# 2D Canonical Forms, Isometric PEPS

## 1. Canonical form for bond in 2D tensor network

For 1D MPS, there is a canonical form for a virtual bond: Schmidt decomposition into left and right parts, yielding diagonal bond matrix:

Method to obtain Schmidt decomposition: SVD

Schmidt decomposition also serves to 'fix gauge' on bond:

bond matrix should be diagonal, with only positive diagonal entries, arranged from large to small.

[Evenbly2018]

Generic question for 2D tensor network: can a canonical form for bonds be defined? The question is nontrivial due to presence of loops, so Schmidt decomposition does not apply.

Evenbly proposes a generic answer in terms of 'bond environment'. [Evenbly2018, Sec. II]

(a) Consider bond between tensors A and B, described by bond matrix  $\sigma_{AB}$ 

(b,c) Its 'bond environment',  $\gamma_{AB}$ , is 4-leg tensor obtained by deleting this bond (twice) from  $\langle \psi | \psi \rangle$ 







Useful properties of bond environment:

E.1 Bond environment of an index is invariant under gauge changes on all other internal indices of network.

E.2 All bond environments of all indices are invariant under unitary transformations on external indices of

network (because external indices are contracted out when constructing  $\langle Y \rangle$ ).



 $A \qquad B \qquad (1)$ 

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## Gauge fixing [Evenbly2018, Sec. III]

Define left and right 'boundary matrices' by contracting  $\sigma^{\dagger} \sigma$ 



FIG. 2. (a)–(b) The left boundary matrix  $\rho_L$  is formed from contracting a bond environment  $\Upsilon$  with (two copies of) the associated bond matrix  $\sigma$ . (b) The right boundary matrix  $\rho_R$ . (c) The weighted trace gauge (WTG) is the choice of gauge that yields trivial environment matrices,  $\tilde{\rho}_L \propto \mathbb{I}$  and  $\tilde{\rho}_R \propto \mathbb{I}$ .

or  $\sigma \sigma^{\dagger}$  onto  $\gamma$  from left or right:

contract left index of 6 with matching index of  $6^+$ 

contract right index of  $\checkmark$  with matching index of  $\sigma^{\dagger}$ 

Index is in 'weighted trace gauge' (WTG) if both left and right boundary matrices are proportional to  $\underline{1}$  and bond matrix  $\sigma$  itself is diagonal, with positive diagonal elements, arranged from large to small.

If bond is bridge index, so that bond environment factorizes, WTG implies



## 2. Full environment truncation (FET)

[Evenbly2018, Sec. V]

Goal: replace  $|\psi\rangle$ , with bond dimension  $\chi$  on bond between A and B, by  $(\tilde{\psi})$ , with bond dimension  $\tilde{\chi} < \chi$ 

 $\sigma_{AB}$ Strategy: replace bond matrix

by 
$$\tilde{\sigma}_{AB} v^{\dagger}$$
 (1)

on that bond, while keeping their overlap maximal.

and chose isometries, UV

$$l = 1, \quad \sigma^{\dagger} \sigma = 1, \quad (i)$$

 $\langle \tilde{\psi} | \psi \rangle \langle \psi | \tilde{\psi} \rangle$ 



$$\langle \tilde{\psi} | \psi \rangle \langle \psi | \psi \rangle$$

(d,e,f): this cost function can be expressed through the bond environment,  $\gamma$ , Hence the name: 'full environment trunctation' (FET).

FIG. 5. (a)–(c) The index connecting tensors A and B is truncated to smaller dimension,  $\tilde{\chi} < \chi$ , by replacing  $\sigma_{AB}$  with the product  $u(\tilde{\sigma}_{AB})v^{\dagger}$ , where u, v are isometries and  $\tilde{\sigma}_{AB}$  is a  $\tilde{\chi} \times \tilde{\chi}$  matrix. (d)–(f) The overlaps  $\langle \psi | \psi \rangle$ ,  $\langle \tilde{\psi} | \psi \rangle$ ,  $\langle \tilde{\psi} | \tilde{\psi} \rangle$  of the states from (a)–(b), which have been expressed in terms of the bond environment  $\Upsilon$ .

Initialize optimization protocol by doing SVD on bond matrix:





FIG. 11. Diagrams relating to the full environment truncation (FET) algorithm. (a) The fidelity F between an initial and a truncated state expressed in terms of a bond environment  $\Upsilon$ , see Fig. 5. (b)–(d) Definitions of tensors R, P, and B. (e) The fidelity F can be expressed as a generalized eigenvalue problem in R as F = $(RP^{\dagger}PR^{\dagger})/(RBR^{\dagger})$ . (f) The fidelity is maximized with the choice  $R = PB^{-1}$ . (g) Updated tensor u',  $\tilde{\sigma}'$ , and v' are obtained from the SVD of the product uR.

 $R = \widetilde{\sigma} v^{\dagger}$  using SVD from (4). (b) Initialize

Then seek to solve for optimal R while u is held fixed.

(c-d) Define tensors P, B, such that cost function takes the form

$$F = \frac{R \cap R^{\dagger}}{R \cap R^{\dagger}}, \text{ with } A = P^{\dagger}P$$

(f) Since A is simply outer product of two vectors, optimal choice for R is known analytically:  $\Re = \Re^{-1}$ 

(g) Do SVD on  $\chi R$  to obtain updated  $u', \mathfrak{F}', \mathfrak{T}'$ 

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Next, update the product  $\lambda = (u \tilde{s})$  in similar way, with

Iterate these two steps until convergence is reached (typically 'less than 20 iterations are needed).

#### Benchmark results for FET



FIG. 13. Relative error in the free energy per site of the classical Ising model on a  $2^{16} \times 2^{16}$  lattice of spins at critical temperature, comparing (i) tensor renormalization group [32] (TRG), (ii) tensor renormalization group with enlarged environment [36] (TRG + env) and (iii) tensor renormalization group that includes full environment truncations (TRG + FET).

SRG of [Zhao2010]

FET does better than TRG or SRG.

Evenbly claims (without showing data) that performance of FET is comparable to Gilt.

Gilt is 'smarter' than FET, because Gilt does more than optimize the overlap  $\langle \widehat{\psi} | \psi \rangle$ 

Instead, Gilt eliminates all information flowing out from bond that cannot traverse environment and reach outside world. Gilt and FET actually use same bond environment, but treat its indices differently:



FET successively optimizes  $\sigma$  bond, then  $\overline{\sigma}$  bond, iteratively until convergence.

But it never makes a 'horizontal SVD' through the middle of  $\chi$ , which governs how information flows from inside to outside. For this reason, FET is less efficient than Gilt.

## 3. Isometric PEPS: Moses move

[Zaletel2020]

#### **Motivation**

Canonical forms for 1D MPS are very useful: since constituents are isometries, contractions are trivial:

Standard tool for obtaining canonical form: SVD

## Can we similarly express PEPS state purely through isometries to obtain an 'isometric PEPS' ? YES!



FIG. 1. Schematic representation of the canonical form in 1D and 2D. (a) Left and right isometries are represented by arrows whose orientation indicates whether  $A^{\dagger}A = BB^{\dagger} = 1$ . We view the isometry as an RG-like procedure from the large Hilbert space (incoming arrows) to the smaller one (outgoing arrows). In the case of higher-rank tensors, the contraction  $A^{\dagger}A = 1$  is always over all the incoming arrows. (b) A 1D MPS can be brought into a mixed canonical form with orthogonality center  $\Lambda$ . Note that each dangling physical index implicitly has an incoming arrow. (c) Expectation values of local operators can be directly obtained from  $\Lambda$ . (d) 2D canonical form with "orthogonality hypersurfaces"  $\Lambda$  (column and row highlighted in red). The orthogonality center  $\lambda$  is marked by a red dot. In blue we indicate an example of a subregion with only outgoing arrows, whose boundary map is consequently an isometry.

(red row and column) are isometries:

MPS<sup>2</sup>: all tensors except those in 'orthogonality enter'  $\Lambda$ 



∧ is wave function of the system in an orthonormal basis, because its exterior is an isometry from the physical bonds to the incoming virtual bonds.

This allows local expectation values to be computed as  $\langle \psi | \hat{\delta} | \psi \rangle = \langle \Lambda | \hat{\delta} | \Lambda \rangle$  (2) since tensors A, B outside of orthogonality center  $\Lambda$  contract to  $\mathcal{I}$  by isometry condition (1).

Interesting open question: how does variational power of isometric PEPS differ from general PEPS? One restriction is: many of its correlations decay exponentially, because any two-point function along orthogonality center can be reduced to that of the MPS  $\Lambda$ , whose correlations decay exponentially.



$$\Lambda^{\ell} \mathcal{B}^{\ell+1} = \mathcal{A}^{\ell} \Lambda \mathcal{B}^{\ell+1} = \mathcal{A}^{\ell} \Lambda^{\ell+1}$$
(3)

FIG. 2. The Moses move. (a) The orthogonality hypersurface  $\Lambda^{\ell}$  is split into the product of a left isometry  $A^{\ell}$  and a zerocolumn state  $\Lambda$  with no physical indices. The unzipping is performed by successively applying the splitting procedure shown in panel (b). The legs of the center site  $\lambda$  are grouped into a tripartite state  $|\alpha \beta \rangle$  which is "split" into three tensors in two steps: first find  $|\alpha \beta \rangle \approx u_0 U^{\dagger} |\alpha \beta_{\iota}, \beta_{\kappa} \rangle$  for an initial guess of the isometry  $\overline{u}_0$  and unitary U which minimizes the entanglement across the vertical bond highlighted in red; second set  $a = \overline{u}_0 U^{\dagger}$  and split  $|\alpha \beta_{\iota}, \beta_{\kappa} \rangle$  in two via SVD. The resulting a comprise the tensors in  $A^{\ell}$ , and the choice of U will produce a  $\Lambda$ with minimal vertical entanglement.

At central cite (red dot), three 'regions' meet: top ( $\ll$ ), left/bottom ( $\beta$ ), bottom/right ( $\chi$ ). We need to split three-partite entanglement into two-partite entanglement, top/left ( $\alpha', \beta$ ) vs. bottom-right ( $\beta_{\alpha'}, \chi$ ). Needed: the optimal isometry B which 'splits' the composite index  $\beta$  into two sub-indices  $\beta_{L}$ ,  $\beta_{R}$ 



General question: find U which splits given system into two minimally entangled subsystems:

$$|\psi\rangle = |\psi\rangle_{R}|\beta'_{N}|\omega\rangle_{L}\psi^{R}\beta'\gamma \xrightarrow{\ell} |\psi\rangle = U|\psi\rangle = |\psi\rangle_{R}|\beta_{R}\rangle|\beta_{L}|\omega\rangle_{L}\psi^{R}\beta_{L}\beta_{R}\gamma$$

$$\beta'_{M}|\psi\rangle = \sqrt{\frac{1}{2}}\psi^{R}\beta'\gamma \xrightarrow{\ell} |\psi\rangle = \psi^{R}|\psi\rangle = |\psi\rangle_{R}|\beta_{R}\rangle|\beta_{L}|\varphi\rangle = \psi^{R}|\psi\rangle = \psi^{R}|\psi\rangle$$

$$\beta'_{M}|\psi\rangle = \sqrt{\frac{1}{2}}\psi^{R}|\psi\rangle = \psi^{R}|\psi\rangle = \psi^{R}|\psi\rangle = \psi^{R}|\psi\rangle = \psi^{R}|\psi\rangle = \psi^{R}|\psi\rangle$$

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$$\beta'_{L}|\psi\rangle = \psi^{R}|\psi\rangle$$

$$\beta'_{L}|\psi\rangle$$

Tool: construct reduced density matrix,  $\hat{\beta}_L = T_{r_R} I \tilde{4} \times \tilde{4} I$ 

 $S_{LR}^{(l)}$ 

and choose U such that it minimizes von Neumann (or Shannon) entropy:

$$S_{LR}^{(1)}(\tilde{p}_{L}) = - \operatorname{Tr} \tilde{p}_{L} \log_{2} \tilde{p}_{L} \qquad (9)$$

(8)

is always 
$$\geq \circ$$
  
is maximal if all weights are equal,  $\Rightarrow |\tilde{\psi}\rangle$  is 'maximally entangled'  
is minimal if one weight = 1, all others zero,  $\Rightarrow |\tilde{\psi}\rangle$  is 'product state'  $\begin{pmatrix} (\circ) \\ (\circ) \end{pmatrix}$ 

$$\tilde{\beta}_{L} = \bigcap_{\substack{i=1\\i\neq i}}^{i+1} \tilde{\beta}_{L} = \stackrel{i=1\\i\neq i}{\underset{\substack{i=1\\i\neq i}}{\underset{\substack{i=1\\i\neq i}}{\underset{\substack{i=1\\i\atop i=1}}{\underset{\substack{i=1\\i\neq i}}{\underset{\substack{i=1\\i\neq i}}{\underset{\substack{i=1\\i\neq i}}{\underset{\substack{i=1\\i\neq i}}{\atop\substack{i=1\\i\atop i}}{\atopi=1\\i\atop i}}{\atop\substack{i=1\\i\atop i}}{\atop\substack{i=1\\i\atop i}}{\atopi=1\atopi\atop i}}{\atopi=1\atopi\atop i}}{\atopi=1\atopi\atop i}}{\atopi=1\atopi\atop i}}{\atopi=1\atopi\atop i}}{\atopi=1\atopi\atop i=1\atopi\atop i}}{\atopi=1\atopi\atop i}$$

Practical problem: von Neumann entropy is a highly non-linear function of reduced density matrix, there is no straightforward way to minimize it. Alternative: consider Rényi entropies!

Rényi entropy [Rényi1961] :

$$S^{(\alpha)}(p) = \frac{1}{1-\alpha} \log \left[ T_F p^{\alpha} \right], \quad 0 \le \alpha \le \infty$$
 (12)

 $S_{L/R}^{(\alpha)}(\tilde{\rho}_L)$  for some  $\alpha$ , e.g.  $\alpha = z$ 

Rényi entropy has properties similar to the von Neumann entropy. It reduces to the latter for  $\alpha \rightarrow 1$ :

$$\begin{bmatrix} \operatorname{Proof:} S_{LR}^{(\alpha)}(\rho) = \frac{1}{1-\alpha} \log_2 \left[ \operatorname{Tr}(\rho \cdot \rho^{\alpha-1}) \right] = \frac{1}{1-\alpha} \log_2 \left[ \operatorname{Tr}(\rho e^{(\alpha-1)} \ln \rho) \right] \\ \xrightarrow{\alpha \to 1} \frac{1}{1-\alpha} \log_2 \left[ \operatorname{Tr}\left( \frac{\rho \cdot \left[ 1 + (\alpha-1) \ln \rho + \mathcal{O}((\alpha-1)^2) \right] \right] \right] \\ \left[ \operatorname{use} \operatorname{Tr}\rho = 1 \right] = \frac{1}{1-\alpha} \log_2 \left[ 1 + (\alpha-1) \operatorname{Tr}\rho \cdot \ln\rho + \mathcal{O}((\alpha-1)^2) \right] \\ S_{LR}^{(1)}(\rho) = -\operatorname{Tr}\left[ \rho \log_2 \rho \right] \implies \quad [\text{we used:} \log_2 x = \frac{\ln x}{\ln 2}, \ln(1+y) \xrightarrow{y\to 0} y ] \end{bmatrix}$$

Properties (10) hold also for Rényi entropies, hence they also serve as useful entanglement measures.

To minimize L/R entanglement, we may hence minimize

with 
$$\tilde{\beta}_{L} = \prod_{i=1}^{i+1} \tilde{\beta}_{L} = \sum_{i=1}^{i} \prod_{j=1}^{i+1} \cdots \prod_{j=1}^{i+1} \prod_{j=1}^{i+$$

This constrained nonlinear optimization problem can not be solved directly.

But it can be solved iteratively via line	earization: [Evenbly2009, Sec. IV], [Evenbly2017, Sec. III], TNR.	3
Define environment of 🛛 🕺 via	$Z_2 = t Tr \left[ \int_{\mathcal{U}} \otimes \mathcal{U} \right]$	(17)
Do SVD on environment of $~$ $^{\!$	$\Gamma_u = \hat{u} \tilde{s} \tilde{v}^{\dagger}$	(18)
and update U by the prescription	$u' = \hat{v}\hat{u}^{\dagger}$ :	(19)



(23)







with A, B, C given by:

ß



[Zaletel2020]

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FIG. 3. The MPS to MPS<sup>2</sup>-algorithm: (a) The MPS  $\Lambda^{1:L_x}$ for an  $L_x \times L_y$  strip is fed into the MM by treating the legs of the first column as the left ancilla and the remaining columns as the right ancilla to obtain  $\Lambda^{1:L_x} = A^1 \Lambda^{2:L_x}$ . The renormalized wavefunction  $\Lambda^{2:L_x}$  is then reshaped by viewing the legs of the second column as physical, and the remaining as right-ancilla. Applying the MM again, we can repeat to obtain a canonical TNS. (b) Entanglement entropy  $S_{\ell}$  for the sequence of orthogonality centers (highlighted in pink) after  $\ell$  iterations. y runs from bottom right, to top right, to top left. (c)  $S_{\ell}$  for a cut at  $y \sim L_y/2$ , compared against the bulk area law determined from DMRG.  $L_{\gamma} = 6$ ,  $L_{\gamma} = 20$ 

0.3 b) right top 0.2  $S_{\rho}(y)$ 0.1 MM iter MM 2 area law area law 5 10 15 20 25 0 2 3 4 5 l y

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 $\ell \qquad \qquad \text{left. (c) } S_\ell \text{ for a cut at } y \sim L_y/2, \text{ compared against the bulk} \\ \text{area law determined from DMRG. } L_y = 6, \quad L_y = 20$ 

(a) Start with 'fat' MPS  $\Lambda$ , where each 'site' contains the Use MM to iteratively 'peal off' columns of the wavefunction, producing an MPS<sup>2</sup>.

(b) Entanglement entropy  $S_{\ell}(\gamma)$  for cuts across  $\bigwedge$  (cut runs at fixed  $\gamma$ ), after iteration step  $\ell$ .



(3)

In 'right-region'  $(y < L_y)$ ,  $S_{\ell}$  decreases with  $\ell$ , since  $\Lambda^{\ell:L_x}$  becomes 'thinner'. (c) After initial delay,  $S_{\ell}$  reflects area law:  $S_{\ell}(y = L_y/z) \sim s |\partial A| \sim s(L_x - \ell)$ 

Thus pealing off an isometric column from  $\Lambda$  removes from it a 'unit' 5 of horizontal entanglement.

Initial delay is expected, because any two vertically-entangled degrees of freedom will individually have some entanglement with their horizontal neighbors. The isometries  $\bowtie$  can fully remove them from right-region of  $\land$  only after their entire support is to the left of  $\land$ .

The entanglement removed from right-region of  $\Lambda$  by the isometries A is redistributed to the top-region of  $\Lambda$ , where it is encoded as horizontal entanglement. Its magnitude, given by  $S_{\ell}$  for a vertical cut through the top-region of  $\Lambda$ , is of order of the entanglement 'unit' s.

For  $l = L_{y}$  (= 6), smoothly matches up between right/top regions (despite anisotropic algorithm!)