

Markov quantum networks

quantum states recoverability from bipartite correlations via
Jaynes principle

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Introduction: why quantum GM?

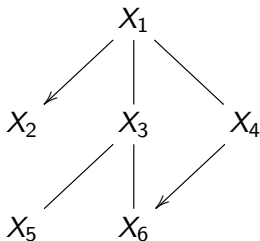
Classical graphical models

Classical RVs $\mathcal{X} = \{X_1, \dots, X_n\} \rightarrow p(\mathcal{X})$?

Representation via *graphical models* (GM)
(Bayesian Networks, Markov random fields)



estimator $\tilde{p}(\mathcal{X}) \approx \{X_1, \dots, X_n\}$



- *direct dependencies*: efficient information collection;
- *conditional independences*: factorization;
- *maximum entropy*: maximal unbiased with the provided info.

Example: BN $\tilde{p}(\mathcal{X}) = \prod p(X_i | \text{pa}(X_i))$

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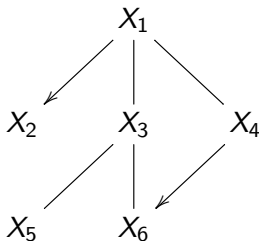
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Quantum graphical models

Quantum system $\mathbb{X} = \{X_1, \dots, X_n\} \rightarrow \rho_{\mathbb{X}} \in \mathcal{L}(\otimes_{i=1}^n \mathcal{H}_{X_i})$?

$$\mathbb{X} \xrightarrow[\text{QM}]{1 \text{ postulate}} \rho \in \mathcal{L}(\mathcal{H}_{\mathbb{X}}) : \rho \succ 0, \rho = \rho^\dagger, \text{Tr}[\rho] = 1.$$

$$\ll \underbrace{\mathbb{X} \dots \mathbb{X}}_{\{\theta_i\} \text{ complete}} \xrightarrow[\text{tomography}]{\text{quantum}} ! \rho_{\mathbb{X}} = f(\theta_i, \langle \theta_i \rangle)$$

Θ_i complete d^{2n} , $d = \dim \mathcal{H}_{X_i}$, $i = 1, \dots, n$

$$\ll \underbrace{\mathbb{X} \dots \mathbb{X}}_{\{\theta_i\} \text{ partial : poly}(n)} \xrightarrow[\text{machine learning}]{\text{quantum}} \tilde{\rho}_{\mathbb{X}} = R(\theta_i, \langle \theta_i \rangle)$$

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Introduction: why quantum GM?

Quantum graphical models

Quantum system $\mathbb{X} = \{X_1, \dots, X_n\} \rightarrow \tilde{\rho}_{\mathbb{X}} \in \mathcal{L}(\otimes_{i=1}^n \mathcal{H}_{X_i})$?

Probability distributions (PD) $p(\mathcal{X}) \rightarrow$ Density operators (DO) $\rho_{\mathbb{X}}$

Quantum graphical model?

$$\tilde{\rho}_{\mathbb{X}} = \mathcal{R}(\{\langle \theta_i \rangle, \theta_i\})$$

efficient recovery procedure

the most likely DO

set of partial information

Problem statement

To compress quantum states finding an **efficient recovery procedure** for learning the DO that maximizes the von Neumann entropy given the set of direct correlations of the unknown quantum state.

Outlines

Problem formalization

- ◁ The maximum entropy estimator, first neighbours approximation, classical Hardness results and restriction to trees.

The tripartite case

- ◁ Result1: efficient procedure for quantum Markov Chains (QMC);
- ◁ Result2: Nec and suff condition for two bipartite marginals compatibility with a QMC.

The multipartite case

- ◁ Result1: quantum Markov networks and Petz factorization;
- ◁ Result2: Nec and suff condition for a tree structured set of bipartite marginals compatibility with a quantum Markov tree.

Conclusion

- ◁ Hints about further results and take home message.

Problem formal statement

The maximum entropy estimator

The maximum entropy-estimate is the least biased estimate possible on the given information, i.e. it is maximally noncommittal with regard to missing information.

$$\begin{array}{ll} \text{PD } p(X) & \longrightarrow \text{DO } \rho_X \quad [\text{Jaynes 1957}] \\ \text{Shannon entropy} & \longrightarrow \text{von Neumann entropy} \\ \text{H}(X) := -\sum_i p(x_i) \log p(x_i) & \longrightarrow \text{S}(X) := -\text{Tr}[\rho_X \log \rho_X] \end{array}$$

Bipartite correlations

- ◀ approximation frequently used in multiparticles physics;
- ◀ efficient measurements collection:

$$\rho_{\mathbb{X}} \text{ on } \mathcal{H}_{\mathbb{X}} = \bigotimes_{i=1}^n \mathcal{H}_{X_i} : \quad O(d^{2n}) \longrightarrow O(n^2 d^4) d := \dim \mathcal{H}_{X_i} < \infty;$$

- ♠ set reduction of the learnable QS ($|GHZ\rangle, \dots$)

Problem formal statement

partial measurements and estimator

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
PD $p(X)$ \longrightarrow DO ρ_X [Jaynes 1957]

Shannon entropy \longrightarrow von Neumann entropy
 $H(X) := -\sum_i p(x_i) \log p(x_i)$ $S(X) := -\text{Tr}[\rho_X \log \rho_X]$

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Problem formalization

Maximum entropy DO given bipartite marginals

$$\mathcal{H}_{X_i} = \text{span} \{ \Lambda_j^{(X_i)}; j = 0, \dots, d-1 \} :$$

$$\Lambda_0^{(X_i)} = \mathbb{I}_{X_i}; \quad \Lambda_j^{(X_i)} = \left(\Lambda_j^{(X_i)} \right)^\dagger; \quad \text{Tr} \left[\Lambda_j^{(X_i)} \right] = 0 \quad \forall j \neq 0$$

measurements $\{ \Lambda_k^{(X_i)} \otimes \Lambda_l^{(X_j)} \otimes \mathbb{I}_{X \setminus X_i X_j} \}$

Maximum entropy principle:

$$\tilde{\rho}_{X_1, \dots, X_n} = \frac{1}{Z} \exp \left(\sum_{\substack{k=0 \\ i^2+j^2 \neq 0}}^{d_{X_i}^2-1} \sum_{l=0}^{d_{X_j}^2-1} \lambda_{kl} \Lambda_k^{(X_i)} \otimes \Lambda_l^{(X_j)} \otimes \mathbb{I}_{X \setminus X_i X_j} \right),$$

$$\{ \lambda_{kl} \} \text{ Lagrange m. : } \text{Tr} \left[\Lambda_k^{(X_i)} \otimes \Lambda_l^{(X_j)} \tilde{\rho} \right] = \alpha_{kl}^{(i,j)}.$$

The set of partial information

Maximum entropy DO given bipartite marginals

$$\mathbb{X} = \{X_1, \dots, X_n\}; \quad \mathcal{H}_{\mathbb{X}} = \bigotimes_{i=1}^n \mathcal{H}_{X_i} = \text{span} \left\{ \bigotimes_{i=1}^n \Lambda_j^{(X_i)} \right\}$$

$$\{ \langle \Lambda_k^{(X_i)} \otimes \Lambda_l^{(X_j)} \rangle = \alpha_{lm}^{(i,j)} \} : \quad \mathcal{C} := \{ \rho_{X_i X_j} = \sum_{kl} \alpha_{lm}^{(i,j)} \Lambda_k^{(X_i)} \otimes \Lambda_l^{(X_j)} \}$$

Maximum entropy principle $\tilde{\rho}_{X_1, \dots, X_n} = \arg \max_{\rho \in \text{Comp}(\mathcal{C})} S(\rho)$

$$\text{Comp}(\mathcal{C}) := \left\{ \rho \in \mathcal{L}(\mathcal{H}_{\mathbb{X}}) : \text{Tr}_{\mathbb{X} \setminus \{X_i, X_j\}}[\rho] = \rho_{X_i X_j}, \forall \rho_{X_i X_j} \in \mathcal{C} \right\}$$

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Maximum entropy DO given bipartite marginals

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$\stackrel{?}{=} R(\{ \rho_{X_i X_j} \})$, $R(\cdot)$ algebraic

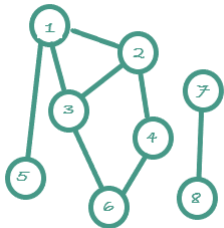
The efficient procedure

Further measurement's set restriction: classical limit

$$\text{PD } \rho(X) \longrightarrow \text{DO } \rho_X$$

Quantum Bayesian network inference

If there is a notion of QBN that generalizes BN, then inferring a QBN cannot be *easier* than inferring a BN (by Cooper reduction).
[P.Mateus 2018]

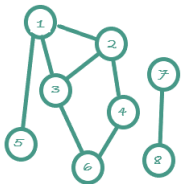


Problem restriction in learning quantum trees:

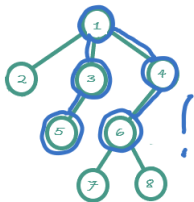
quantum system $\mathbb{X} = \{X_1, \dots, X_n\}$, $\{\rho_{X_i X_j}\}$

$G(\mathbb{X}, E)$ is a tree, $E = \{X_i - X_j, \forall \rho_{X_i X_j}\}$

Classical hardness results



General network



Tree

◀ = $p(X)$ NP-hard [Cooper (1990)]

◀ $\approx \tilde{p}(X)$ NP-hard [Dagum and Luby (1993)]

- = $p(X)$ efficient inference [Edmonds(1967)], [Chow-Liu(1968)]
- efficient optimal tree construction [Edmonds(1967)], [Chow-Liu(1968)]

The efficient procedure

Restriction to quantum trees

$$\{ \rho_{X_i X_j} = \sum_{kl} \alpha_{lm}^{(i,j)} \Lambda_k^{(X_i)} \otimes \Lambda_l^{(X_j)} \} \quad \text{Tree structured}$$

$$\tilde{\rho}_{X_1, \dots, X_n} = \frac{1}{Z} \exp \left(\sum_{\substack{k=0 \\ i^2+j^2 \neq 0}}^{d_{X_i}^2-1} \sum_{l=0}^{d_{X_j}^2-1} \lambda_{kl} \Lambda_k^{(X_i)} \otimes \Lambda_l^{(X_j)} \otimes \mathbb{I}_{\mathbb{X} \setminus X_i X_j} \right),$$

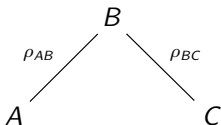
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To compress quantum states finding an **efficient procedure** for learning the DO that maximizes the von Neumann entropy from a **tree-structured set of direct correlations**.

The efficient procedure

The tripartite case

$\{A, B, C\}$ on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$:



$$\left\{ \begin{aligned} \rho_{AB} &= \sum_{kl} A_{kl} \Lambda_k^{(A)} \otimes \Lambda_l^{(B)}, \\ \rho_{BC} &= \sum_{kl} C_{kl} \Lambda_k^{(B)} \otimes \Lambda_l^{(C)} \end{aligned} \right\}$$

$$\tilde{\rho}_{ABC} = \frac{1}{Z_{ABC}} \exp \left(\sum_{\substack{i=0 \\ i^2+j^2 \neq 0}}^{d_A^2-1} \sum_{j=0}^{d_B^2-1} \lambda_{ij} \Lambda_i^{(A)} \Lambda_j^{(B)} + \sum_{i=0}^{d_B^2-1} \sum_{\substack{j=0 \\ i^2+j^2 \neq 0}}^{d_C^2-1} \eta_{ij} \Lambda_i^{(B)} \Lambda_j^{(C)} \right)$$

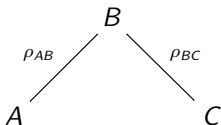
$\{\lambda_{i,j}, \eta_{ij}\}$ Lagrange m.: $\text{Tr}_A [\tilde{\rho}_{ABC}] = \rho_{BC}$, $\text{Tr}_C [\tilde{\rho}_{ABC}] = \rho_{AB}$

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Tripartite case

Quantum Markov chains

Def.: Quantum Markov Chain (QMC)

ρ_{ABC} on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ is a (quantum) Markov Chain $A - B - C$ if \exists a CPTP map $\mathcal{R}_{B \rightarrow BC} : \mathcal{L}(\mathcal{H}_B) \rightarrow \mathcal{L}(\mathcal{H}_{BC})$, recovery map, s.t.

$$\rho_{ABC} = \mathcal{I}_A \otimes \mathcal{R}_{B \rightarrow BC}(\rho_{AB}), \quad [\text{Fawzi2015}]$$

Quantum conditional independence

ρ_{ABC} is a QMC A-B-C if and only if $I_\rho(A : C|B) = 0$ [Hayden2004].

$I_\rho(A : C|B)$ is the quantum conditional mutual Information:

$$I_\rho(\rho_{ABC}) := S(\rho_{AB}) + S(\rho_{BC}) - S(\rho_B) - S(\rho_{ABC}).$$

Tripartite case

Entropic characterisation of QMCs

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For a QMC A-B-C the strong sub-additivity of von Neumann entropy $S(\rho_{ABC}) + S(\rho_B) \geq S(\rho_{AB}) + S(\rho_{BC})$ [Lieb1973] holds with equality.



A QMC ρ_{ABC} A-B-C maximizes the von Neumann entropy given its two bipartite marginals ρ_{AB} and ρ_{BC} .

Tripartite case

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The tripartite case

Algebraic recovery for QMCs

The Petz' recovery map

A QMC ρ_{ABC} A-B-C always admits as recovery channel the *Rotated Petz Recovery Map* [Petz1986,Wilde2015]:

$$\mathcal{P}_{B \rightarrow BC}^{(t)}(\Theta_B) := \rho_{BC}^{\frac{1+t}{2}} \left(\rho_B^{-\frac{1+t}{2}} \Theta_B \rho_B^{-\frac{1+t}{2}} \right) \rho_{BC}^{\frac{1+t}{2}}$$

For $t=0$ CPTP map *Petz Recovery Map* or *transpose map*

$$\mathcal{P}_{B \rightarrow BC}(\cdot) = \rho_{BC}^{\frac{1}{2}} \rho_B^{-\frac{1}{2}} (\cdot) \rho_B^{-\frac{1}{2}} \rho_{BC}^{\frac{1}{2}}$$

⇓

A QMC ρ_{ABC} A-B-C can be recovered algebraically from its marginals ρ_{AB} and ρ_{BC} via Petz Recovery map:

$$\tilde{\rho}_{ABC} = \rho_{BC}^{\frac{1}{2}} \rho_B^{-\frac{1}{2}} \rho_{AB} \rho_B^{-\frac{1}{2}} \rho_{BC}^{\frac{1}{2}} = \rho_{AB}^{\frac{1}{2}} \rho_B^{-\frac{1}{2}} \rho_{BC} \rho_B^{-\frac{1}{2}} \rho_{AB}^{\frac{1}{2}}$$

Tripartite case: result1

Problem solution for the subset of QMCs

- ◀ A QMC ρ_{ABC} A-B-C maximizes the von Neumann entropy given its two bipartite marginals ρ_{AB} and ρ_{BC} .
- ◀ A QMC ρ_{ABC} A-B-C can be recovered algebraically from its marginals ρ_{AB} and ρ_{BC} via Petz Recovery map.



Theorem 1

Given bipartite marginals quantum states $\rho_{AB} \in \mathcal{L}(\mathcal{H}_{AB})$, $\rho_{BC} \in \mathcal{L}(\mathcal{H}_{BC})$ compatible with a QMC state, say ρ_{ABC} , then the solution to the maximum entropy estimator is $\tilde{\rho}_{ABC} = \rho_{ABC}$. Moreover $\tilde{\rho}_{ABC}$ can be algebraically recovered via the Petz map, concretely:

$$\tilde{\rho}_{ABC} = \rho_{BC}^{\frac{1}{2}} \rho_B^{-\frac{1}{2}} \rho_{AB} \rho_B^{-\frac{1}{2}} \rho_{BC}^{\frac{1}{2}} = \rho_{AB}^{\frac{1}{2}} \rho_B^{-\frac{1}{2}} \rho_{BC} \rho_B^{-\frac{1}{2}} \rho_{AB}^{\frac{1}{2}}.$$

Tripartite case

the compatibility problem

Def.: Compatible quantum states

$\rho_{AB} \in \mathcal{L}(\mathcal{H}_{AB})$ and $\rho_{BC} \in \mathcal{L}(\mathcal{H}_{BC})$ are compatible if

$$\text{Comp}(\rho_{AB}, \rho_{BC}) \neq 0$$

Classical scenario

$\{A, B, C\}$ classical RVs, finite domains, $p(A, B)$ and $p(B, C)$ PDs.

Prop: classical compatibility $p(A, B)$ and $p(B, C)$ are compatible iff $\sum_a p(A = a, B) = \sum_c p(C = c, B)$.

Prop: compatibility with a Markov chain

$\mathcal{C} = \{p(A, B), p(B, C)\} \Rightarrow \exists p(A, B, C) \in \text{Comp}(\mathcal{C})$ s.t. $A \perp C|B$

Tripartite case

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Classical scenario

$\{A, B, C\}$ classical RVs, finite domains, $p(A, B)$ and $p(B, C)$ PDs.

Prop: classical compatibility $p(A, B)$ and $p(B, C)$ are compatible iff $\sum_a p(A = a, B) = \sum_c p(C = c, B)$.

Prop: compatibility with a Markov chain

$\mathcal{C} = \{p(A, B), p(B, C)\} \Rightarrow \exists p(A, B, C) \in \text{Comp}(\mathcal{C})$ s.t. $A \perp C|B$

Tripartite case

the compatibility problem

Def.: Compatible quantum states

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Quantum scenario

Hard problem: quantum compatibility or marginal problem

$$\mathbb{X} = \{X_1, \dots, X_n\} : \text{Comp}\{\rho_{\mathcal{J}} \mid \mathcal{J} \in \mathbb{X}\} \neq 0 \text{ np-complete [Liu2007].}$$

Problem: compatibility with a QMC

$$\mathcal{C} = \{\rho_{AB}, \rho_{BC}\} \stackrel{?}{\Rightarrow} \exists \text{QMC } \tilde{\rho}_{ABC} \in \text{Comp}(\mathcal{C})$$

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Tripartite case: result2

Compatibility with QMCs

Theorem 2

$\rho_{AB} \in \mathcal{L}(\mathcal{H}_{AB})$, $\rho_{BC} \in \mathcal{L}(\mathcal{H}_{BC})$ are compatible with a QMC A-B-C on \mathcal{H}_{ABC} iff both the following conditions hold:

- i) $\text{Tr}_A[\rho_{AB}] = \text{Tr}_C[\rho_{BC}] = \rho_B$;
- ii) $\Theta_{ABC} := (\mathbb{I}_A \otimes \rho_{BC}^{1/2}) (\mathbb{I}_A \otimes \rho_B^{-1/2} \otimes \mathbb{I}_C) (\rho_{AB}^{1/2} \otimes \mathbb{I}_C)$ is normal.

Corollary

The space of bipartite marginals ρ_{AB} and ρ_{BC} compatible with a QMC on \mathcal{H}_{ABC} is strictly included in the space of bipartite compatible marginals with at least one tripartite state on \mathcal{H}_{ABC} .

Multipartite case

Quantum Markov trees

$$\mathbb{X} = \{X_1, \dots, X_n\}; \quad \mathcal{H}_{\mathbb{X}} = \bigotimes_{i=1}^n \mathcal{H}_{X_i} = \text{span} \left\{ \bigotimes_{i=1}^n \Lambda_j^{(X_i)} \right\}$$

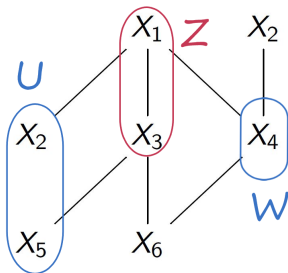
$$\mathcal{C} = \{ \rho_{X_i X_j} \in \mathcal{L}(\mathcal{H}_{X_i X_j}) : i \neq j \in \{1, \dots, n\} \} \text{ s.t.}$$

$\mathcal{G}_{\mathcal{C}}$ is a spanning tree.

Maximum entropy principle:

$$\tilde{\rho}_{X_1, \dots, X_n} = \arg \max_{\rho \in \text{Comp}(\mathcal{C})} S(\rho) \stackrel{?}{=} P(\{\rho_{X_i X_j}\})$$

Quantum Markov networks



Quantum Markov network

Quantum graph $(\mathcal{X}, \{\mathcal{H}_X\}_{X \in \mathcal{X}}, \rho, \mathcal{G})$, where ρ satisfies the global Markov property: $\forall U, W \subset \mathcal{X}$ s.t. \exists a separator Z for U and W

$$I_\rho(U : W | Z) = 0.$$

Markov quantum tree: Markov quantum net with \mathcal{G} a tree.

Markov quantum tree

Efficient recovery

$$\mathbb{X} := \{X_1, \dots, X_n\}, \mathcal{H} = \bigotimes_{i=1}^n \mathcal{H}_{X_i}, \rho \in \mathcal{L}(\mathcal{H}), \rho \succ 0,$$

$$\mathcal{C} := \{\rho_{X_i X_j} \in \mathcal{L}(\mathcal{H}_{X_i X_j}), i \neq j \in \{1, \dots, n\} : \text{Tr}_{\mathbb{X} \setminus \{X_i X_j\}}[\rho] = \rho_{X_i X_j}\}$$

Petz factorization

ρ is factorizable via Petz if its square root $\Theta \in \mathcal{L}(\mathcal{H})$, i.e. $\rho = \Theta \Theta^\dagger$, admits a decomposition

$$\Theta = \prod \rho_{X_i X_j}^{\frac{1}{2}} \left(\mathbb{I}_{X_i} \otimes \rho_{X_j}^{-\frac{1}{2}} \right) \otimes \mathbb{I}_{\mathbb{X} \setminus \{X_i X_j\}}.$$

Result1

A Markov quantum tree admits a factorization in terms of its bipartite marginals via Petz.

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compatibility condition

$$\mathbb{X} := \{X_1, \dots, X_n\}, \quad \mathcal{H} = \bigotimes_{i=1}^n \mathcal{H}_{X_i},$$

Constructive ordering

$$\mathcal{C} := \{\rho_{X_k X_{j_k}} \in \mathcal{L}(\mathcal{H}_{X_k X_{j_k}}), k \in \{2, \dots, n\}, j_k \in \{1, \dots, k-1\}\}$$

Result2

The estimator $\tilde{\rho} := \arg \max_{\rho \in \text{Comp}(\mathcal{C})} S(\rho)$ exists (i.e. $\text{Comp}(\mathcal{C}) \neq \emptyset$) and moreover factorizes over its bipartite marginals according to the Petz-factorization iff

$$I_\rho(X_k : \text{ad } X_{j_k} | X_{j_k}) = 0, \text{ ad } X_{j_k} \in \{X_1, \dots, X_{k-1}\} \quad \forall k = 3, \dots, n.$$

Markov quantum tree

compatibility condition

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Conclusion

The problem:

To compress quantum states finding an *efficient procedure* for learning *the most likely DO* given a *chosen set of partial information* about the unknown multipartite quantum system.

Solution:

The subset of multipartite DO compatible with a quantum Markov tree can be efficiently approximated by its closest quantum Markov tree via Petz factorization. The tree can be efficiently determined via the quantum generalization of the Chow-Liu algorithm.

Take home message

Classical graphical models techniques for discrete RV, ranged on finite domains, can be extended to the set of multipartite density operators, invertible and defined on finite dimensional Hilbert spaces, that form a *quantum Markov network*.

S. Di Giorgio, B.Mera, P.Mateus - March 2019
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