

APPLYING THE TRIAD NETWORK REPRESENTATION TO FOUR-DIMENSIONAL ATRG METHOD

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ABOUT TENSOR RENORMALIZATION GROUP

[M. Levin and C. P. Nave, (2007).]

Tensor Renormalization Group = Numerical Real space Renormalization Group

 \rightarrow A candidate for overcoming sign problems in LQCD

TRG is applicable for sign problem region, but has large cost at higher dimensions



OTHER APPROACHES TO HIGHER DIMENSIONS

	HOTRG [Xie et al, (2012).]	ATRG [D. Adachi, T. Okubo, and S. Todo, (2020).]	Triad TRG [D. Kadoh and K. Nakayama, (2019).]	MDTRG Triad rep. [K. Nakayama, (2023).]
cost	$O(\chi^{4d-1})$	$O(\chi^{2d+1})$	$O(\chi^{d+3})$	$O(qr^3\chi^{d+3})$
Fundamental tensor	$O(\chi^{2d})$	$O(\chi^{d+1})$	$O(\chi^3)$	$O(\chi^{d+1})$
methods	Exact Contraction	 Bond-swapping via RSVD Exact Contraction 	 Triad Contraction via RSVD 	 Decomposition of unit-cell tensor Triad Internal line oversampling Contraction via RSVD

Our motivation is to search for a more efficient algorithm for four-dimensional theories.

COST REDUCTION FOR HIGHER DIMENSIONS – ATRG

[D. Adachi, T. Okubo, and S. Todo, (2020).]

Two reason for the cost reduction

- ✓ The fundamental tensor has d+1 legs.
- \checkmark By performing bond swapping, the number of isometries is reduced by 1/2.

The cost of ATRG is χ^{2d+1} ! (HOTRG was χ^{4d-1}) RSVD is used in the bond-swapping step



COST REDUCTION FOR HIGHER DIMENSIONS – MDTRG TRIAD REP.

[K. Nakayama, (2023).]

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Difference from ATRG is

- ✓ Using RSVD with QR iteration in contraction step (approximated SVD scheme)
- ✓ Oversampling of internal line $\chi \to r \chi$
- Decomposition of Unit-cell tensor

MDTRG is more accurate than Triad TRG , almost same accuracy of HOTRG

→ MDTRG-Triad rep. is improved version of Triad TRG, which cost is $O(qr^3\chi^{d+3})$



CONSIDERATION ON VARIOUS METHOD IN 4D

• In 4D systems, it is Trade-off between accuracy and computation cost

	HOTRG [Xie et al, (2012).]	ATRG [D. Adachi, T. Okubo, and S. Todo, (2020).]	MDTRG Triad rep. [K. Nakayama, (2023).]
cost	$O(\chi^{15})$	$O(\chi^9)$ \bigcirc	$O(qr^3\chi^7)$
Accuracy		•••	?
Problem	• Large cost, difficult to enlarge χ	 Large cost The convergence of free energy is not as good in the 2D cases. 	 Investigation is needed

PROPOSAL

We aim for faster algorithms!

	ATRG [D. Adachi, T. Okubo, and S. Todo, (2020).]	Triad-MDTRG [K. Nakayama, (2023).]
Cost in 4D	$O(\chi^9)$	$O(qr^3\chi^7)$
methods	 Bond-swapping via RSVD Exact Contraction 3 isometry in the contraction step 	 Decomp. of Unit- cell tensor Triad Internal line oversampling
		 Contraction via RSVD

Triad-ATRG ?

Research

TRIAD REPRESENTATION OF ATRG

- We consider triad representation of ATRG
- Consider HOSVD of unit cell tensor $\Gamma = AX\sigma YD$ after the Bond swapping
- SVD of. $AX\sigma$ and σYD provides SVD of Γ thanks to canonical form [S. Akiyama, phd, 2022.]
- Make triad representation in the same manner as MDTRG
- Triad legs are oversampled $\chi \rightarrow r \chi$



TRIAD REPRESENTATION OF ATRG

- However, in four dimensions, the order of computational cost does not change even if not all tensors are converted into triad form. Therefore, we use a form with as few decompositions as possible.
- We obtain <u>4 legs tensors E, F, G, H ∈ C^{χ×χ×χ×rχ}</u> and 3 legs tensors I, J, K, L ∈ C^{χ×χ×rχ} (we call this form as triad rep.)



TRIAD REPRESENTATION OF ATRG

- Computational cost of this procedure is $O(\chi^7)$ (If we use RSVD, $O(qr\chi^6)$)
- All decomposition in this procedure are SVD of the Unit-Cell Tensor



MAKING SQUEEZERS

- We derive squeezers in the same manner of ATRG [S. Akiyama, phd, 2022.]
- since Γ is not canonical form anymore, we must decompose $\Gamma \simeq EFGHIJKL$
- We can calculate separately by introducing the Gramm-matrix of. *EFIJ* and *GHKL*



MAKING SQUEEZERS

- Computational cost of this procedure is $\min(O(\chi^7), O(r^2\chi^6))$
- All decomposition in this procedure are SVDs of $\Gamma(n)\Gamma(n+\hat{\mu})$ as in the improved ATRG

[S. Akiyama, phd, 2022.] [S. Iino, S. Morita, and N. Kawashima, (2019).] [D. Adachi, T. Okubo, and S. Todo, (2022).]



CONTRACTION STEP

- Thanks to the Triad form, Computational cost is reduced to $O(r^2\chi^7)$, smaller than ATRG ($O(\chi^9)$) Bottleneck
- We do not use RSVD since we already used it once in the bond-swapping step



SUMMARY OF COMPUTATIONAL COST

	Step	ATRG	Triad ATRG	
	Bond Swapping	$O(qr\chi^6)$	$O(qr\chi^6)$	
Â	Make Triad	None	$O(\chi^7)$	
$\hat{\uparrow}$ $\hat{2}$	Squeezer	$O(\chi^7)$	$O(\min(\chi^7, r^2\chi^6))$	
$\hat{3}$ $\hat{1}$	Contraction <	$O(\chi^9)$	$O(r^2\chi^7)$	
		Bot	tleneck	
	$r\chi^{6}$ $O(\gamma$	(⁷)	$O(r^2\chi^6)$	

表1 Computational cost

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Numerical results on 4D Ising model

FREE ENERGY

• We investigate the convergence of free energy at 4D Ising model in r=7, L=1024,T=6.65035



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COMPUTATIONAL TIME ON A CPU

- We investigate the computational time in r=7 using a single CPU calculation
- Scaling of the computational time is $O(\chi^7)$



COMPUTATIONAL TIME ON GPUS

- We investigate the computational time in r=7 ,L=1024 by 2 GPU parallelized calculation
- Scaling of the computational time improved significantly



PHASE TRANSITION POINT

To determine the transition point, we evaluate the following value at each coarse-graining step. $X^{(m)} = \frac{(\mathrm{Tr}A^{(m)})^2}{\mathrm{Tr}(A^{(m)})^2}, \text{ with } A^{(m)}_{kl} = \sum T^{(m)}_{i_1 i_2 i_3 k i_1 i_2 i_3 l}$ If X=2, the system is in an ordered phase, and if X=1, it is in a disordered phase

HOTRG(D=13): $T_c = 6.650365(5)$ [S. Akiyama, Y. Kuramashi, T. Yamashita, and Y. Yoshimura, (2019).]

[Z.-C. Gu and X.-G. Wen, (2009).]





PHASE TRANSITION POINT



HOTRG(χ =13): $T_c = 6.650365(5)$ [S. Akiyama, Y. Kuramashi, T. Yamashita, and Y. Yoshimura, (2019).]

Monte-Carlo: $T_c = 6.6803069(58)$ [P. H. Lundow and K. Markström, (2023).]

Difference from the ATRG results at χ =54 is ~0.1% for r=7, and ~0.04% for r=10

*results of ATRG has not converged well

Further investigation for larger χ_{-} is needed

SUMMARY AND FUTURE WORKS

- The results of Triad-ATRG are highly consistent with the ATRG results
- Triad-ATRG significantly improves the computational cost on CPU and GPUs

Triad ATRG would be a powerful tool for 4D systems

Future works

- Investigate the accuracy of internal energy
- Calculate in more large χ
- Apply to other 4D systems

END

ABOUT TENSOR NETWORK

The tensor network method was developed in condensed matter physics (Hamiltonian formalism) For Quantum Field Theory, we use Lagrangian approach

	Hamiltonian	Lagrangian
Target	Many body system	Path integral
Method	Variational	Renormalization
Physics	Ground state Partial function Real time evolution Green function	

We use TRG for higher dimensions

ABOUT SUMMATION RULES

Tensor is multidimensional array! We use convention of tensor network diagrams below.



Tensor Network = Diagram representation of tensor contraction

Theorem Let $m, n \in \mathbb{N}$ Any comprex matrix with rank $r, A \in \mathbb{C}^{m \times n}$ is decomposed by using singular value $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r \geq 0$,

$$A = U\Sigma V^{\dagger} \tag{1}$$

with $U \in \mathbb{C}^{m \times m}$, $V \in \mathbb{C}^{n \times n}$ is unitaly matrix, and

$$\Sigma = \begin{pmatrix} \operatorname{diag}(\sigma_1, \dots, \sigma_r) & O_{r,m-r} \\ O_{m-r,r} & O_{m-r,n-r} \end{pmatrix}$$
(2)

$$AA^{\dagger} = U\Sigma^2 U^{\dagger}, \quad A^{\dagger}A = V\Sigma^2 V^{\dagger}$$

Singular values have important information of the matrix. (next page)

BEST LOW RANK APPROXIMATION

Theorem The comprex matrix $X \in \mathbb{C}^{m \times n}$ which satisfies $||A - X||_F = \min_{\operatorname{rank} X' = k} ||A - X'||_F$ with rank k < r is

k

$$||A||_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2}$$
(1)

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$$X = \sum_{m=1} \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^{\dagger}$$
(1)
$$= \begin{pmatrix} \boldsymbol{u}_1 \ \cdots \ \boldsymbol{u}_k \end{pmatrix} \begin{pmatrix} \sigma_1 \\ & \ddots \\ & & \sigma_k \end{pmatrix} \begin{pmatrix} \boldsymbol{v}_1^{\dagger} \\ \vdots \\ \boldsymbol{v}_k^{\dagger} \end{pmatrix}$$
(2)

 \boldsymbol{u} and \boldsymbol{v} is columns of U, V

Truncated-SVD,(RSVD,Arnordi,...)

SVD is the best approximation for matrix

[N. Halko, P.-G. Martinsson, and J. A. Tropp, (2010).]

Let $A \in \mathbb{C}^{m \times n}$ be a target matrix, and let $\Omega \in \mathbb{C}^{n \times l}$ be a random matrix with $l = \chi + p$ with a target rank χ . We compute $Q = qr(A\Omega)$. Then we iterate the following procedure for q times:

 $\Omega = \operatorname{qr}(A^{\dagger}Q)$ $Q = \operatorname{qr}(A\Omega)$

We obtain $A \simeq QQ^{\dagger}A$. Finally, by computing the SVD

 $Q^{\dagger}A\simeq \overline{U}\Sigma V^{\dagger}$

we obtain the truncated SVD of $A \simeq Q\overline{U}\Sigma V^{\dagger}$ with $\Sigma \in \mathbb{C}^{\chi \times \chi}$. Total cost is $O(qmn\chi)$

RSVD is powerful tool in the TRG calculations

ABOUT TENSOR RENORMALIZATION GROUP

[M. Levin and C. P. Nave, (2007).]

Tensor Renormalization Group = Numerical Real space Renormalization Group Partial function can be expressed in Tensor network form if interaction is



Tensor Renormalization Group (TRG) method has no sign problems ! TRG is applicable for sign problem region, but has large cost at higher dimensions

TENSOR RENORMALIZATION GROUP

[M. Levin and C. P. Nave, (2007).]

Applying SVD, we decompose subnetwork, and contract inner bonds $T \in \mathbb{C}^{\chi \times \chi \times \chi \times \chi}$



Rotating the system, we get new network, but the number of tensors became 1/4

 \rightarrow Renormalization , total computational cost is $\chi^6 \log V$

HOTRG

[Z. Y. Xie, J. Chen, M. P. Qin, J. W. Zhu, L. P. Yang, and T. Xiang, (2012).]

For higher dimensions, HOTRG renormalize each direction separately.

We multiply <u>truncated unitary matrix</u> $U_{x_1x_2x} \in \mathbb{C}^{\chi \times \chi \times \chi}$ from each side. $UU^{\dagger} \simeq I$ $\hat{2}$ isometry



 $T_{i_{1}(n^{*})i_{2}(n^{*})j_{1}(n^{*})j_{2}(n^{*})}^{R} = U_{j_{1}(n+\hat{1})j_{1}(n)j_{1}(n^{*})}^{*}T_{i_{1}(n+\hat{1})i_{2}(n+\hat{1})j_{1}(n+\hat{1})j_{2}(n+\hat{1})}T_{i_{1}(n)i_{2}(n)j_{1}(n)j_{2}(n)}U_{i_{1}(n+\hat{1})i_{1}(n)i_{1}(n^{*})}$ U is obtained by SVD of subnetwork TT; this is optimal for y direction.

HOTRG PROCEDURE

Renormalize each direction anisotropically

Applicable to 3d,4d systems



https://smorita.github.io/TN_animation/

- $computational cost = \chi^{lpha} \log V
 ightarrow$ Easy to take thermodynamic limit (MC $ightarrow V^{eta}$)
- No Sign Problem
- Easy to treat Fermion

HOTRG

[Z. Y. Xie, J. Chen, M. P. Qin, J. W. Zhu, L. P. Yang, and T. Xiang, (2012).] For 3d or higher dimensions, this procedure can be also done by separatory We multiply truncated unitary matrices $U_{x_1x_2x}^{(1)}$, $U_{y_1y_2y}^{(2)}$ from x and y axis. contract $U^{(1)}$ $U^{(1)\dagger}$ 7(2) $U^{(2)}$

 $T^R = U^{*(2)} U^{*(1)} T T U^{(1)} U^{(2)}$

U is obtained by Eigen Value Decomposition of subnetwork TT

HOTRG

[Z. Y. Xie, J. Chen, M. P. Qin, J. W. Zhu, L. P. Yang, and T. Xiang, (2012).]

HOTRG can be applied to any dimensional systems, but it has large computational cost. HOTRG has χ^{4d-1} for contraction step, it is too large for 4d systems like QCD



CONSTRACT TENSOR REPRESENTATION

Partial function can be expressed in Tensor network form if interaction is local



We can constract Tensor Network Representations of the spin system as follows.

Consider following Hamiltonian

Ising model
$$W[\sigma_n, \sigma_{n+\hat{\mu}}] = -J\sigma_n\sigma_{n+\hat{\mu}}, \quad K[\sigma_n] = h\sigma_n$$

$$Z = \sum_{\sigma_n} \left[\prod_{n} \exp\left(\sum_{\mu} \underbrace{W[\sigma_n, \sigma_{n+\hat{\mu}}]}_{\text{hopping term}} + \underbrace{K[\sigma_n]}_{\text{on-site term}} \right) \right]$$

CONSTRACT TENSOR REPRESENTATION

Let
$$X_{\sigma_n\sigma_{n+\hat{\mu}}} = \exp\left(W[\sigma_n, \sigma_{n+\hat{\mu}}]\right)^{\underset{i_{\mu}(n)}{\overset{\mathsf{SVD}}{=}}} \sum_{i_{\mu}(n)} U_{\sigma_n}S_{i_{\mu}(n)}V_{\sigma_{n+\hat{\mu}}i_{\mu}(n)}^* \xrightarrow{\sigma_n} \underbrace{X_{\sigma_{n+\hat{\mu}}}}_{\sigma_{n+\hat{\mu}}} = \underbrace{\sigma_n}_{i_{\mu}(n)} \underbrace{V[\sigma_n, \sigma_{n+\hat{\mu}}]}_{i_{\mu}(n)} + \underbrace{K[\sigma_n]}_{on-site \ term}\right) = \sum_{\sigma} \left[\prod_n \prod_{\mu} X_{\sigma_n\sigma_{n+\hat{\mu}}}\right] \exp(K[\sigma_n])$$

$$= \underbrace{X_{\sigma_n\sigma_n+\hat{\mu}}}_{X \ \sigma_n\sigma_{n+\hat{\mu}}} = \underbrace{\Phi_{\sigma_n\sigma_n}}_{i_{\mu}(n)} \underbrace{\Phi_{\sigma_n\sigma_n}}_{i_{\mu$$

COST REDUCTION FOR HIGHER DIMENSIONS – ATRG

[D. Adachi, T. Okubo, and S. Todo, (2020).]

In d-dimensional system, The tensor T has 2d legs, which results in high memory cost! One way to reduce cost is the ATRG method. -Adachi et al (2020)

- 1. Decompose a fundamental tensor to d+1 legs. $TT \rightarrow ABCD$
- 2. Decompose $BC \rightarrow X\sigma Y$ with the bond swapping
- 3. Using isometry (called squeezer), make GH and next ABCD







COST REDUCTION FOR HIGHER DIMENSIONS – MDTRG

[K. Nakayama, (2023).]

MDTRG-Triad rep. is improved version of Triad TRG, which cost is $O(qr^3\chi^{d+3})$ Difference from Triad TRG is

- ✓ Oversampling of internal line $\chi \to r \chi$
- ✓ Using RSVD with QR iteration in contraction step (approximated SVD scheme)
- ✓ Decomposition of Unit-cell tensor
- → MDTRG is more accurate than Triad TRG , same accuracy of HOTRG



RSVD IN 4D SYSTEM

The numerical instability caused by RSVD is serious in four dimensions [H. Oba, (2019).]

Is there any efficient triad algorithms for 4D system?

- In ATRG, q = O(D) is sufficient in Bond swapping step, total cost is $O(\chi^9)$
- If we take q = O(D) in MDTRG, the cost is $O(r^3\chi^8)$, difficult to enlarge χ and r simultaneously



COST REDUCTION FOR HIGHER DIMENSIONS – TRIAD TRG

[D. Kadoh and K. Nakayama, (2019).]

Cost of Triad TRG is. χ^{d+3} !

Two reason of cost reduction

- ✓ Fundamental tensor has 3 legs
- ✓ Using RSVD in contraction step

But Triad TRG is less accurate than HOTRG, due to the additional decomposion



COMPUTATIONAL TIME ON GPUS

- We investigate the computational time in r=7 ,L=1024by 2 GPU parallelized calculation
- Scaling of the computational time improved significantly



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HOTRG

HOTRG decomposes subnetwork TT unlike original TRG, which decomposes T



HOTRG has small error from the exact solution. -Xie et al (2012)

FIG. 4. (Color online) Comparison of the relative errors of free energy with respect to the exact results for the 2D Ising model obtained by various methods with D = 24. The critical temperature $T_c = 2/\ln(1 + \sqrt{2})$.

Decomposing large network reduces the systematic error!

Definition Let $A \in \mathbb{R}^{m \times n}$ The norm of A is defined by

$$||A||_F = \sqrt{\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2}$$

This norm satisfies the following properties.

$$||A||_{F}^{2} = \operatorname{tr}[A^{\dagger}A] = \sum_{i=1}^{r} \sigma_{i}^{2}$$
(2)

(1)

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TENSOR RENORMALIZATION GROUP

Consider Network



(subnetwork)

Apply SVD for Tensor $T \in \mathbb{C}^{\chi \times \chi \times \chi \times \chi}$ (χ is called the bond dimension, often take 50~100)

$$T_{ijkl} = \sum_{m}^{\chi^2} U_{(ij)m} \sigma_m V_{(kl)m}^* \stackrel{\text{truncated}}{\simeq} \sum_{m}^{\chi} U_{(ij)m} \sigma_m V_{(kl)m}^* = \sum_{m}^{\chi} S_{(ij)m}^{[1]} S_{(kl)m}^{[2]}$$

Apply for another pair of indices, we can decompose T below



BEST LOW RANK APPROXIMATION

SVD is the best approximation for matrix. It compress the necessary information of the matrix.



Large singular values is dominant for the norm of the matrix

BEST LOW RANK APPROXIMATION

SVD is the best approximation for matrix. It compress the necessary information of the matrix.

128 x 128 pixels



$$\sum_{l=1}^{r} \sqrt{\lambda_l} \mathbf{u}_l \mathbf{v}_l^T$$

Original image



Using SVD for tensor contraction!

TENSOR RENORMALIZATION GROUP

Consider Network



(subnetwork)

Apply SVD for Tensor $T \in \mathbb{C}^{D \times D \times D \times D}$ (D is called the bond dimension, often take 50~100)

$$T_{ijkl} = \sum_{m}^{D^2} U_{(ij)m} \sigma_m V_{(kl)m}^* \stackrel{\text{truncated}}{\simeq} \sum_{m}^{D} U_{(ij)m} \sigma_m V_{(kl)m}^* = \sum_{m}^{D} S_{(ij)m}^{[1]} S_{(kl)m}^{[2]}$$

Apply for another pair of indices, we can decompose T below



BOND-SWAPPING

Two reason of cost reduction

[D. Adachi, T. Okubo, and S. Todo, (2020).]

- ✓ Fundamental tensor has less legs
- \checkmark By doing bond swapping, the # of isometry is reduced to $\frac{1}{2}$

