

Optimization on Tensor Network Varieties

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Tensor networks

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- Quantum Physics (Quantum Many-body Systems)
- Algebraic Complexity Theory (Algebraic Branching Programs)
- Machine Learning (Linear Networks)
- Algebraic Statistics (Graphical Models)
- Numerical Linear Algebra (Tensor Trains)

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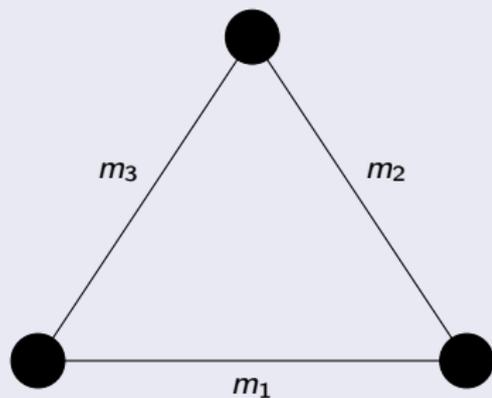
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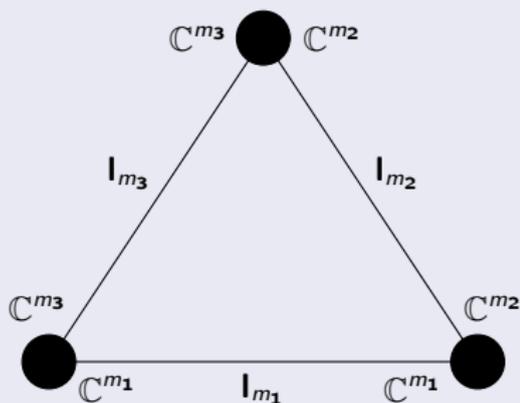
They give rise to

Algebraic varieties with rich representation theoretic structure



Fix a weighted graph $\Gamma = (\mathbf{v}(\Gamma), \mathbf{e}(\Gamma))$ with weights $\mathbf{m} = (m_e : e \in \mathbf{e}(\Gamma))$ called *bond dimensions*. Let $L = \#\mathbf{v}(\Gamma)$.

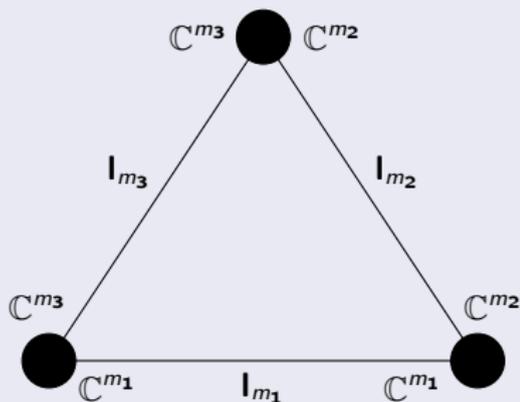
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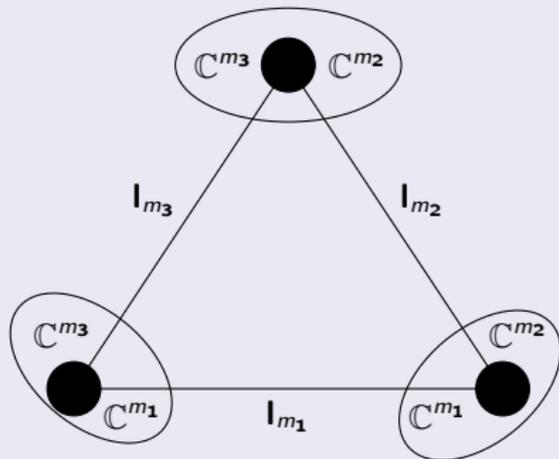
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$$\bigotimes_{v \in \mathbf{v}(\Gamma)} \left[\bigotimes_{e \ni v} \mathbb{C}^{m_e} \right] = \bigotimes_{v \in \mathbf{v}(\Gamma)} W_v$$

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Group together spaces on the same vertex, to obtain a tensor of order L

This is $T(\Gamma, \mathbf{m})$, the graph tensor associated to Γ with bond dimension \mathbf{m} .

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Define

$$\begin{aligned} \Phi : \prod_{v \in \mathbf{v}(\Gamma)} \text{Hom}(W_v, V_v) &\rightarrow V_1 \otimes \cdots \otimes V_L \\ (X_1, \dots, X_L) &\mapsto (X_1 \otimes \cdots \otimes X_L)(T(\Gamma, \mathbf{m})). \end{aligned}$$

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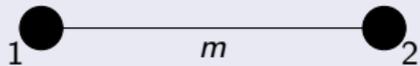
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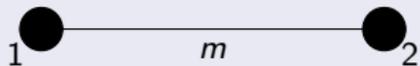
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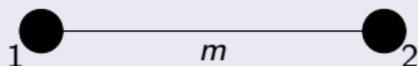
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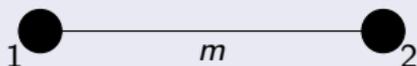
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So

$$\mathcal{TNS}_\Gamma^\circ(m, \mathbf{n}) = \{T \in V_1 \otimes V_2 : \text{rank}(T) \leq m\}$$

In this case $\mathcal{TNS}_\Gamma(m, \mathbf{n}) = \mathcal{TNS}_\Gamma^\circ(m, \mathbf{n})$.

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- Irreducibility and invariancy under rescaling:

We can think of (the projectivization of) $\mathcal{TNS}_\Gamma(\mathbf{m}, \mathbf{n})$ as a projective irreducible variety in $\mathbb{P}(V_1 \otimes \cdots \otimes V_L)$.

Who cares?

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Strategy. Given $T \in \mathbb{C}^n \otimes \cdots \otimes \mathbb{C}^n$

- choose a graph Γ and small \mathbf{m} , so that evaluating $T(\Gamma, \mathbf{m})$ is easy;
- hope to find linear maps X_1, \dots, X_L such that

$$(X_1 \otimes \cdots \otimes X_L)(T(\Gamma, \mathbf{m})) = T;$$

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Questions

- What if $T \in \mathcal{TNS}_\Gamma(\mathbf{m}, \mathbf{n}) \setminus \mathcal{TNS}_\Gamma^\circ(\mathbf{m}, \mathbf{n})$?
- How large is this boundary?
- How to sample points from the boundary?

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Theorem. [Landsberg, Qi, Ye'12; Barthel, Lu, Friesecke'21]

- If Γ does not have cycles, then $\mathcal{TNS}_\Gamma^\circ(\mathbf{m}, \mathbf{n})$ is Zariski closed.
- If Γ does have cycles, then “we expect”

$$\mathcal{TNS}_\Gamma(\mathbf{m}, \mathbf{n}) \setminus \mathcal{TNS}_\Gamma^\circ(\mathbf{m}, \mathbf{n}) \neq \emptyset$$

unless it is empty for trivial reasons (e.g. $\mathcal{TNS}^{\Gamma^\circ}(\mathbf{m}, \mathbf{n})$ fills the space).

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In [Christandl, G., Stilck-França, Werner'20], we determine a new ansatz class with two properties:

- evaluation is *easy*
- the class includes tensors at the boundary

We use the geometry of osculating spaces to $\mathcal{TNS}_\Gamma(\mathbf{m}, \mathbf{n})$.

Restriction and degeneration

Consider two tensors $S \in W_1 \otimes \cdots \otimes W_L$ and $T \in V_1 \otimes \cdots \otimes V_L$.

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Degeneration: S degenerates to T if there exist $X_i(\varepsilon) : W_i \rightarrow V_i$ depending on ε such that

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With these definitions:

- $\mathcal{TNS}^{\Gamma^\circ}(\mathbf{m}, \mathbf{n})$ is the set of all restrictions of $T(\Gamma, \mathbf{m})$;
- $\mathcal{TNS}^{\Gamma}(\mathbf{m}, \mathbf{n})$ is the set of all degenerations of $T(\Gamma, \mathbf{m})$.

Frist ideas to enlarge the ansatz class

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Theorem [classical; CGSW]

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With this strategy, pass from a spanning tree for Γ to the entire Γ .

How do degenerations look like?

Fact. If S degenerates to T , it is possible to choose $X_i(\varepsilon)$ depending polynomially in ε and obtain

$$(X_1(\varepsilon) \otimes \cdots \otimes X_L(\varepsilon))[S] = \varepsilon^a T_0 + \cdots + \varepsilon^{a+e} T_e$$

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Note. From a geometric point of view:

- e is the degree of the approximating curve,
- a is more complicated.

Using e : An interpolation argument

Theorem [Bini; Strassen; CLVW]

Let $T \in \mathcal{TN}\mathcal{S}^\Gamma(m, n)$ with error degree e .

There exists $M \leq (e + 1)m$ such that $T \in \mathcal{TN}\mathcal{S}^{\Gamma^\circ}(M, n)$ for some $M \leq (e + 1)m$.

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Classical fact: Every $e + 1$ generic points on a curve of degree e have the same span as the whole curve.

So, $e + 1$ points on the approximating curve span the limit point!

Increase the bond dimension enough to get $e + 1$ simultaneous restrictions, then interpolate to get the limit point.

The role of a

Recall

$$(X_1(\varepsilon) \otimes \cdots \otimes X_L(\varepsilon))[S] = \varepsilon^a T + \text{higher order terms.}$$

Write

$$X_j(\varepsilon) = X_{j,0} + X_{j,1}\varepsilon + X_{j,2}\varepsilon^2 + \cdots$$

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so that

$$X_1(\varepsilon) \otimes \cdots \otimes X_L(\varepsilon) = \sum_P \left[\sum_{p_1 + \cdots + p_L = P} X_{1,p_1} \otimes \cdots \otimes X_{L,p_L} \right] \varepsilon^P.$$

The role of a

Recall

$$(X_1(\varepsilon) \otimes \cdots \otimes X_L(\varepsilon))[S] = \varepsilon^a T + \text{higher order terms.}$$

Write

$$X_j(\varepsilon) = X_{j,0} + X_{j,1}\varepsilon + X_{j,2}\varepsilon^2 + \cdots$$

so that

$$X_1(\varepsilon) \otimes \cdots \otimes X_L(\varepsilon) = \sum_p \left[\sum_{p_1 + \cdots + p_L = p} X_{1,p_1} \otimes \cdots \otimes X_{L,p_L} \right] \varepsilon^p.$$

Two things must happen:

- for $p < a$, $\left(\sum_{p_1 + \cdots + p_L = p} X_{1,p_1} \otimes \cdots \otimes X_{L,p_L} \right) [S] = 0$,
- for $p = a$, $\left(\sum_{p_1 + \cdots + p_L = a} X_{1,p_1} \otimes \cdots \otimes X_{L,p_L} \right) [S] = T$.

The role of a – cont'd

Consider a vector space \mathbb{C}^{a+1} , with basis $\{v_0, \dots, v_a\}$ and define

$$\chi_{a,L} = \sum_{p_1 + \dots + p_L = a} v_{p_1} \otimes \dots \otimes v_{p_L} \in \mathbb{C}^{a+1} \otimes \dots \otimes \mathbb{C}^{a+1}$$

These are generalizations of tangent vectors to the variety of rank-one tensors in $(\mathbb{C}^{a+1})^{\otimes L}$.

The role of a – cont'd

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Observation. If S degenerates to T with approximation degree a , then T is a restriction of

$$S \boxtimes \chi_{a,L}.$$

The role of a – cont'd

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Observation. If S degenerates to T with approximation degree a , then T is a restriction of

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New ansatz class [CGSW]

Define

$$\partial TNS_{\mathbf{m},n,a}^{\Gamma} = \{\text{all restrictions of } T(\Gamma, \mathbf{m}) \boxtimes \chi_{a,L}\}$$

This contains all degenerations of $T(\Gamma, \mathbf{m})$ with approximation degree a .

Properties of the new ansatz class

New class:

$$\partial\mathcal{TN}\mathcal{S}_{\mathbf{m},\mathbf{n},a}^{\Gamma} = \{ \text{all restrictions of } T(\Gamma, \mathbf{m}) \boxtimes \chi_{a,L} \}$$

- $\partial\mathcal{TN}\mathcal{S}_{\mathbf{m},\mathbf{n},a}^{\Gamma}$ contains tensors at the boundary!

Properties of the new ansatz class

New class:

$$\partial \mathcal{TNS}_{\mathbf{m}, \mathbf{n}, a}^{\Gamma} = \{ \text{all restrictions of } T(\Gamma, \mathbf{m}) \boxtimes \chi_{a, L} \}$$

- $\partial \mathcal{TNS}_{\mathbf{m}, \mathbf{n}, a}^{\Gamma}$ contains tensors at the boundary!
- We prove that *good evaluation properties* of $T(\Gamma, \mathbf{m})$ pass to $T(\Gamma, \mathbf{m}) \boxtimes \chi_{a, L}$:
 - $\chi_{a, L}$ has minimal *border rank*;
 - $\chi_{a, L}$ has a small tensor network representation.

Summary and final remarks

- Tensor network representations are useful to evaluate tensors.
- Sometimes, one wants to evaluate tensors at the boundary.
- We can enlarge the bond dimension to include elements of the boundary.
- We can define a new ansatz class which includes elements of the boundary.
- In both cases, we can control the *overhead in the complexity* of evaluation.

Summary and final remarks

- Tensor network representations are useful to evaluate tensors.
- Sometimes, one wants to evaluate tensors at the boundary.
- We can enlarge the bond dimension to include elements of the boundary.
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- In both cases, we can control the *overhead in the complexity* of evaluation.

What next?

The new classes contain many new tensors, not just boundary ones.

- How much bigger is the new class?
- What are the new tensors?
- Are they useful?