

# Corner Transfer Matrix Renormalization Group

Efficient Contraction of 2D Classical Lattice Models

Your Name

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# Outline

- 1 From 1D to 2D: The Contraction Issue
- 2 Going to 2D: A Fundamentally Harder Problem
- 3 CTMRG: Extending to 2D
- 4 Results
- 5 Summary

# Review: 1D Transfer Matrix (Your Pre-knowledge)

## 1D Ising Model:

$$H = -J \sum_i \sigma_i \sigma_{i+1}$$

### Partition function as contraction:

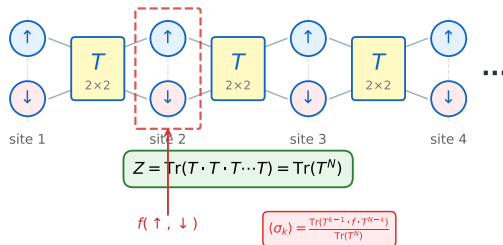
$$Z = \text{Tr}(T \cdot T \cdot T \cdots T) = \text{Tr}(T^N)$$

where  $T \in \mathbb{R}^{2 \times 2}$  encodes local interactions.

### Local observable:

$$\langle \sigma_k \rangle = \frac{\text{Tr}(T^k \cdot f(\uparrow, \downarrow) \cdot T^{N-k})}{\text{Tr}(T^N)}$$

All  $T$  identical  $\Rightarrow$  commute  $\Rightarrow$  diagonalize once!

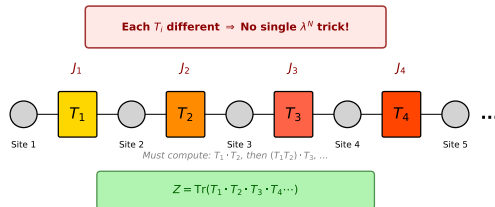


# When Even 1D Classical Needs Renormalization Group

**Recall:** For uniform 1D Ising,  $Z = \text{Tr}(T^N)$  has no contraction issues.

**But what if...**

- Couplings  $J_i$  are **site-dependent**?
- Random disorder:  $J_i \sim \mathcal{N}(\bar{J}, \sigma)$ ?
- Open boundary conditions (no translation symmetry)?



**Then:** Cannot diagonalize  $T$  once!

$$Z = \text{Tr}(T_1 \cdot T_2 \cdot T_3 \cdots T_N)$$

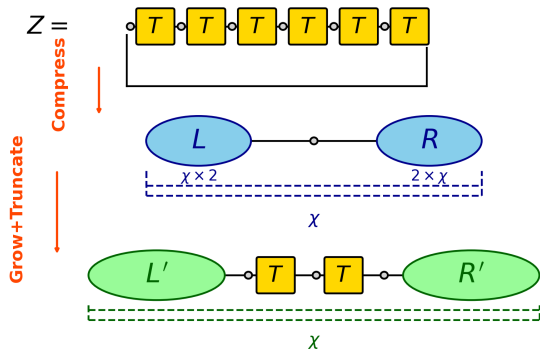
Each  $T_i$  is different  $\Rightarrow$  no simple  $\lambda^N$  formula.

## The Problem

For  $N$  sites: need  $O(N)$  matrix multiplications.  
Not exponential, but **no closed-form solution**.

# Solution: Transfer Matrix Renormalization Group (TMRG)

**Insight:** Not all configurations contribute equally to  $Z \Rightarrow$  Keep only the **most relevant** ones!



$\chi$  = bond dimension (most relevant configurations in compressed basis)

## TMRG Algorithm:

- 1 **Grow:**  $L' = L \cdot T$ ,  $R' = T \cdot R$   
(add sites)
- 2 **Truncate:** SVD  $\rightarrow$  keep  $\chi$  largest  
(coarse-grain)

## RG Fixed Point

Iterate until  $L^*, R^*$  converge  $\Rightarrow$   
Thermodynamic limit!

*Kind-of like infinite-DMRG by adding new  
of sites*

## 2D: The Transfer Matrix Becomes a **Network**

**1D:** Ordered product of matrices

$$Z = \text{Tr}(T_1 \cdot T_2 \cdots T_N)$$

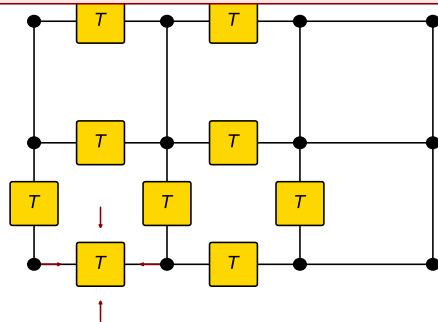
Contract left-to-right:  $O(N)$ .

**2D:** Each site couples to **4 neighbors!**

$$T_{\sigma_{\text{up}}, \sigma_{\text{down}}, \sigma_{\text{left}}, \sigma_{\text{right}}}^{\sigma_i}$$

This is a **rank-4 tensor**, not a matrix!

**2D: Each  $T$  has 4 legs  $\Rightarrow$  No simple contraction order!**



**Rank-4 tensor**

## The Fundamental Problem

# One Approach: Row-to-Row Transfer (DMRG-style)

**Idea:** Group one row of  $L$  spins  $\rightarrow$  treat as a “super-spin” with  $2^L$  states.

[Figure: Row  $\rightarrow$  super-spin,  $T_{\text{row}} \in \mathbb{R}^{2^L \times 2^L}$ ]

## Apply DMRG/TMRG ideas:

- Row config space  $\rightarrow$  MPS
- Row-to-row transfer  $\rightarrow$  MPO
- Truncate via SVD

## Pros & Cons

- + Systematic, well-understood
- Breaks 2D symmetry
- Hard to generalize to other lattices

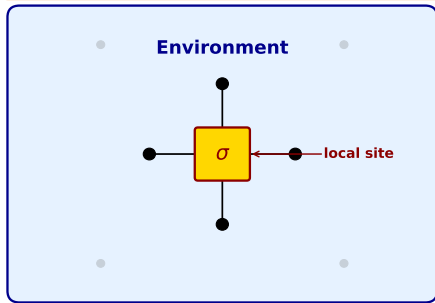
Then  $Z = \text{Tr}(T_{\text{row}}^M)$  looks like 1D!

(Details in Appendix)

# A More Natural Approach: Think in 2D!

**Question:** If we only want **local observables**  $\langle \sigma_{i,j} \rangle$ , do we really need to contract the *entire* infinite lattice?

Only need local  $\langle \sigma \rangle$ ?  $\Rightarrow$  Compress the environment!



$$\langle \sigma \rangle = \frac{\text{Tr}(\text{Environment} \cdot \sigma)}{\text{Tr}(\text{Environment})}$$

## Key Insight:

Decompose the infinite 2D environment into **geometrically natural** pieces:

- 4 **Corners** (quarter-planes)
- 4 **Edges** (half-infinite strips)

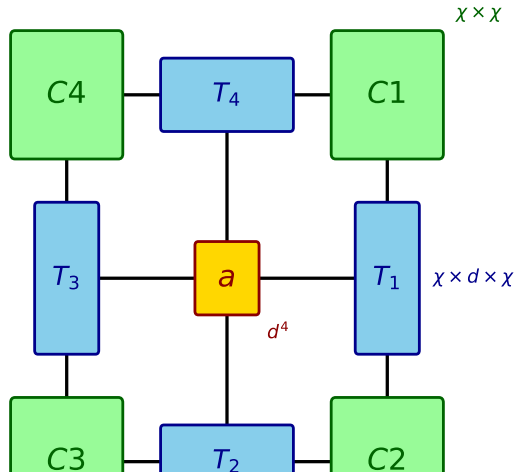
## Baxter's Insight (1968)

The **Corner Transfer Matrix** encodes a quarter of the infinite plane!



## 2D Analog: Four Corners + Four Edges

**CTMRG: Decompose 2D environment into 4 Corners + 4 Edges**



# The Local Tensor: Building Block

Local Boltzmann weight tensor  $a$ :

*[Figure: Local tensor  $a$  with 4 legs]*

For 2D Ising:

$$a_{u,d,l,r} = \sum_{\sigma} W_{\sigma,u} W_{\sigma,d} W_{\sigma,l} W_{\sigma,r}$$

where

$$W_{\sigma,\sigma'} = e^{\frac{\beta J}{2} \sigma \sigma'}$$

## Physical Meaning

$a$  encodes the Boltzmann weight at one site, with bond weights split symmetrically.

# CTMRG Iteration: Step 1 — Grow (Absorb Row/Column)

**Absorption:** Add one row **and** one column to expand the environment.

*[Figure: Absorption step — corner grows by absorbing a and edges]*

## CTMRG Iteration: Step 2 — Truncate (The Key Difference!)

**Truncation in 2D:** Use the **full environment** to determine projectors.

*[Figure: Building density matrix from environment for truncation]*

**Compute projector  $P$ :**

**Apply truncation:**

# CTMRG: Complete Algorithm

*[Figure: CTMRG algorithm flowchart]*



# Computing Observables with CTMRG

**Partition function:**

$$Z \propto \text{Tr}(C_1 T_1 C_2 T_2 C_3 T_3 C_4 T_4)$$

*[Figure: Computing  $\langle \sigma \rangle$  by inserting operator]*

# Numerical Results: 2D Ising Model

*[Results to be added: magnetization, critical behavior, etc.]*



# Summary: The Core of CTMRG

## CTMRG in Three Steps

- 1 **Decompose:** Infinite 2D lattice  $\rightarrow$  4 corners + 4 edges
- 2 **Grow:** Absorb local tensors (add row/column)
- 3 **Truncate:** SVD-based RG to keep  $\chi$  most relevant states

*[Figure: Visual summary — Decompose  $\rightarrow$  Grow  $\rightarrow$  Truncate]*



## Comparison: iDMRG vs CTMRG

Aspect	iDMRG (1D)	CTMRG (2D)
Dimension	1D chain	2D square lattice
Environment	Left + Right	4 Corners + 4 Edges
Grow step	Add site pair	Add row + column
Truncation	SVD on center bond	SVD on corner boundaries
Bond dimension	$\chi$ (MPS)	$\chi$ (environment)
Fixed point	$L^*, R^*$	$C_i^*, T_i^*$
Computational cost	$O(\chi^3)$	$O(\chi^6)$ or $O(\chi^5)$

# Thank You!

Questions?

## Appendix: TMRG Setup in Detail

**Goal:** Compute  $Z = \text{Tr}(T_1 \cdot T_2 \cdots T_N)$  for large  $N$ .

*[Figure: Left environment  $L$ , local site  $T$ , right environment  $R$ ]*

**Left Environment  $L$ :**

$$L_\sigma = \sum T_1 \cdot T_2 \cdots T_{k-1}$$

**Right Environment  $R$ :**

$$R_\sigma = \sum T_{k+1} \cdots T_N$$

## Appendix: TMRG Step 1 — Grow (Absorption)

**Absorption:** Add one more site to the environment.

*[Figure:  $L' = L \cdot T_k$ , growing the left environment]*

**Mathematically:**

$$L'_{\sigma_k} = \sum_{\sigma_{k-1}} L_{\sigma_{k-1}} \cdot (T_k)_{\sigma_{k-1}, \sigma_k}$$

## Appendix: TMRG Step 2 — Truncate (SVD)

**Idea:** Compress  $L'$  back to dimension  $\chi$  using SVD.

**Form the “density matrix”:**

$$\rho = L' \cdot R'^T$$

**SVD:**

$$\rho = U \Sigma V^\dagger$$

**Truncate:**

$$P = U_{:,1:\chi}$$

**New environment:**

$$L_{\text{new}} = P^\dagger L'$$

*[Figure: SVD spectrum, keep  $\chi$  largest]*

Eckart-Young Theorem

SVD gives the **optimal** rank- $\chi$  approximation

# Appendix: TMRG Convergence and Observables

**Iterate:** Grow  $\rightarrow$  Truncate  $\rightarrow$  Grow  $\rightarrow$  Truncate  $\rightarrow \dots$

**Convergence criterion:**

Fixed point:  $L^*, R^*$  such that

$$L^* \xrightarrow{\text{grow+truncate}} L^*$$

**Free energy:**

$$\begin{aligned} f &= -k_B T \lim_{N \rightarrow \infty} \frac{1}{N} \ln Z \\ &= -k_B T \ln \sigma_1^* \end{aligned}$$

**Local observables:**

$$\langle \sigma_k \rangle = \frac{L^* \cdot \sigma_k \cdot R^*}{L^* \cdot R^*}$$

**Correlation functions:**

$$\langle \sigma_i \sigma_j \rangle = \frac{L^* \cdot \sigma_i \cdot T^{|i-j|} \cdot \sigma_j \cdot R^*}{Z}$$

**Physical Meaning**

$L^*, R^*$  encode the **thermodynamic limit**.



## Appendix: 2D Row-to-Row — Row as Super-Spin

**Idea:** Treat one row of  $L$  spins as a single “super-spin”.

**Row configuration:**

$$\vec{\sigma} = (\sigma_1, \sigma_2, \dots, \sigma_L)$$

Total states:  $2^L$ .

**Row-to-row transfer:**

$$(T_{\text{row}})_{\vec{\sigma}, \vec{\sigma}'} = \prod_{i=1}^L e^{\beta J \sigma_i \sigma'_i} \prod_{i=1}^{L-1} e^{\beta J \sigma_i \sigma_{i+1}}$$

$$T_{\text{row}} \in \mathbb{R}^{2^L \times 2^L}.$$

*[Figure: Row  $\rightarrow$  super-spin with  $2^L$  states]*

### Key Point

Now  $Z = \text{Tr}(T^M)$  looks like 1D problem with  $2^L$  dimensional transfer matrix

# Appendix: Row Transfer Matrix = MPO

**Key insight:**  $T_{\text{row}}$  has a **tensor network** structure!

**Decompose**  $T_{\text{row}}$  into local tensors:

$$T_{\vec{\sigma}, \vec{\sigma}'} = \sum_{\alpha_1, \dots} W_{\alpha_0 \alpha_1}^{\sigma_1 \sigma'_1} W_{\alpha_1 \alpha_2}^{\sigma_2 \sigma'_2} \dots$$

*[Figure: MPO structure of  $T_{\text{row}}$ ]*

**Local tensor  $W$ :**

$W_{\alpha\beta}^{\sigma\sigma'}$  = local Boltzmann weight

- $\sigma, \sigma'$ : spins in rows  $n, n+1$
- $\alpha, \beta$ : auxiliary (horizontal bonds)

**No Quantum!**

“MPO” is just a factorization of the classical transfer matrix.

## Appendix: Boundary = MPS

**MPS:** Efficient representation of row configuration space.

**Full vector:**

$$|R\rangle = \sum_{\vec{\sigma}} R_{\vec{\sigma}} |\vec{\sigma}\rangle$$

has  $2^L$  components.

**MPS compression:**

$$R_{\vec{\sigma}} = A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_L}$$

Only  $L \cdot \chi^2 \cdot 2$  parameters!

*[Figure: MPS tensor network]*

### Physical Meaning

MPS compresses  $2^L$  row configs into  $\chi$  effective states with **limited entanglement**.

# Appendix: Row-to-Row DMRG Algorithm

**Combine:** MPS (boundary) + MPO (transfer) + SVD (truncation).

- 1 Initialize MPS  $|L\rangle$ ,  $|R\rangle$  for boundaries
- 2 **Grow:** Apply MPO  $T_{\text{row}}$  to boundaries

$$|L'\rangle = T_{\text{row}}|L\rangle$$

- 3 **Truncate:** SVD to compress bond dimension back to  $\chi$
- 4 Iterate until convergence to fixed point  $|L^*\rangle$ ,  $|R^*\rangle$

## Pros

- Systematic, well-understood
- Controlled approximation

## Cons

- Breaks 2D rotational symmetry
- Hard to generalize to other lattices

## Appendix: No Monte Carlo Sign Problem

**Classical models:** All Boltzmann weights are **positive**!

$$W = e^{-\beta H} > 0 \quad \text{always}$$

*[Figure: Classical (positive) vs Quantum (sign problem)]*

## Appendix: Why is 3D Difficult?

**In 2D:** Environment tensors are **1D objects** (edges).

**In 3D:** Environment would be **2D surfaces** — back to exponential!

*[Figure: 2D boundary problem in 3D systems]*

## Beyond square lattice Ising:

### Different lattices:

- Honeycomb
- Triangular
- Kagome

### Different models:

- Potts model
- Clock model
- Vertex models

### Quantum systems (via iPEPS):

- 2D Heisenberg model
- Frustrated magnets
- Topological phases

### Improvements:

- Directional CTMRG
- Full-update vs simple-update
- Gradient optimization

## Appendix: Computational Complexity

### CTMRG scaling:

Operation	Cost	Bottleneck?
Corner absorption	$O(\chi^4 d^2)$	✓
Edge absorption	$O(\chi^3 d^2)$	
Build density matrix	$O(\chi^4)$	
SVD for projector	$O(\chi^3 d^3)$	
Apply truncation	$O(\chi^3 d)$	
<b>Total per iteration</b>	$O(\chi^3 d^3)$ to $O(\chi^6)$	

### Comparison

- iDMRG (1D):  $O(\chi^3)$  per sweep
- CTMRG (2D):  $O(\chi^5) - O(\chi^6)$  per iteration
- More expensive, but still **polynomial** in  $\chi$ !



## Appendix: Key References

### Original works:

- R. J. Baxter, *J. Math. Phys.* **9**, 650 (1968) — Corner transfer matrices
- R. J. Baxter, *J. Stat. Phys.* **19**, 461 (1978) — CTM method

### Modern CTMRG:

- T. Nishino & K. Okunishi, *J. Phys. Soc. Jpn.* **65**, 891 (1996)
- T. Nishino & K. Okunishi, *J. Phys. Soc. Jpn.* **66**, 3040 (1997)

### CTMRG for iPEPS:

- R. Orús & G. Vidal, *Phys. Rev. B* **80**, 094403 (2009)
- P. Corboz et al., *Phys. Rev. B* **84**, 041108(R) (2011)

### Reviews:

- R. Orús, *Ann. Phys.* **349**, 117 (2014) — Tensor networks review