assuming that a ground state $|\Omega\rangle$ of a known local Hamiltonian H?

Expectation value from a local patch

Main Problem

Given a g.s. $|\Omega\rangle$ of a known local Hamiltonian H in the form of a PEPS and a local observable B, approximate $\langle\Omega|B|\Omega\rangle$ using only a local patch L of the PEPS around B.



$\dim(V_L) = d^{O(|\partial L|)}$

- *Local patch* $V_L = \mathrm{span}\{|v_\alpha\rangle\}$
- *Environment* $V_L^c = \mathrm{span}\{|v_\alpha^c\rangle\}$

internal states (local patch)

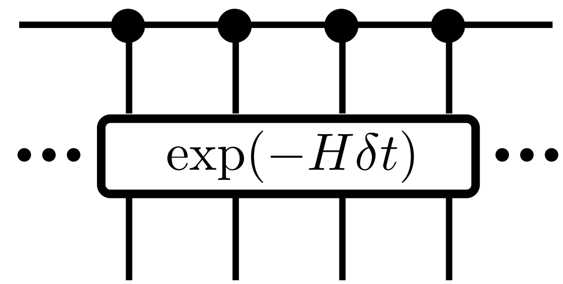
external states (environment)

$$|\Omega\rangle = \sum_\alpha |v_\alpha\rangle \otimes |v_\alpha^c\rangle$$

Finding the g.s. by imaginary time evolution

1. Given a local Hamiltonian H with ***non-degenerate*** g.s., then

$$|\Omega\rangle = \lim_{t\to\infty} \frac{e^{-Ht}|\psi_0\rangle}{\|e^{-Ht}|\psi_0\rangle\|} = \lim_{t\to\infty} \frac{\prod e^{-H\delta t}|\psi_0\rangle}{\|e^{-Ht}|\psi_0\rangle\|}$$

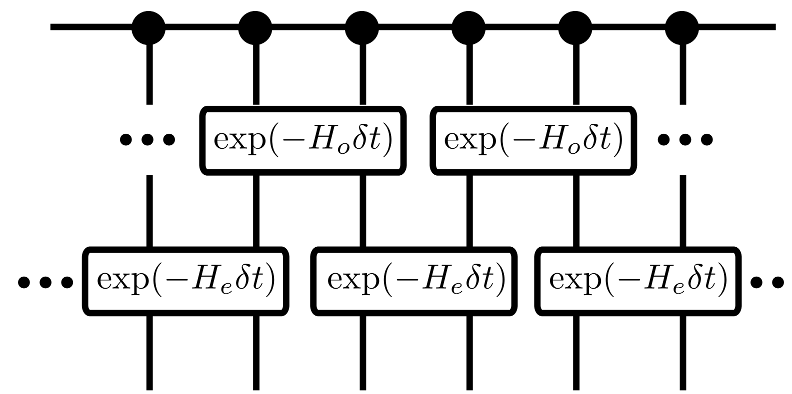


2. Simulating imaginary time evolution e^{-Ht}

- Suzuki-Trotter expansion

$$(e^{-H_o\delta t}e^{-H_e\delta t})^m = e^{-(H_o+H_e)t} + O(mh^2\delta t^2),$$

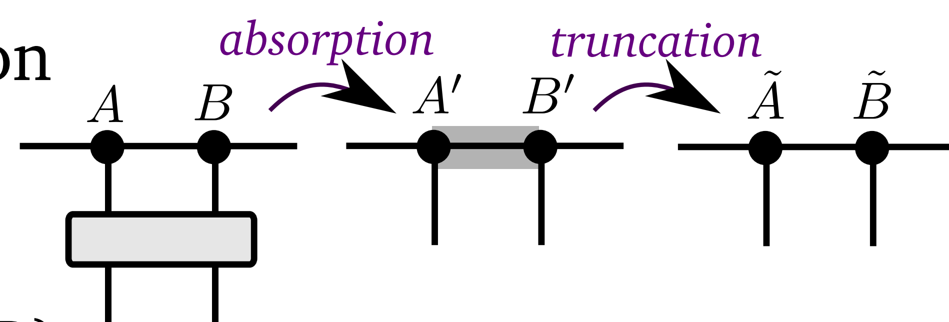
where $\delta t = \frac{t}{m}$ and $h = \max\{\|H_1\|, \|H_2\|\}$.



- Taylor expansion *arXiv:1701.05039*

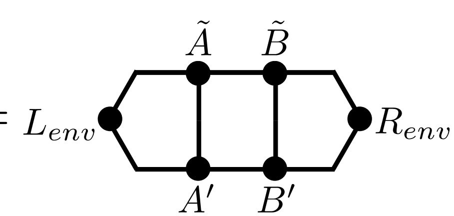
$$e^{-iH\delta t} \approx \sum_{k=0}^{K} \frac{1}{k!}(-iH\delta t)^k,$$ where $K = O(\frac{\log(r/\epsilon)}{\log\log(r/\epsilon)})$ for the given precision ϵ/r.

3. Truncation: finding low-rank approximation



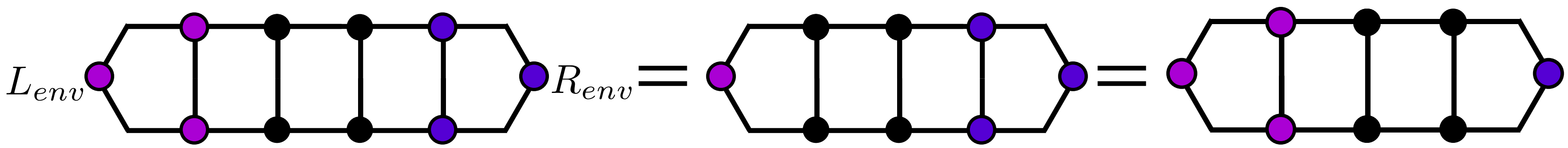
- SVD with ***the canonical form*** of MPS

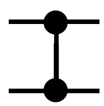
- Alternating least sqaure method (also for *2D*)

Minimize $\||\psi_{A'B'}\rangle - |\psi_{\tilde{A}\tilde{B}}\rangle\|^2$ where $\langle\psi_{A'B'}|\psi_{\tilde{A}\tilde{B}}\rangle =$  .

Translation-Invariance Optimization (TIO)

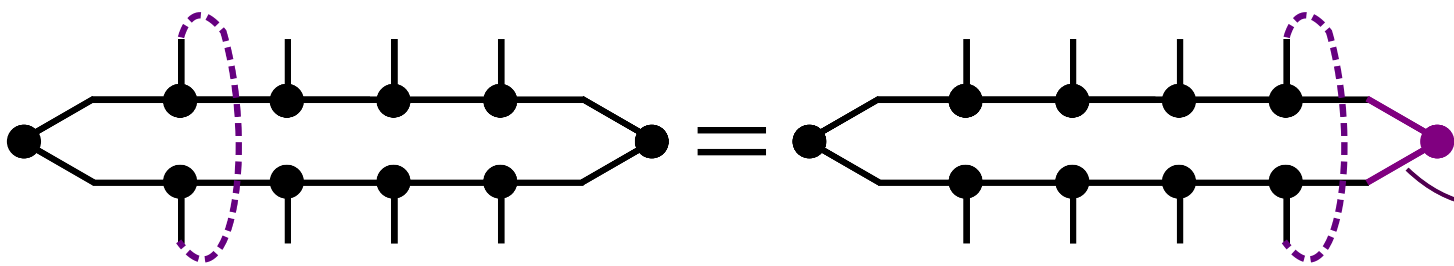
- Transfer matrix method in *1D*

$\langle\psi|\psi\rangle =$ 

Let $E =$ , we have $ER_{env} = R_{env}$ and $E^\dagger L_{env} = L_{env}$.

- Equality constraints of axises $\rho_{left} = \rho_{right}$

#Constraints $= e^{O(|L|)}$



Over-determined!

#Variables $= e^{O(|\partial L|)}$

☆ TIO works for both frustrated and frustration-free systems.

- Approximating constraints by l_2-norm $\|A\| = \sqrt{\mathrm{Tr}(A^\dagger A)}$

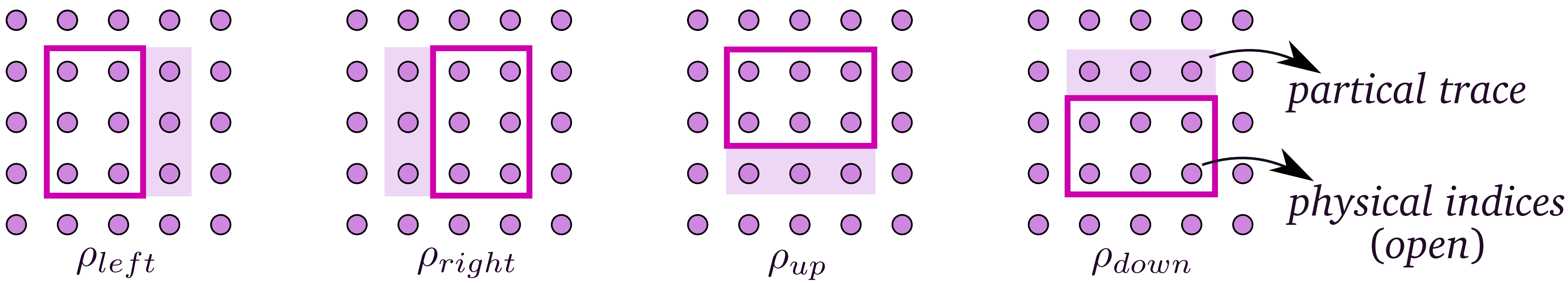
Semi-definite quadratic programming (SDQP) problem

- Approximating $\rho_{left} - \rho_{right} = 0$ by $\|\rho_{left} - \rho_{right}\| = 0$, with constraints $\mathrm{Tr}(\rho) = 1$ and $\rho \succeq 0$, i.e. any reduced density matrix.
- Minimizing $\|\rho_{left} - \rho_{right}\|^2 + \|\rho_{up} - \rho_{down}\|^2$ for 2D systems on the square lattice.

Solving SDQP by the primal-dual interior method

Separating environments from ρ_L on a local patch

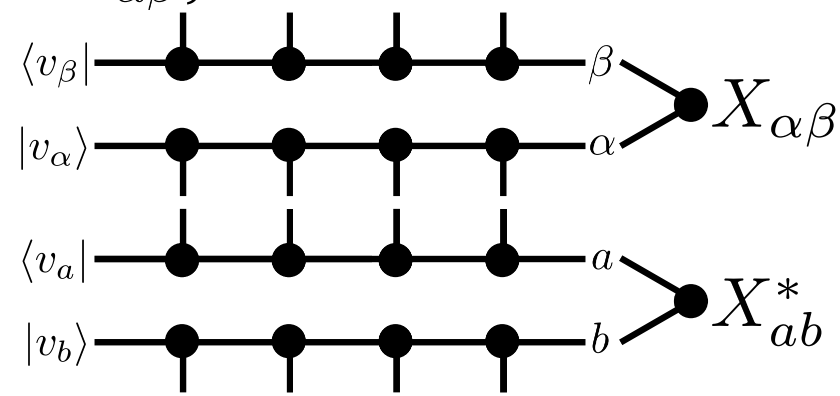
- Reconstruct a *reduced density matrix* ρ_L from $V_L = \mathrm{span}\{|v_1\rangle, \cdots, |v_N\rangle\}$, since $\rho_L = \sum_{\alpha,\beta} \rho_{\alpha\beta} |v_\alpha\rangle\langle v_\beta|$ where $\rho_{\alpha\beta} \in \mathbb{C}^N$ is an unknown *trace 1 PSD matrix*.
- Taking TIO as an example, we have $\rho_{left} = \rho_{right}$ and $\rho_{up} = \rho_{down}$.



- Now consider $\rho^\dagger_{left}\rho_{left}$, let environments be $X_{\alpha\beta}$, we have

$$\rho = \sum_{\alpha\beta} \rho_{\alpha\beta} |v_\alpha\rangle\langle v_\beta| = \sum_{\alpha\beta} X_{\alpha\beta} |v_\alpha\rangle\langle v_\beta|,$$

$$\rho^\dagger = (\sum_{ab} \rho_{ab} |v_a\rangle\langle v_b|)^\dagger = \sum_{ab} X_{ab} |v_b\rangle\langle v_a|.$$



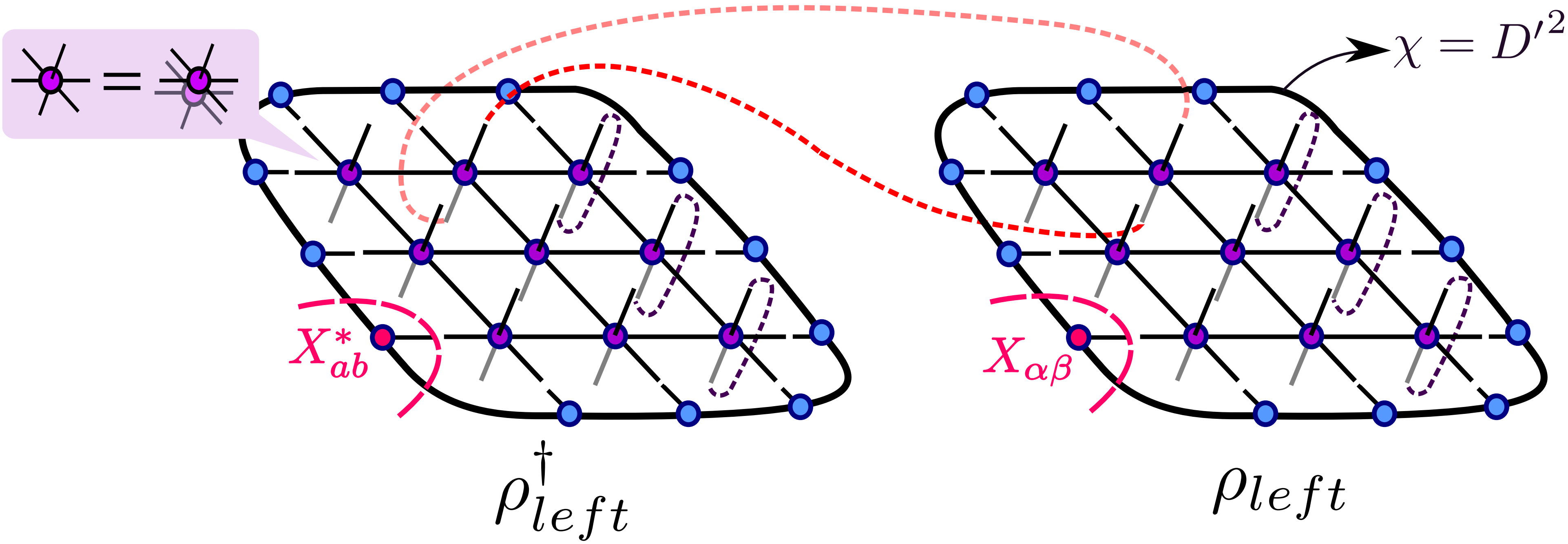
- Finally, the SDQP in practial is the following.

$$\min_X \quad F(X) := \sum_{\alpha,\beta,a,b} X^*_{\alpha\beta} K_{(\alpha\beta),(ab)} X_{ab}$$

$$\text{subject to} \quad X \succeq 0, \mathrm{Tr}(CX) = 1$$

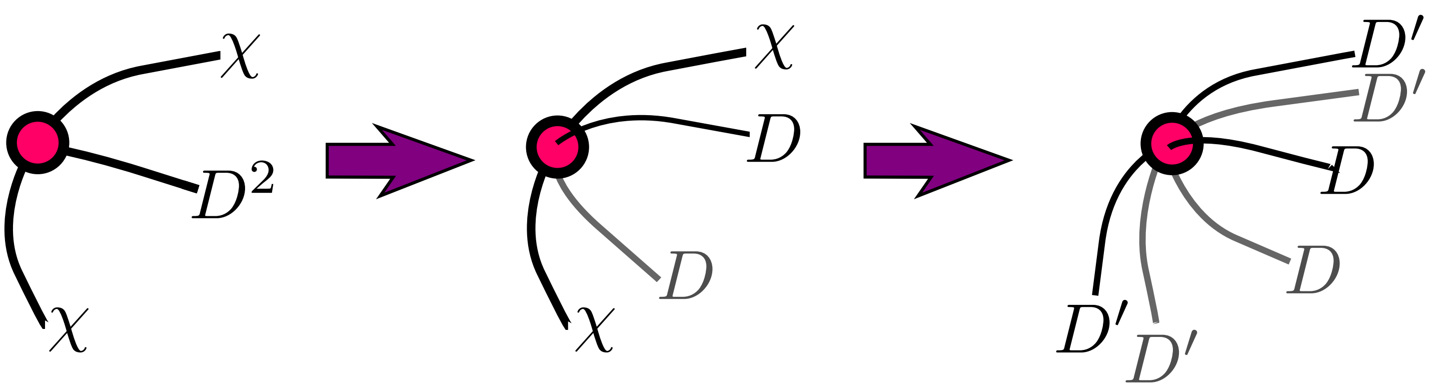
Constructing tensor networks of the SDQP

- Taking TIO as an example, we have $\rho_{left}^{\dagger}\rho_{left}$ in its objective function $F(X)$.



Only labels of open indices are important!

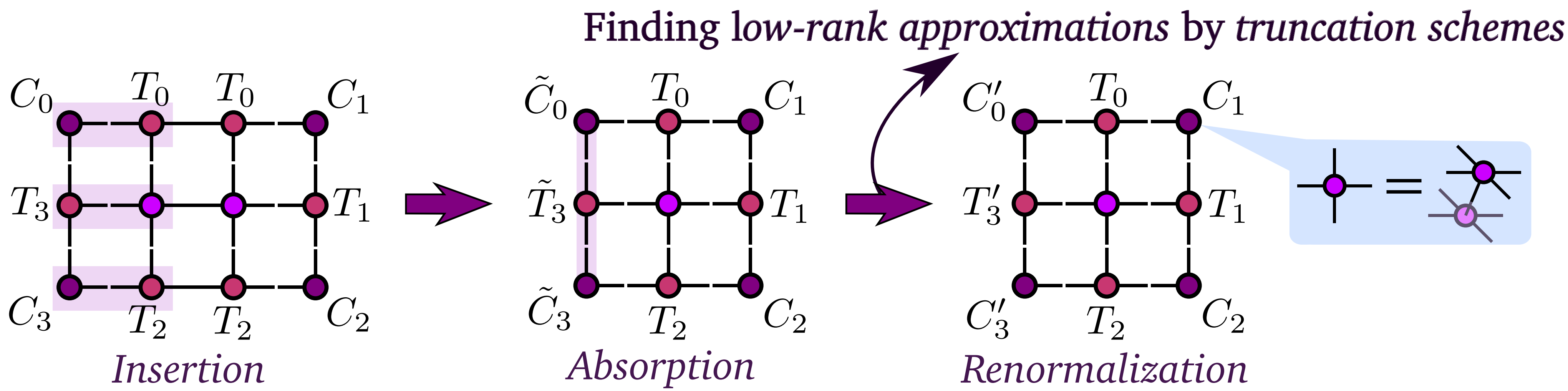
- Transformation between environments and the variable of SDQP.



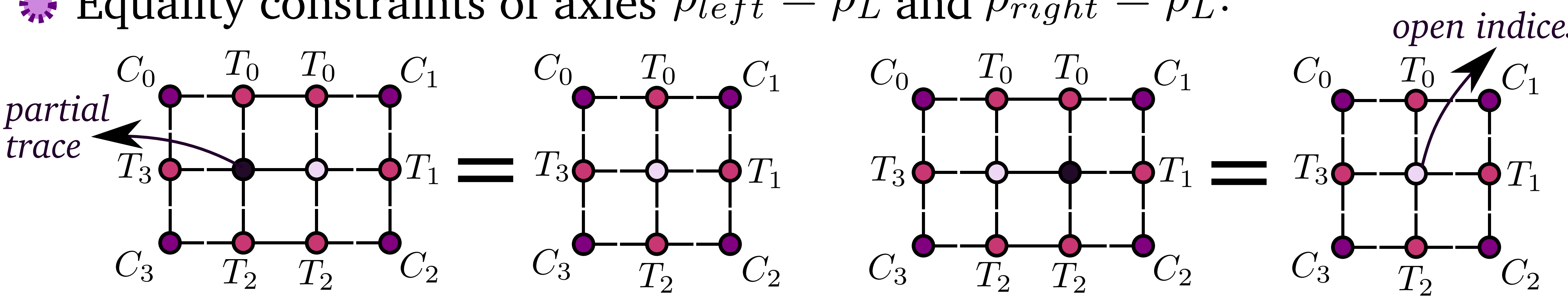
PSD matrix
(positive semi-definite)
$X_{\text{black;gray}}$

Variational Corner Transfer Matrix (varCTM)

- Corner transfer matrix (CTM): directional coarse-graining move.



- Equality constraints of axies $\rho_{left} = \rho_L$ and $\rho_{right} = \rho_L$.



☆ varCTM works for both frustrated and frustration-free systems.

- Approximating constraints: SDQP problem with same structure.

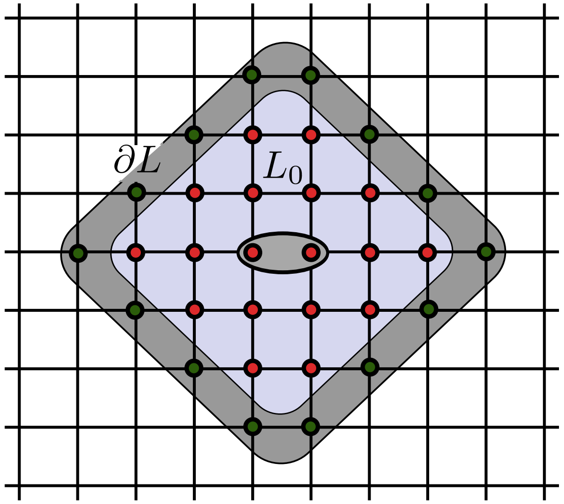
$$
\begin{aligned}
\min_{\rho} \quad & F(\rho) = \|\rho_{left} - \rho_L\|^2 + \|\rho_{right} - \rho_L\|^2 + \|\rho_{up} - \rho_L\|^2 + \|\rho_{down} - \rho_L\|^2 \\
\text{subject to} \quad & \rho \succeq 0, \ \mathrm{Tr}(\rho) = 1
\end{aligned}
$$

Commutator Gauge Optimaization (CGO)

Approximating environments

Ref: Phys. Rev. B 94, 195143 (2016)

The CGO lemma



Given a local patch $L = L_0 \cup \partial L$, consider a local observable $B \in V_{L_0}$ and an *eigenstates* $|\psi\rangle$ of local Hamiltonian H, then

$$\langle\psi|[H_L, B]|\psi\rangle = \langle\psi|H_L B|\psi\rangle - \langle\psi|B H_L|\psi\rangle = 0.$$

Using the cyclicity of trace, we have

$$\langle\psi|[H_L, B]|\psi\rangle = \mathrm{Tr}_L(\rho_L[B, H_L]) = \mathrm{Tr}_L(B[H_L, \rho_L]).$$

Notice that $\mathrm{Tr}_L(B[H_L, \rho_L]) = \mathrm{Tr}_{L_0}(B\mathrm{Tr}_{\partial L}[H_L, \rho_L]) = 0, \forall B$, we got the lemma:

$$\mathrm{Tr}_{\partial L}[H_L, \rho_L] = 0.$$

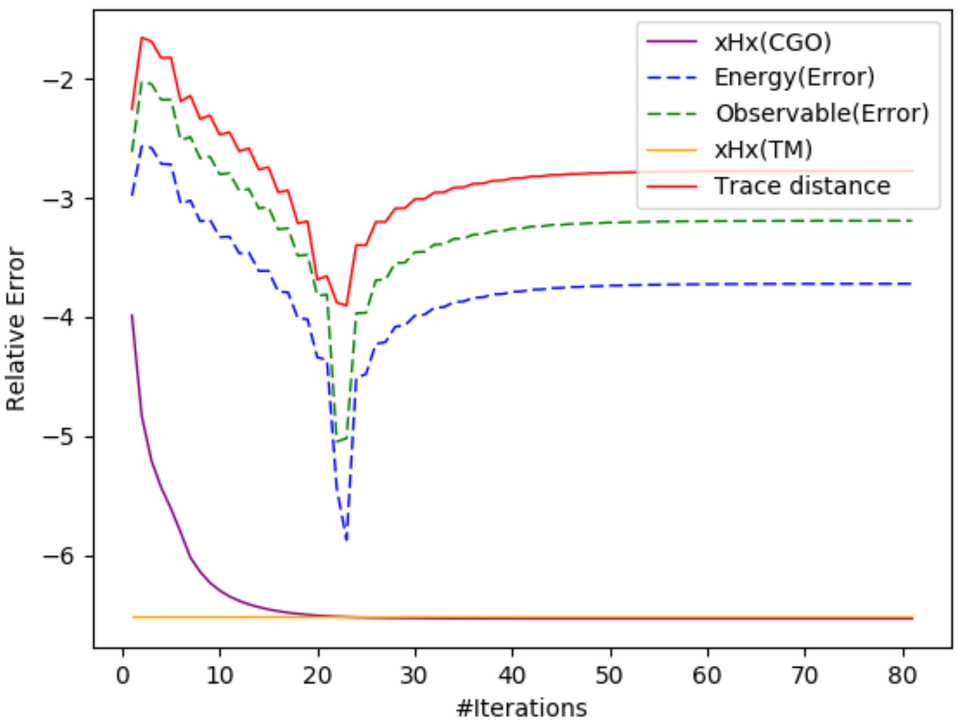
- *Area law* (conjecture) guarantees that information of g.s. is local!
- CGO only works for frustrated systems, since frustration-free systems ($[H_L, \rho_L] = 0$) satisfy it trivially.

Approximating constraints: the SDQP problem

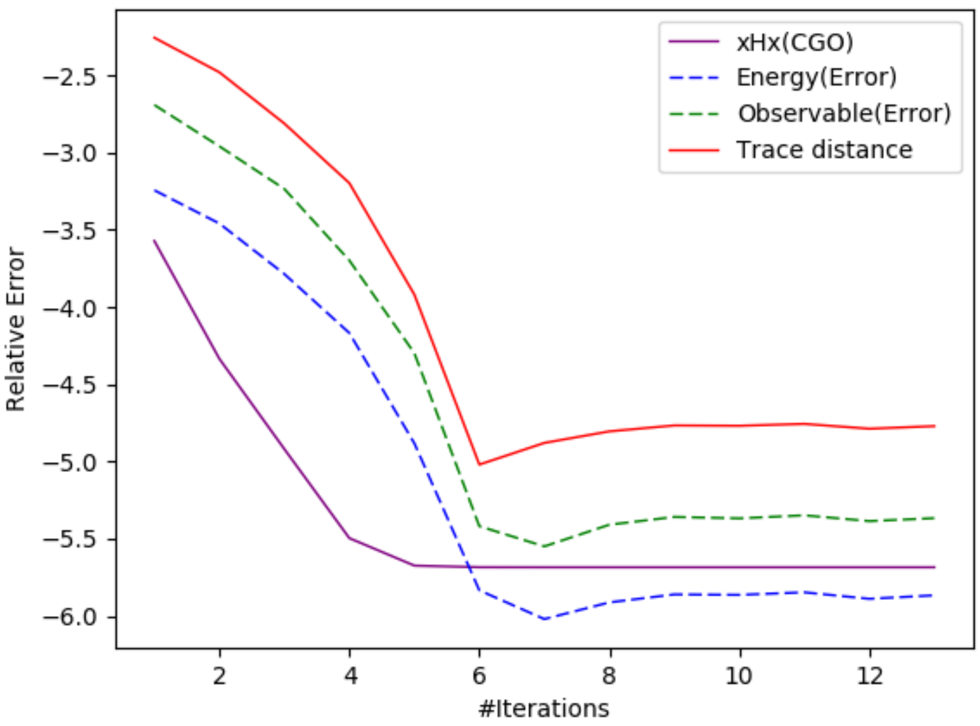
$$\begin{array}{ll} \min\limits_{\rho_L} & F(\rho_L) := \mathrm{Tr}_{L_0}\|\mathrm{Tr}_{\partial L}[H_L, \rho_L]\|^2 \\ \text{subject to} & \rho_L \succeq 0,\ \mathrm{Tr}(\rho_L) = 1 \end{array}$$

Numerical results of CGO

Testing CGO for approximating environments
on the transverse Ising model:



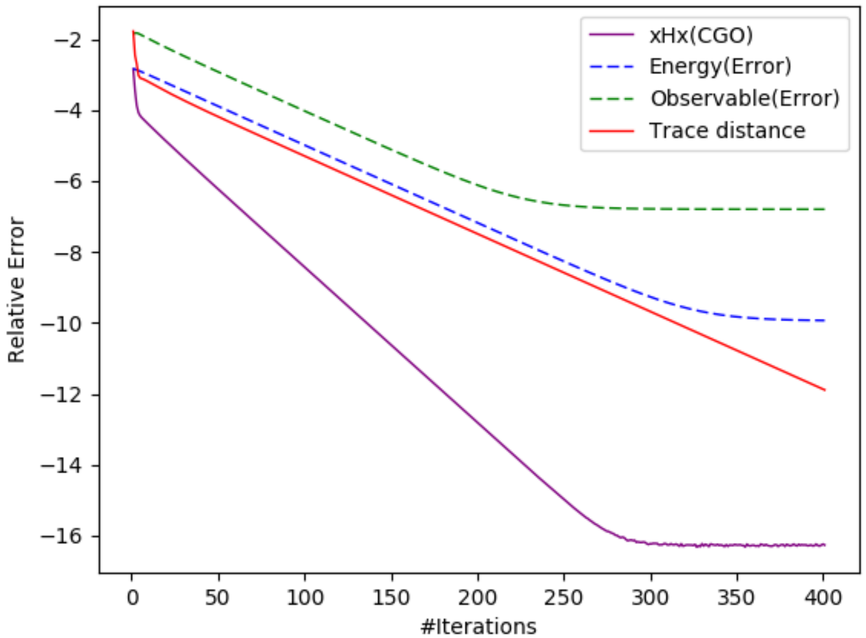
local patch (l=5)



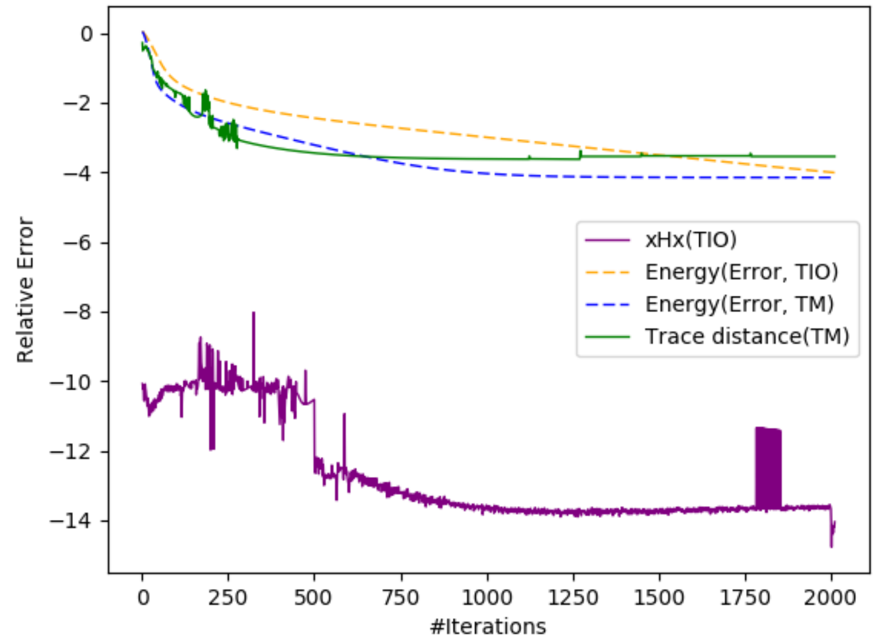
local patch (l=12)

Numerical results of TIO

- Approximating environments and finding g.s. on the tranverse Ising model.

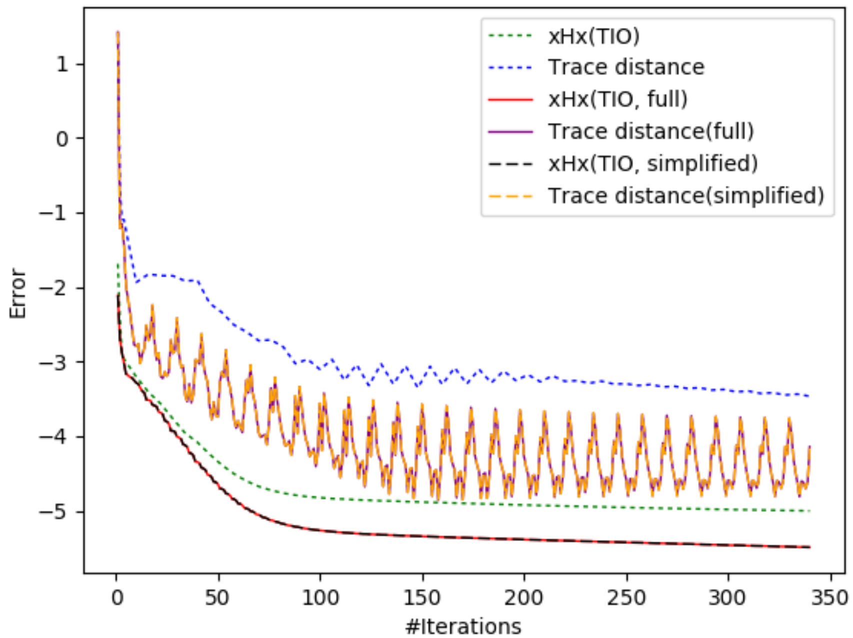


approx. environments: l=7

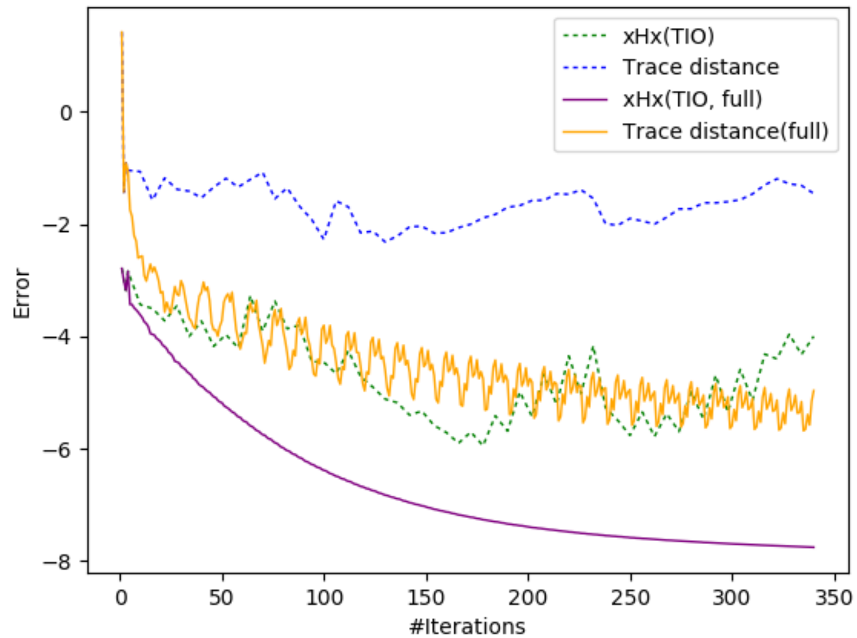


finding g.s. with iTEBD: l=7

- Approximating environments on the 2D AKLT model with 3×3 square lattices.



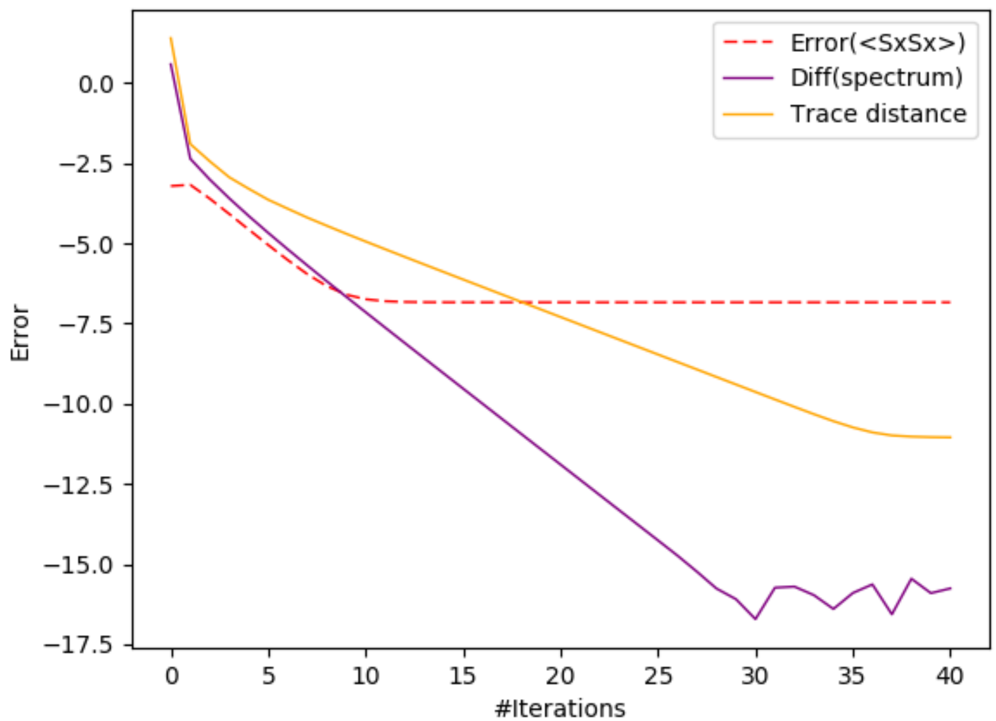
$D' = 2$



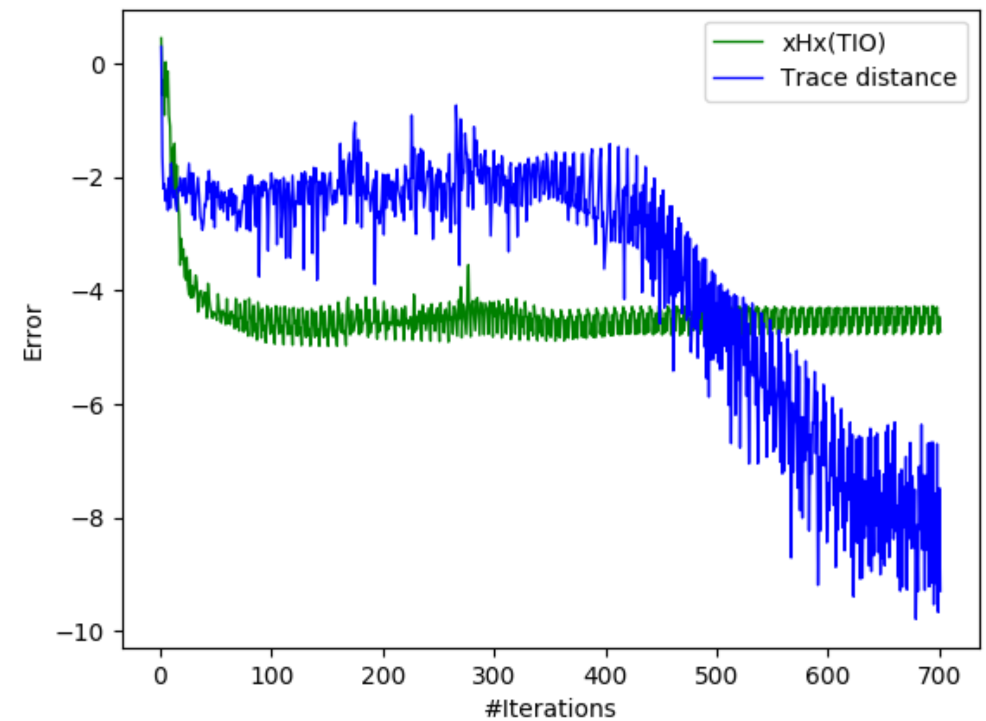
$D' = 3$

Numerical results of varCTM

Testing CTM and varCTM for approximating environments on the *2D* AKLT model with the square lattice:



CTM (D'=4) on 3×3 lattice



varCTM (D'=4) on 3×3 lattice

$\mathrm{CTM}(D' = 20)$	$\mathrm{CTM}(D' = 2)$	$\mathrm{CTM}(D' = 3)$	$\mathrm{CTM}(D' = 4)$	$\mathrm{varCTM}(D' = 4)$
-1.1688	-1.1685	-1.1684727	-1.1684726	-1.150430023457

$\mathrm{TIO}(D' = 2)$	$\mathrm{TIO}(D' = 2,\mathrm{full})$	$\mathrm{TIO}(D' = 3)$	$\mathrm{TIO}(D' = 3,\mathrm{full})$
$(-1.18030, -1.18028)$	$(-1.17907, -1.17894)$	$(-1.183, -1.179)$	$(-1.18392, -1.18386)$

Summary

- Efficient contraction of a *2D* tensor-network is the main obstacle for good *2D* tensor-based algorithms.
- If we assume that the T.N. is a good approximation to the g.s., then local patches can be used to approximate a local expectation value.
- Non-trivial local constraints (translation-invariance and commutator gauge properties) for glocal g.s. of local Hamiltonian *H* guaranteed by area laws: $\#\mathrm{Variables} = e^{O(|\partial L|)}$ and $\#\mathrm{Constraints} = e^{O(|L|)}$.
- To approximate environments, these constraints can be written as *semi-definite quadratic programming* (SDQP) problems, and then solving them by the *primal-dual interior point methods.*
- Separate a series of environment tensors E_i from g.s. ρ_L, and it will leads us to some practical algorithms (optimizing them alternatively).
- Interesting numerical results in 2D among CGO, TIO and varCTM. But how to understand the structure of g.s.' environment by comparing TIO and varCTM?

Thanks for listening!

Q&A