Tensor Networks, RNNs and Weighted Automata

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Outline

1 An Introduction to Tensor Networks

- 2 Weighted Automata Vs. RNNs
- 3 Tensor Network Models for Sequences
- A Tensor Network View of the Spectral Learning Algorithm

An Introduction to Tensor Networks

Tensors



$$\begin{split} \mathbf{M} \in \mathbb{R}^{d_1 \times d_2} & \mathcal{T} \in \mathbb{R}^{d_1 \times d_2 \times d_3} \\ \mathbf{M}_{ij} \in \mathbb{R} \text{ for } i \in [d_1], j \in [d_2] & (\mathcal{T}_{ijk}) \in \mathbb{R} \text{ for } i \in [d_1], j \in [d_2], k \in [d_3] \end{split}$$

Tensors: Multiplication with Matrices







 $\mathbf{AMB}^{\top} \in \mathbb{R}^{m_1 \times m_2}$

 $\mathcal{T} imes_1 \mathbf{A} imes_2 \mathbf{B} imes_3 \mathbf{C} \in \mathbb{R}^{m_1 imes m_2 imes m_3}$

ex: If $\mathcal{T} \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ and $\mathbf{A} \in \mathbb{R}^{m_1 \times d_1}$, $\mathbf{B} \in \mathbb{R}^{m_2 \times d_2}$, $\mathbf{C} \in \mathbb{R}^{m_3 \times d_3}$, then $\mathcal{T} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C} \in \mathbb{R}^{m_1 \times m_2 \times m_3}$ is defined by



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$$(\mathcal{T} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C})_{i_1, i_2, i_3} = \sum_{k_1=1}^{n_1} \sum_{k_2=1}^{n_2} \sum_{k_3=1}^{n_3} \mathcal{T}_{k_1 k_2 k_3} \mathbf{A}_{i_1 k_1} \mathbf{B}_{i_2 k_2} \mathbf{C}_{i_3 k_3}$$

for all $i_1 \in [d_1], i_2 \in [m_2], i_3 \in [d_3]$.





Matrix product:

$$\underline{m} \land \underline{n} \land \underline{B} \not p \qquad (AB)_{i_1,i_2} = \sum_{k=1}^n A_{i_1k} B_{ki_2}$$



Inner product:

$$\mathbf{u} \quad \mathbf{v} \quad \mathbf{v} = \sum_{k=1}^{n} \mathbf{u}_{k} \mathbf{v}_{k}$$



$$\mathsf{Edge} \equiv \mathsf{contraction}$$

Inner product between tensors:

$$(\mathcal{S}, \mathcal{V}) = \sum_{i_1=1}^{d_1} \sum_{i_2=1}^{d_2} \sum_{i_3=1}^{d_3} \mathcal{S}_{i_1 i_2 i_3} \mathcal{T}_{i_1 i_2 i_3}$$



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Frobenius norm of a tensor:

$$S \xrightarrow{d_1}_{d_2} S \|S\|_F^2 = \sum_{i_1=1}^{d_1} \sum_{i_2=1}^{d_2} \sum_{i_3=1}^{d_3} (S_{i_1 i_2 i_3})^2$$



Trace of an $n \times n$ matrix:



 $\operatorname{Tr}(\mathbf{M}) = \sum_{i=1}^{n} \mathbf{M}_{ii}$



Weighted Automata Vs. RNNs

Most of what I will talk about today is based on joint work with Tianyu Li (PhD student) and Doina Precup:

- Rabusseau, Guillaume, Tianyu Li, and Doina Precup. "Connecting weighted automata and recurrent neural networks through spectral learning." The 22nd International Conference on Artificial Intelligence and Statistics. PMLR, 2019.
- Li, Tianyu, Doina Precup, and Guillaume Rabusseau. "Connecting Weighted Automata, Tensor Networks and Recurrent Neural Networks through Spectral Learning." arXiv preprint arXiv:2010.10029 (2020).



Tianyu Li:

Weighted Automata Vs. Recurrent Neural Networks



- Weighted automata are "robust" models for sequence data
- Recurrent neural networks can also deal with sequence data
 - Remarkably expressive models, impressive results in speech and audio recognition
 - \ominus Less tractable than WA, limited understanding of their inner working
- Connections between WA and RNN:
 - Can RNN learn regular languages? [Giles et al, 1992], [Avcu et al., 2018]
 - Can we extract finite state machines from RNNs? [Giles et al, 1992], [Weiss et al., 2018], [Ayache et al., 2018]
 - Can we combine FSMs with WA? [Rastogi et al., 2016], [Dyer et al., 2016]
 - To which extent Weighted Automata are linear RNNs?

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- Recall: a Deterministic Finite Automaton (DFA) recognizes a language (subset of Σ^*).



 \hookrightarrow a DFA computes a function $f: \Sigma^* \to \{\top, \bot\}.$

Weighted Automata: States and Weighted Transitions

Example with 2 states and alphabet $\Sigma = \{a, b\}$



slide credits: B. Balle, X. Carreras, A. Quattoni - ENMLP'14 tutorial

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Operator Representation



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- A WA computes a function $f: \Sigma^* \to \mathbb{R}$
- Weighted Automaton: $A = (oldsymbol{lpha}, \{oldsymbol{A}^\sigma\}_{\sigma\in\Sigma}, oldsymbol{\omega})$ where

$$\begin{split} & \boldsymbol{\alpha} \in \mathbb{R}^n \text{ initial weights vector} \\ & \boldsymbol{\omega} \in \mathbb{R}^n \text{ final weights vector} \\ & \mathbf{A}^{\sigma} \in \mathbb{R}^{n \times n} \text{ transition weights matrix for each } \boldsymbol{\sigma} \in \boldsymbol{\Sigma} \end{split}$$

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- A computes a function $f_A : \Sigma^* \to \mathbb{R}$ defined by

$$f_A(\sigma_1\sigma_2\cdots\sigma_k)= oldsymbol{lpha}^{ op}oldsymbol{A}^{\sigma_1}oldsymbol{A}^{\sigma_2}\cdotsoldsymbol{A}^{\sigma_k}oldsymbol{\omega}$$



2nd order RNNs

• Recurrent Neural Network (RNN):

$$(\textbf{x}_1,\textbf{x}_2,\textbf{x}_3,\cdots)\mapsto(\textbf{y}_1,\textbf{y}_2,\textbf{y}_3,\cdots)$$

• Vanilla RNN:

$$\mathbf{h}_t = g(\mathbf{U}\mathbf{x}_t + \mathbf{V}\mathbf{h}_{t-1}), \quad \mathbf{y}_t = g(\mathbf{M}\mathbf{h}_t)$$

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• Second-order RNN [Giles et al., NIPS'90]:

$$\mathbf{h}_t = g(\boldsymbol{\mathcal{W}} \times_2 \mathbf{x}_t \times_3 \mathbf{h}_{t-1})$$

 \rightarrow order 2 multiplicative interactions: $[\mathbf{h}_t]_i = g\left(\sum_{j,k} \mathcal{W}_{ijk}[\mathbf{x}_t]_j[\mathbf{h}_{t-1}]_k\right)$.

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→ order 2 multiplicative interactions: $[\mathbf{h}_t]_i = g\left(\sum_{j,k} \mathcal{W}_{ijk}[\mathbf{x}_t]_j[\mathbf{h}_{t-1}]_k\right)$. \hookrightarrow (side note) 2nd order RNN subsume vanilla RNN Weighted Automata and Recurrent Neural Networks

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Weighted Automata and Recurrent Neural Networks

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Weighted Automata and Recurrent Neural Networks

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Theorem

WAs are expressively equivalent to second-order linear RNNs for computing functions over sequences of discrete symbols.

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- But 2-RNNs can compute functions over sequences of continuous vectors (e.g., word embeddings), what about WAs?
- \hookrightarrow We can extend the definitions of WAs to continuous vectors!

Continuous WA / linear 2-RNN

Definition

A continuous WA is a tuple $A = (\alpha, \mathcal{A}, \omega)$ where

 $oldsymbol{lpha} \in \mathbb{R}^n$ initial weights vector $oldsymbol{\omega} \in \mathbb{R}^n$ final weights vector $oldsymbol{\mathcal{A}} \in \mathbb{R}^{n imes d imes n}$ is the transition tensor.

A computes a function $f_A : (\mathbb{R}^d)^* \to \mathbb{R}$ defined by



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- \hookrightarrow We can extend the definitions of WAs to continuous vectors!
 - Can we learn linear 2-RNNs from data?
 - * Over sequences of discrete symbols?
 - $\,\hookrightarrow\,$ Yes: spectral learning of WA
 - * Over sequences of continuous vectors?
 - \hookrightarrow Yes: technical contribution of [AISTATS'19]
- Extension to tree models:
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 - ► Continuous extension of WTA and spectral learning algorithm.

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- What do linear counterparts of neural sequential models (LSTMs, bi-directionnal RNNs, etc.) correspond to?
- Spectral initialization of RNNs (ongoing work of Maude Lizaire).
- More accurate map of equivalences between WA and RNNs (e.g. Multiplicative interaction RNNs are special case of 2nd order RNNs)...

Tensor Network Models for Sequences

• Tensor Train decomposition [Oseledets, 2011]:



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• If the ranks are all the same $(R_1 = R_2 = \cdots = R)$, can represent a vector of size 2^n with $\mathcal{O}(nR^2)$ parameters!

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- If the ranks are all the same $(R_1 = R_2 = \cdots = R)$, can represent a vector of size 2^n with $\mathcal{O}(nR^2)$ parameters!
- We can also efficiently perform operations on TT tensors:
 - Inner product, sum, component-wise product, ... all in time linear in n for vectors of size dⁿ.

Tensor Train / Matrix Product States



• We can parameterize linear classification models with MPS [Stoudenmire & Schwab, 2016]:

$$f(\boldsymbol{\mathcal{X}}) = \operatorname{sign}(\langle \boldsymbol{\mathcal{W}}, \boldsymbol{\mathcal{X}} \rangle) = \operatorname{sign}\left(\begin{array}{c} \mathbf{\mathcal{G}}_{1} \xrightarrow{R} \mathbf{\mathcal{G}}_{3} \xrightarrow{R} \mathbf{\mathcal{G}}_{3} \\ \mathbf{\mathcal{X}} \end{array} \right)$$

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• We can also model probability distributions with MPS [Han et al., 2018]:

$$\mathbb{P}(\mathcal{X}) = \underbrace{\begin{array}{c} \mathcal{G}_1 \xrightarrow{R} \mathcal{G}_2 \xrightarrow{R} \mathcal{G}_3 \xrightarrow{R} \mathcal{G}_4 \\ \mathcal{X} \end{array}}_{\mathcal{X}}$$

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MPS for sequence modeling

• We can also use MPS to model functions and distributions over fixed length sequences:

$$\mathbb{P}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) = \begin{pmatrix} \mathbf{G}_1 & \mathbf{F}_1 & \mathbf{G}_2 & \mathbf{F}_2 & \mathbf{G}_3 & \mathbf{F}_1 & \mathbf{G}_4 \\ \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & \mathbf{x}_4 \end{pmatrix} \text{ or } \mathbb{P}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) = \begin{pmatrix} \mathbf{G}_1 & \mathbf{F}_2 & \mathbf{F}_2 & \mathbf{G}_3 & \mathbf{F}_2 & \mathbf{G}_4 \\ \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & \mathbf{x}_4 \end{pmatrix}^2$$

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 \hookrightarrow How to model distributions over variable length sequences?

Uniform MPS

• **uniform MPS** (uMPS) decomposition \equiv MPS with same core at each site:

$$\underbrace{\mathcal{W}}_{\begin{array}{c} d \end{array}} = \underbrace{\boldsymbol{\alpha}}_{R} \underbrace{\mathcal{A}}_{R} \underbrace{\mathcal{A}}$$

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• With uMPS, we can model functions and distributions over variable length sequences:

 $\,\hookrightarrow\,$ Nothing else than the continuous WA we defined previously!

Guillaume Rabusseau

Tensor networks, RNNs and Weighted Autom

• A uMPS is given by a tuple ($\alpha \in \mathbb{R}^n, \mathcal{A} \in \mathbb{R}^{n \times d \times n}, \omega \in \mathbb{R}^n$) and maps any sequence of vectors $\mathbf{x}_1, \cdots, \mathbf{x}_k \in \mathbb{R}^d$ to a scalar:



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- If the inputs are one-hot encoding, $uMPS \equiv Weighted Automata (generalization of HMMs)$
 - ▶ \hookrightarrow If the probability of a sequence is $f(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_k)^2 \equiv$ Quadratic weighted automata (Bailly, 2011) / MPS from quantum physics

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- Linear second order RNNs \equiv uMPS
- For a thorough discussion of connections between uMPS, stochastic processes and automata, see

Srinivasan, S., Adhikary, S., Miller, J., Rabusseau, G. and Boots, B.

Quantum Tensor Networks, Stochastic Processes, and Weighted Automata (AISTATS 2021).

- Versatile sampling algorithm:
 - We can exactly sample from a uMPS/WFA distribution projected onto the support of a regular language / context free grammar.

Jacob Miller, Guillaume Rabusseau, and John Terilla. *Tensor Networks for Language Modeling.* arXiv preprint arXiv:2003.01039 (AISTATS 2021).

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- Training uMPS/WFA with word embeddings for language modeling (work of Jacob Miller).
- Learning dynamics in uMPS/WFA trained by gradient based method could provide theoretical insights on training RNN.

A Tensor Network View of the Spectral Learning Algorithm

Hankel matrix

- We consider the case where inputs are sequences of discrete symbols:
 - Σ a finite alphabet of size d (e.g. $\{a, b\}$)
 - Σ^* strings on Σ (e.g. *abba*)
 - A uMPS computes a function $f: \Sigma^* \to \mathbb{R}$:

$$f(\sigma_1\cdots\sigma_k) = \frac{\alpha}{\int_{d}^{n} \frac{\partial}{\partial t} \int_{d}^{n} \frac{\partial}{\partial t} \int_{d}^{n} \frac{\partial}{\partial t} \int_{d}^{n} \frac{\partial}{\partial t} \int_{d}^{n} \frac{\partial}{\partial t} \frac{\partial}{\partial t} \int_{d}^$$

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• $\mathbf{H}_f \in \mathbb{R}^{\Sigma^* \times \Sigma^*}$: Hankel matrix of $f : \Sigma^* \to \mathbb{R}$

• Definition: prefix p, suffix $s \Rightarrow (\mathbf{H}_f)_{p,s} = f(ps)$

	а	Ь	aa	ab		
а	f(aa) f(ba)	f(ab)]	
Ь		f(bb)				
aa	f(aaa)	f(aab)				
ab	÷	÷	÷	÷	÷	
÷	:	÷		÷	·	

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Spectral Learning of uMPS

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• Fundamental theorem [Carlyle and Paz, 1971; Fliess 1974]:

 $\mathsf{rank}(\mathbf{H}_f) < \infty \Longleftrightarrow f$ can be computed by a uMPS

Spectral Learning of uMPS

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 $\mathsf{rank}(\mathbf{H}_f) < \infty \Longleftrightarrow f$ can be computed by a uMPS

 \hookrightarrow Proof is constructive! From a low rank factorization of \mathbf{H}_f we can recover a uMPS computing f...

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 \rightarrow Efficient and consistent learning algorithms for uMPS/weighted automata [Hsu et al., 2009; Bailly et al. 2009; Balle et al., 2014, ...].
Spectral Learning: when does it work?

Theorem (Exact case)

If the set of prefixes and suffixes $\mathcal{P}, \mathcal{S} \subset \Sigma^*$ are such that

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 we have

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 \hookrightarrow When f is a probability distribution, we get an unbiased and consistent estimator! [c.f. work of B. Balle]

- Let $f:\Sigma^* o \mathbb{R}$ be the function computed by a uMPS $(\alpha, \mathcal{A}, \omega)$.
- Define the ℓ th order Hankel tensor $\mathcal{H}^{(\ell)} \in \mathbb{R}^{\Sigma \times \Sigma \times \dots \times \Sigma}$ by

$$\mathcal{H}^{(\ell)}_{\sigma_1,\sigma_2,\cdots,\sigma_\ell} = f(\sigma_1\sigma_2\cdots\sigma_\ell)$$

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$$\underbrace{\mathcal{H}^{(\ell)}}_{d \mid d \cdots \mid d} = \underbrace{\left(\begin{array}{c} \alpha & \overset{n}{\longrightarrow} &$$

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• It follows that the Hankel matrix $\mathbf{H}_f \in \mathbb{R}^{\Sigma^* \times \Sigma^*}$ can be decomposed in sub-blocks of low uMPS rank:

		а	Ь	aa	ab	
$H_f =$	а	f(aa) f(ba) f(aaa)	f(ab)]
	Ь	f(ba)	f(bb)			
	aa	f(aaa)	f(aab)			
	ab	÷	÷	÷	÷	÷
	÷		÷	÷	÷	·]

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		а	Ь		ab				a b	aa ab	ba bb	aaa aab	
a	а	f(aa)	f(ab)					a b	$\mathcal{H}^{(2)}_{\Sigma \times \Sigma}$	H	(3) Σ×Σ²	$\mathcal{H}^{(4)}_{\Sigma imes \Sigma^3}$	
	Ь	f(ba)	f(bb)					аа					
	aa	f(aaa)	f(aab)					aa ab ba	$\mathcal{H}^{(3)}_{\Sigma^2 imes \Sigma}$	$\mathcal{H}^{(4)}_{\Sigma^2 imes \Sigma^2}$	$\mathcal{H}^{(5)}_{\Sigma^2 imes \Sigma^3}$		
	ab	÷	÷	÷	÷	÷		bb					
	:		÷					aaa aab	$\mathcal{H}^{(4)}_{\Sigma^3 \times \Sigma}$	$\mathcal{H}_{\Sigma}^{()}$	5) $3 \times \Sigma^2$	$\mathcal{H}^{(6)}_{\Sigma^3 \times \Sigma^3}$	
	•	·	•	•	•	• -		÷	L:	:		:	

In the spectral algorithm, we need to estimate
 (h_P)_u = f(u), (h_S)_v = f(v), (H_{P,S})_{u,v} = f(uv) and (H_{P,Σ,S})_{u,σ,v} = f(uσv)
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- \hookrightarrow All the quantities we need to estimate are matricization of low uMPS rank tensors!
 - This leads to an efficient learning algorithm:
 - Estimate $\mathcal{H}^{(\ell)}, \mathcal{H}^{(2\ell)}, \mathcal{H}^{(2\ell+1)}$ directly in the MPS/TT format
 - Use the spectral algorithm to convert the MPS decomposition into a uniform MPS model.

Spectral Learning \equiv Conversion from MPS to uMPS

• Let $f: \Sigma^* \to \mathbb{R}$ be a function for which we have access to an MPS decomposition of the Hankel tensors $\mathcal{H}^{(\ell)}, \mathcal{H}^{(2\ell)}, \mathcal{H}^{(2\ell+1)}$.

 \rightarrow f can be a probability distribution, or the wave function of a quantum system.

Spectral learning algorithm = efficient way to recover a uMPS computing *f* from the 3 Hankel tensors

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- Spectral learning algorithm \equiv efficient way to recover a uMPS computing *f* from the 3 Hankel tensors
- \hookrightarrow From $\mathcal{H}^{(\ell)}, \mathcal{H}^{(2\ell)}, \mathcal{H}^{(2\ell+1)}$, we can compute the value of f on sequences of arbitrary length!

 $[\]rightarrow$ f can be a probability distribution, or the wave function of a quantum system.

$$\textbf{Input:} \ \boldsymbol{\mathcal{H}}^{(\ell)} = \begin{array}{c} A_1 \quad A_2 \quad \cdots \quad A_{l-1} \quad A_l \\ \boldsymbol{\varphi} - \boldsymbol{\varphi} - \boldsymbol{\varphi} - \boldsymbol{\varphi} \end{array}, \ \boldsymbol{\mathcal{H}}^{(2\ell)} = \begin{array}{c} B_1 \quad B_2 \quad \cdots \quad B_{2l-1} \quad B_{2l} \\ \boldsymbol{\varphi} - \boldsymbol{\varphi} - \boldsymbol{\varphi} - \boldsymbol{\varphi} \end{array}, \ \boldsymbol{\mathcal{H}}^{(2\ell+1)} = \begin{array}{c} C_1 \quad C_2 \quad \cdots \quad C_{2l} \quad C_{2l+1} \\ \boldsymbol{\varphi} - \boldsymbol{\varphi} - \boldsymbol{\varphi} - \boldsymbol{\varphi} - \boldsymbol{\varphi} \end{array}$$

Output: uMPS $(\alpha, \mathcal{A}, \omega)$ computing f

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1. Left-orthonormalisation of B_1, \cdots, B_ℓ (first half of $\mathcal{H}^{(2\ell)}$)

2. Right-orthonormalisation of $B_{\ell+1}, \cdots, B_{2\ell}$ (second half of $\mathcal{H}^{(2\ell)}$)

$$- \underbrace{B_{l+1}B_{l+2}\cdots B_{2l-1}B_{2l}}_{- \underbrace{O} - \underbrace{O$$

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3. Computation of the uMPS parameters:



Spectral Learning with Tensor Networks

- Recap:
 - More structure than matrix rank in the Hankel matrix.
 - ► When $\mathcal{P} = \mathcal{S} = \Sigma^{\ell}$, the spectral learning algorithm can be performed efficiently in the MPS/TT format.
 - $\hookrightarrow \text{ Time complexity is reduced from } \mathcal{O}\left(n|\Sigma|^{2\ell} + n^2|\Sigma|^{\ell+1}\right) \text{ to } \mathcal{O}\left(n^3\ell|\Sigma|\right).$

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 - \hookrightarrow Time complexity is reduced from $\mathcal{O}\left(n|\Sigma|^{2\ell} + n^2|\Sigma|^{\ell+1}\right)$ to $\mathcal{O}\left(n^3\ell|\Sigma|\right)$.
- Future directions:
 - ► Spectral learning of continuous WA/uMPS for RL (work of Tianyu Li)
 - Similar connections and algorithms can be derived for models on trees
 - What about graphs? (e.g. potential connections between TN and GNN)
 - Lots of connections between quantum TN, probabilistic models, formal languages, machine learning, etc. to explore!
 (e.g., using density matrices to model languages (see work of
 - Tai-Danae Bradley)

That's all, folks!

Thanks for listening! Questions?