Blocking versus Sampling

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Work done with Alexei Bazavov, Shailesh Chandrasekharan, Alan Denbleyker, Yuzhi "Louis" Liu, Chen-Yen Lai, Shan-Wen Tsai, Li Ping Yang, Judah Unmuth-Yockey, Tao Xiang, Zhiyuan Xie, Ji-Feng Yu, and Haiyuan Zou

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The Tensor Renormalization Group (TRG)

- Exact blocking (spin and gauge, PRD 88 056005)
- Applies to many lattice models (talks: O(3), Schwinger model)
- Can blocking and sampling be complementary?
- Recent numerical progress with TRG
 - Truncation methods
 - Solution of sign problems (PRD 89, 016008)
 - Critical exponents
- O(2) model with a chemical potential (arxiv 1403.5238)
 - Phase diagram
 - Comparison with the worm algorithm
 - Microscopic control of the systematic errors
 - Optical lattice realization? (poster)
 - Onclusions

Motivation: study of non trivial fixed points

Irrelevant directions can be slow: problem for small volumes. Blocking?



Figure : Schematic flows for SU(3) with 12 flavors (picture by Yuzhi Liu).



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Block Spining in Configuration Space is difficult!



Figure : Ising 2, Step 1, Step 2,write the formula!



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TRG: simple and exact! (Levin, Wen, Xiang ..)

For each link, we use the Z_2 character expansion:

$$\exp(\beta\sigma_1\sigma_2) = \cosh(\beta)(1 + \sqrt{\tanh(\beta)}\sigma_1\sqrt{\tanh(\beta)}\sigma_2) = \cosh(\beta)\sum_{n_{12}=0,1} (\sqrt{\tanh(\beta)}\sigma_1\sqrt{\tanh(\beta)}\sigma_2)^{n_{12}}.$$

Regroup the four terms involving a given spin σ_i and sum over its two values ± 1 . The results can be expressed in terms of a tensor: $T_{xx'yy'}^{(i)}$ which can be visualized as a cross attached to the site *i* with the four legs covering half of the four links attached to *i*. The horizontal indices *x*, *x'* and vertical indices *y*, *y'* take the values 0 and 1 as the index n_{12} .

$$T_{xx'yy'}^{(i)} = f_x f_{x'} f_y f_{y'} \delta \left(\text{mod}[x + x' + y + y', 2] \right) ,$$

where $f_0 = 1$ and $f_1 = \sqrt{\tanh(\beta)}$. The delta symbol is 1 if x + x' + y + y' is zero modulo 2 and zero otherwise.



TRG blocking (graphically)

Exact form of the partition function: $Z = (\cosh(\beta))^{2V} \operatorname{Tr} \prod_i T_{xx'yy'}^{(i)}$. Tr mean contractions (sums over 0 and 1) over the links. Reproduces the closed paths of the HT expansion. TRG blocking separates the degrees of freedom inside the block which are integrated over, from those kept to communicate with the neighboring blocks. Graphically :





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PRD 88 056005

- Higher dimensions
- O(2) model
- O(3) model (Judah Unmuth-Yockey's talk, Thursday 14:35, 329)
- Principal chiral models
- Abelian gauge theories
- SU(2) gauge theories

Yuya Shimizu and Yoshinobu Kuramashi, 1 flavor of Wilson fermion Schwinger model, arxiv 1403.0642 (talk on Tuesday)



Blocking defines a new rank-4 tensor $T'_{XX'YY'}$ where each index now takes four values.

$$\begin{aligned} T'_{X(x_1,x_2)X'(x_1',x_2')Y(y_1,y_2)Y'(y_1',y_2')} &= \\ \sum_{x_U,x_D,x_R,x_L} T_{x_1x_Uy_1y_L} T_{x_Ux_1'y_2y_R} T_{x_Dx_2'y_Ry_2'} T_{x_2x_Dy_Ly_1'} , \end{aligned}$$

where $X(x_2, x_2)$ is a notation for the product states e.g., X(0,0) = 1, X(1,1) = 2, X(1,0) = 3, X(0,1) = 4. The partition function can be written as

$$Z = \operatorname{Tr} \prod_{2i} T_{XX'YY'}^{\prime(2i)} ,$$

where 2*i* denotes the sites of the coarser lattice with twice the lattice spacing of the original lattice.

Practical Implementation: Truncations

- For numerical calculations, we restrict the indices *x*, *y*,... to a finite number *N*_{states}.
- We use the smallest blocking: $M_{XX'yy'}^{(n)} = \sum_{y''} T_{x_1x'_1yy''}^{(n-1)} T_{x_2x'_2y''y'}^{(n-1)}$ where $X = x_1 \otimes x_2$ and $X' = x'_1 \otimes x'_2$ take now N_{states}^2 values.
- We make a truncation $N_{states}^2 \rightarrow N_{states}$ using $T_{xx'yy'}^{(n)} = \sum_{IJ} U_{xI}^{(n)} M_{IJyy'}^{(n)} U_{x'J}^{(n)*}$

The unitary matrix U diagonalizes a matrix which is either

• $\mathbb{G}_{XX'} = \sum_{X''yy'} M_{XX''yy'} M^*_{X'X''yy'}$ (Xie et al. PRB86, HOTRG)

• $\mathbb{T}_{XX'} = \sum_{v} M_{XX''yy}$ (YM PRB87, Transfer Matrix)

and we only keep the N_{states} eigenvectors corresponding the the largest eigenvalues of one of these matrices.

Overlap of the eigenvectors of $\mathbb{G}_{XX'}$ and $\mathbb{T}_{XX'}$

The overlap matrix $O_{ij} = \sum_X U_{iX} \tilde{U}_{Xj}^*$ seems to have remarkable properties. One example with O(2) indicates that the eigenvectors are approximately the same but the eigenvalues are sometimes in a different order:

	/1.	0.	0.	0.	0.	0.	0.	0. \	
O _{ij} =	0.	0.	0.9983	0.	0.	0.	0.0576	0.	
	0.	0.9999	0.	0.	0.	0.	0.	0.	
	0.	0.	0.	1.	0.	0.	0.	0.	
	0.	0.	0.	0.	0.9997	0.	0.	0.	
	0.	0.	0.	0.	0.	1.	0.	0.	
	0.	0.	0.0576	0.	0.	0.	0.9983	0.	
	\0.	0.	0.	0.	0.	0.	0.	0.9996/	ii
									- <u>'</u>

Values smaller than 10^{-7} in absolute value have been replaced by 0.



- The linear algebra seems insensitive to the fact that the values of the initial tensor become complex
- This allows us to deal with complex β, chemical potential (no apparent sign problem)
- However, when one approaches a zero of the partition function, larger truncations are necessary
- The TRG allows us to study the analyticity in complex β and μ planes
- There are subtleties with parity at complex β (H. Zou's thesis); need for CP or PT considerations?



Comparing with Onsager-Kaufman (PRD 89, 016008)



Figure : Zeros of Real (\blacksquare) and Imaginary (\square) part of the partition function of the Ising model at volume 8 × 8 from the HOTRG calculation with $D_s = 40$ are on the exact lines. Gray lines: MC reweighting solution. Thick Black curve: the "radius of confidence" for MC reweighting result, above this line, the error is large.

Calculated zeros confirms KT FSS ($1 + \nu = 1.5$) (PRD 89, 016008)



Figure : Zeros of XY model with linear size L = 4, 8, 16, 32, 64, 128 (from up-left to down-right) calculated from HOTRG with $D_s = 40, 50$ and zeros with L = 4, 8, 16, 32 from MC. The curve is a model for trajectory of the lowest zeros. Fit: $\text{Im}\beta_z = 1.27986 \times (1.1199 - \text{Re}\beta_z)^{1.49944}$.

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Accurate exponents from approximate tensor renormalizations (YM, PRB 87, 064422)

- For the Ising model on square and cubic lattices, truncation method (HOSVD) sharply singles out a surprisingly small subspace of dimension two.
- In the two states limit, the transformation can be handled analytically yielding a value 0.964 for the critical exponent ν much closer to the exact value 1 than 1.338 obtained in Migdal-Kadanoff approximations. Alternative blocking procedures that preserve the isotropy can improve the accuracy to $\nu = 0.987$ (isotropic G) and 0.993 (T) respectively.
- More than two states: adding a few more states does not improve the accuracy (Efrati et al. RMP 86 (2014))



The simplest example of quantum rotors (arxiv 1403.5238)

O(2) model with one space and one Euclidean time direction. The $N_x \times N_t$ sites of the lattice are labelled (x, t). We assume periodic boundary conditions in space and time.

$$Z = \int \prod_{(x,t)} \frac{d\theta_{(x,t)}}{2\pi} e^{-S}$$

$$S = -\beta_t \sum_{(x,t)} \cos(\theta_{(x,t+1)} - \theta_{(x,t)} + i\mu)$$

$$-\beta_s \sum_{(x,t)} \cos(\theta_{(x+1,t)} - \theta_{(x,t)}).$$

In the isotropic case, we have $\beta_s = \beta_t = \beta$.

In the limit $\beta_t >> \beta_s$ we reach the time continuum limit.

For $\mu \neq 0$ and real, the MC method does not work (complex action).

For large μ , there is a correspondence with the Bose-Hubbard model (Sachdev, Fisher, ..)

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Phase diagram



Figure : Phase diagram for 2D O(2) isotropic model in β - μ plane (left) and in the β - $\beta e^{\mu}/2$ plane (right) which resembles the anisotropic case. The lines labeled by "3s" stand for the phase separation lines of a 3-states system

Comparing TRG with the worm algorithm

β	μ	$\langle N \rangle$ (worm)	$\langle N \rangle$ (HOTRG)
1.12	0.01	0.00726(1)	0.00728(8)
0.46	1.8	0.98929(1)	0.9892(3)
0.28	2.85	1.98980(2)	1.989(2)
0.2	3.53	2.96646(3)	2.967(1)
0.12	4.3	3.96206(4)	3.965(1)

Table : Comparison of $\langle N \rangle$ between worm algorithm and HOTRG



Microscopic Analysis of Systematic Errors



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Eigenvalue distribution ($\beta = 0.06, \mu = 3.5$)





Entropy of the eigenvalue distribution

The eigenvalues of the transfer matrix are all positive, and after normalization can be interpreted as probabilities: $\sum_i p_i = 1$. We can then define an invariant entropy $S = \sum_i p_i \ln(p_i)$





Evolution of eigenvalue distribution with μ (β = 0.3)





11 states for the initial tensor and then enough states in the first blocking to stabilize $\langle N \rangle$ with 5 digits (in progress, estimated error less of order 1 in the last digit, preliminary).

size	β	μ	$\langle N \rangle$ (worm)	$\langle N \rangle$ (HOTRG)	number of states
2 × 2	0.06	3.5	0.69156	0.69155	31
2 imes 4	0.06	3.5	0.54080	0.54079	15
2 imes 2	0.3	1.8	0.61204	0.61204	34
2 imes 4	0.3	1.8	0.47929	0.47930	18



Optical Lattice Implementations? (A. Bazavov's poster)



Figure : (Color Online) Two-species (green and red) bosons in optical lattice with species-dependent optical lattice (with the same green and red). The nearest neighbor interaction is coming from overlap of Wannier gaussian wave functions. We assume the difference between intra-species interactions, are small $U \gg \delta$.

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- TRG: Exact blocking with controllable approximations
- Deals well with sign problems, reliable at larger $\text{Im}\beta$ than reweighting MC
- Ising case: checked with the complex Onsager-Kaufman exact solution
- Finite Size Scaling of Fisher zeros of *O*(2) agrees with Kosterlitz-Thouless
- Robust estimations of the eigenvalues of the transfer matrix
- Agreement with the worm algorithm at 5 digit level
- Understanding of the systematic errors
- Real time evolution?

Thanks!