Refuting spectral compatibility of quantum marginals

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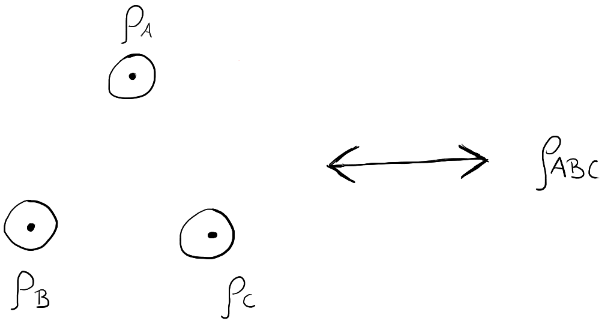
Quantum marginal problem I

Problem.

Given a set of marginals (reduced density matrices), does there exist a joint state?



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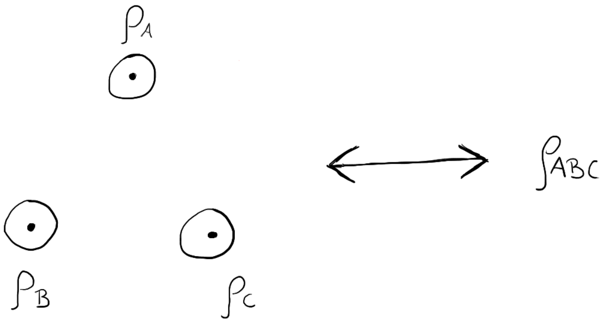

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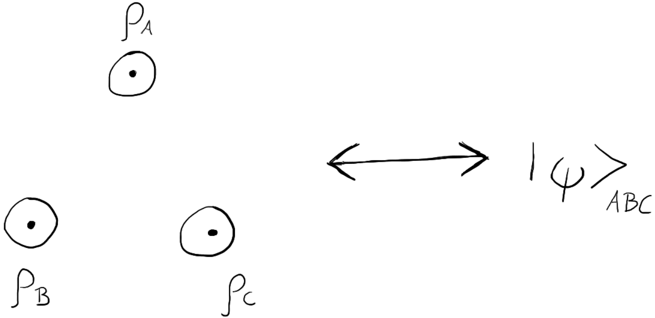
Given a set of marginals (reduced density matrices), does there exist a **pure** joint state?



Rather easy: $|\psi\rangle_{ABC}$ exists, iff linear constraints on local spectra $\lambda(\rho_A)$, $\lambda(\rho_B)$, $\lambda(\rho_C)$ are fulfilled.[1]

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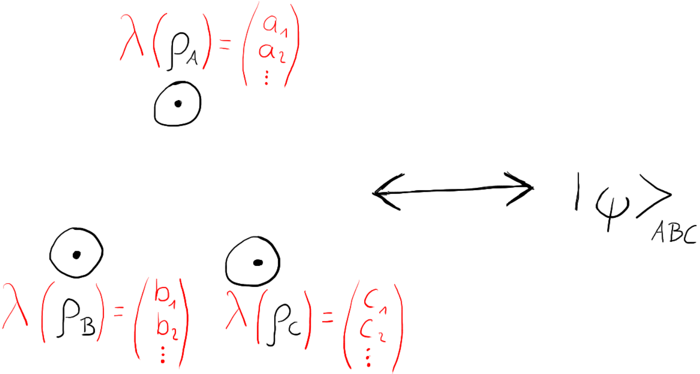

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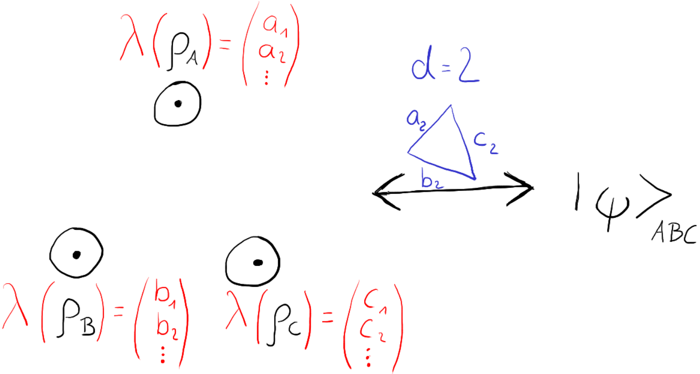

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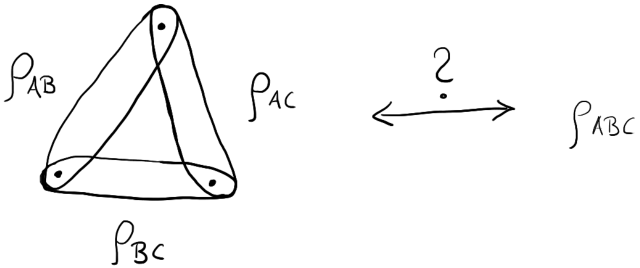

Rather easy: Formulate semidefinite program:

$$\text{find } \rho_{ABC}$$
$$\text{s.t. } \rho_{ABC} \geq 0$$
$$\mathrm{Tr}_A(\rho_{ABC}) = \rho_{BC}, \cdots$$

Efficiently solvable, ~~sometimes~~ usually infeasibility can be certified.

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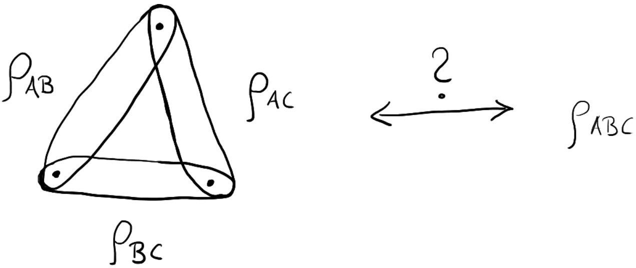

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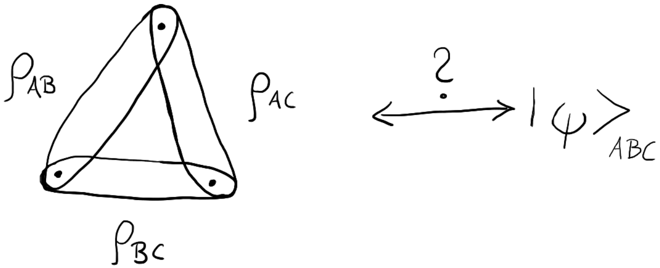

Hard (QMA-complete)![2]

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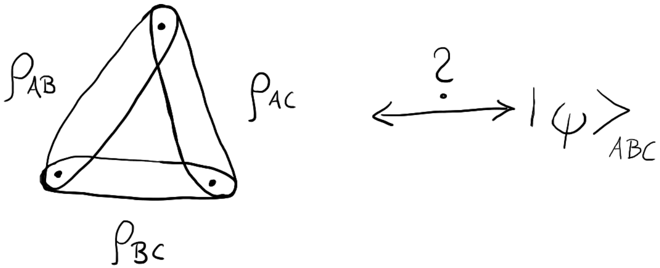

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Why should we care?

Compatibility problem is relevant:

- Quantum chemistry: properties of fermionic system are governed by its one- and two-body marginals (Pauli principle + generalizations).
- Monogamy of Entanglement: $E(\rho_{AB}) + E(\rho_{AC}) + E(\rho_{BC}) \leq \text{const.}$
- Existence of Quantum Error Correcting Codes/Absolutely Maximally Entangled States.[3]
- [Can be decided by a hierarchy of semidefinite programs[4]]

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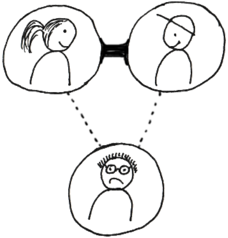

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ARTICLE

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A complete hierarchy for the pure state marginal problem in quantum mechanics

Xiao-Dong Yu [1✉], Timo Simnacher [1], Nikolai Wyderka [1,2], H. Chau Nguyen [1] & Otfried Gühne [1]

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But often we could care less!

Often, we do not care about the actual marginals, but only their **spectrum**!
E.g., entropic inequalities

- Strong subadditivity of von Neumann Entropy $S(\rho) = -\operatorname{Tr}(\rho \log \rho) = -\sum_i \lambda_i \log \lambda_i$:

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- Other entropies, e.g.,
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Spectral marginal problem

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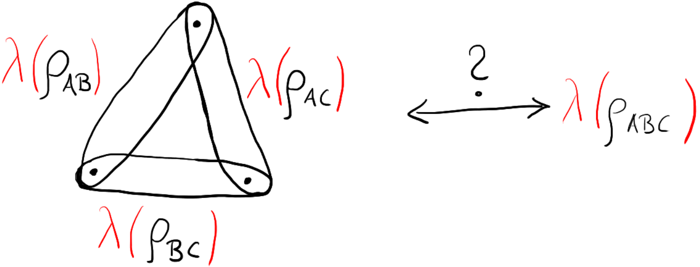
Given a set of spectra of marginals, does there exist a joint state with given spectrum?



Equivalent to sum-of-hermitian matrices problem: Given hermitian matrices A, B and C, which spectra $\underbrace{\lambda(A),\lambda(B),\lambda(A+B)}_{\text{Horn's inequalities}},\lambda(C),\lambda(A+C),\lambda(B+C),\lambda(A+B+C)$ are compatible?

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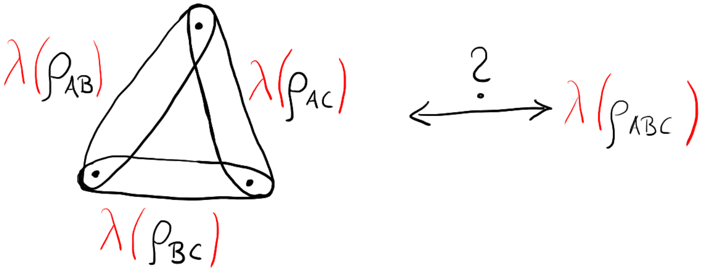

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A first trial I

Can we formulate it as a semidefinite program?

1. Replace $\lambda(\rho) = (\lambda_1, \ldots, \lambda_d)$ by $(\,\mathrm{Tr}(\rho), \mathrm{Tr}(\rho^2), \ldots, \mathrm{Tr}(\rho^d)\,)$ $\rightarrow$ input data is $\mathrm{Tr}(\rho_A^\ell) \equiv q_A^{(\ell)}, \ldots, \mathrm{Tr}(\rho_{AB}^\ell) \equiv q_{AB}^{(\ell)}, \ldots, \mathrm{Tr}(\rho_{ABC}^\ell) \equiv q_{ABC}^{(\ell)}$
2. Write down "SDP":

$$
\begin{aligned}
\text{find}\ & \rho_{ABC} \\
\text{s.t.}\ & \rho_{ABC} \geq 0, \\
& \mathrm{Tr}(\rho_{ABC}^\ell) = q_{ABC}^{(\ell)} \quad \forall \ell, \\
& \mathrm{Tr}[\mathrm{Tr}_C(\rho_{ABC})^\ell] = q_{AB}^{(\ell)} \quad \forall \ell, \\
& \ldots
\end{aligned}
$$

is not linear!

A first trial II

3. Use trick: Let $\sigma \in S_k$ be a permutation, s.t.

$$\sigma \left|v_1\right\rangle \otimes \left|v_2\right\rangle \otimes \cdots \otimes \left|v_k\right\rangle = \left|v_{\sigma^{-1}(1)}\right\rangle \otimes \left|v_{\sigma^{-1}(2)}\right\rangle \otimes \cdots \otimes \left|v_{\sigma^{-1}(k)}\right\rangle$$

   For example:

$$(143)(2) \left|v_1\right\rangle \otimes \left|v_2\right\rangle \otimes \left|v_3\right\rangle \otimes \left|v_4\right\rangle$$

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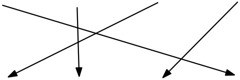

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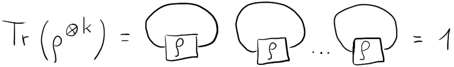

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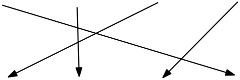

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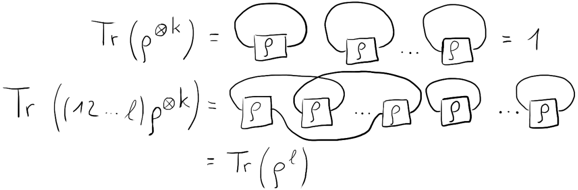

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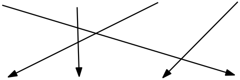

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   Then: $\mathrm{Tr}((1 \ldots \ell)\rho^{\otimes k}) = ... = \mathrm{Tr}(\rho^{\ell})$.

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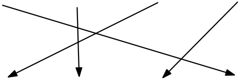

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4. Multipartite:

$$\mathrm{Tr}\left[\begin{matrix}(1\ldots\ell)_A\\ \otimes\\ (1\ldots\ell)_B\\ \otimes\\ ()_C\end{matrix}\cdot \boxed{\rho_{ABC}} \otimes \ldots \otimes \boxed{\rho_{ABC}}\right] = \mathrm{Tr}[(1\ldots\ell)_{AB}\rho^{\otimes k}] = \mathrm{Tr}[\rho_{AB}^{\ell}]$$

A first trial III

Combine tricks:

$$\begin{aligned}
\text{find}\ & \rho_{ABC} \\
\text{s.t.}\ & \rho_{ABC} \geq 0, \\
& \mathrm{Tr}[(1\ldots\ell)_{ABC}\,\rho_{ABC}^{\otimes k}] = q_{ABC}^{(\ell)} \quad \forall \ell, \\
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Still not linear!

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$$\begin{aligned} &\text{find } X_k \\ &\text{s.t. } X_k \geq 0, \\ &\quad \mathrm{Tr}[(1\dots\ell)_{ABC} X_k] = q^{(\ell)}_{ABC} \quad \forall \ell, \\ &\quad \mathrm{Tr}[(1\dots\ell)_{AB} X_k] = q^{(\ell)}_{AB} \quad \forall \ell, \\ &\quad \dots \\ &\quad \pi_{ABC} X_k \pi^{-1}_{ABC} = X_k \quad \forall \pi \in S_k \end{aligned}$$

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If SDP is **infeasible** for some k, then this proves **incompatibility** of spectra! But will it detect all incompatible spectra?

Quantum de Finetti theorem

Let X_k be such that for all $m \geq k$, there exists an X_m satisfying

$$\pi X_m \pi^{-1} = X_m \,, \qquad \mathrm{Tr}_{m\setminus k}(X_m) = X_k \,.$$

Then

$$X_k = \int \rho^{\otimes k} \, \mathsf{d}\mu(\rho) \,.$$

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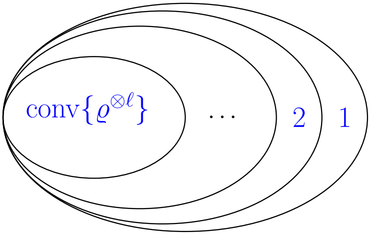
Yields sequence of outer approximations of conv$(\rho^{\otimes k})$



But we want $X_k = \rho^{\otimes k}$!

Quadratic constraints

- If we can demand $\mathrm{Tr}[(1\ldots\ell)_{ABC}X_k] = q^{(\ell)}_{ABC}$, then also

$$\mathrm{Tr}[((1\ldots\ell)(\ell+1\ldots2\ell)_{ABC}X_k] = (q^{(\ell)}_{ABC})^2.$$

- Write

$$\begin{aligned} 0 &= \mathrm{Tr}[[(1\ldots\ell)_{ABC} - q^{(\ell)}_{ABC}][(\ell+1\ldots2\ell)_{ABC} - q^{(\ell)}_{ABC}]X_k] \\ &= \int |\mathrm{Tr}[[(1\ldots\ell)_{ABC} - q^{(\ell)}_{ABC}]\rho^{\otimes\ell}]|^2 \, \mathrm{d}\mu(\rho). \end{aligned}$$

- Average over non-negative numbers $= 0 \Rightarrow$ almost all of them must vanish!

$$\Rightarrow \text{There exists a } \rho_{ABC} \text{ with correct } \mathrm{Tr}(\rho^{\ell}_{ABC})$$

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Result

Add quadratic constraints to hierarchy makes it complete:

Theorem

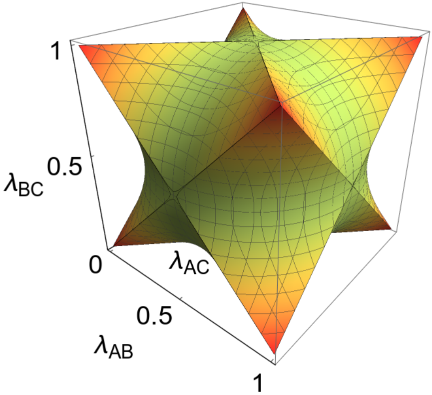
The spectra $\lambda(\rho_{AB}), \lambda(\rho_{AC}), \lambda(\rho_{BC})$ *are compatible iff the SDP*

$$\begin{aligned}
&\textit{find}\, X_k \\
&\textit{s.t.}\, X_k \geq 0, \\
&\quad \mathrm{Tr}[(1\dots\ell)_S X_k] = q_S^{(\ell)}, \\
&\quad \mathrm{Tr}[(1\dots\ell)(\ell+1\dots 2\ell)_S X_k] = (q_S^{(\ell)})^2 \quad \forall \ell = 1,\dots,\dim(\rho_S), S \in \{AB, AC, BC\} \\
&\quad \pi_{ABC} X_k \pi_{ABC}^{-1} = X_k \quad \forall \pi \in S_k
\end{aligned}$$

is feasible for each k.

Example

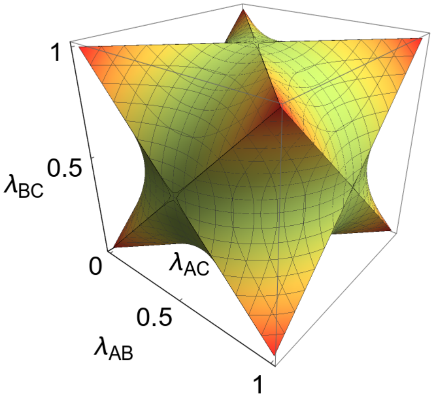
$$\lambda(\rho_{AB}) = \begin{pmatrix} \lambda_{AB} \\ 1-\lambda_{AB} \\ 0 \\ \dots \end{pmatrix} \quad \lambda(\rho_{AC}) = \begin{pmatrix} \lambda_{AC} \\ 1-\lambda_{AC} \\ 0 \\ \dots \end{pmatrix} \quad \lambda(\rho_{BC}) = \begin{pmatrix} \lambda_{BC} \\ 1-\lambda_{BC} \\ 0 \\ \dots \end{pmatrix}, k=2$$



Example

How good is it?

- If $\rho_{ABC} = |\psi\rangle\langle\psi|_{ABC}$, then $\lambda(\rho_{AB}) = \lambda(\rho_C), \ldots$
- $\lambda(\rho_A), \lambda(\rho_B), \lambda(\rho_C)$ compatible iff



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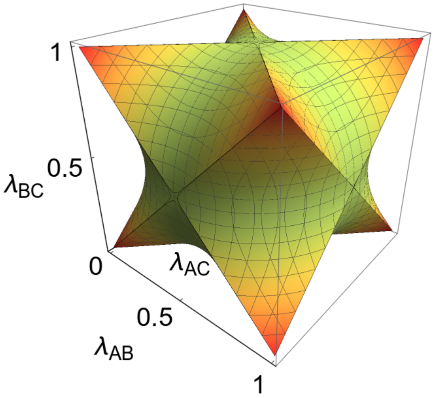
- If $\rho_{ABC} = |\psi\rangle\langle\psi|_{ABC}$, then $\lambda(\rho_{AB}) = \lambda(\rho_C), \ldots$
- $\lambda(\rho_A), \lambda(\rho_B), \lambda(\rho_C)$ compatible iff 



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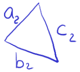
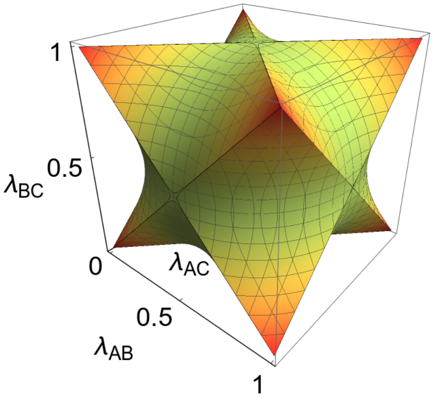
- $\lambda(\rho_A), \lambda(\rho_B), \lambda(\rho_C)$ compatible iff 



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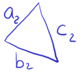
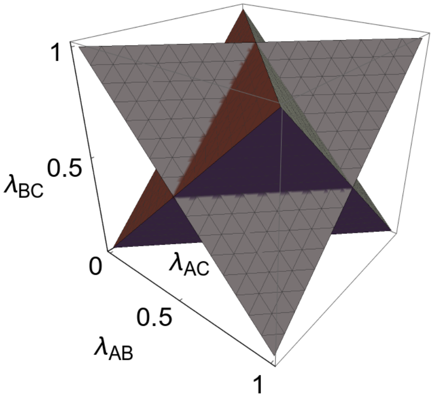
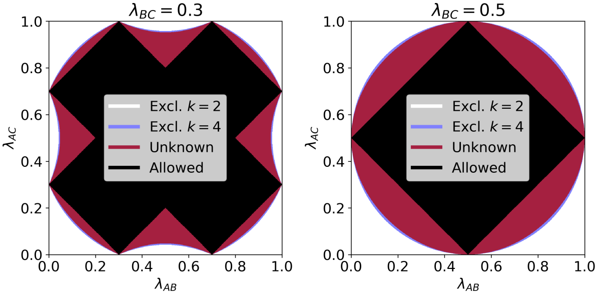
- $\lambda(\rho_A), \lambda(\rho_B), \lambda(\rho_C)$ compatible iff 



Example

More copies?

- Use symmetry reduction to check $k = 2, 3, 4, (5)$:



- Use dual representation to obtain purity inequalities:

$k = 2$: For all tripartite states (Shadow ineq.),

$$1 - \mathrm{Tr}(\rho_{AB}^2) - \mathrm{Tr}(\rho_{AC}^2) + \mathrm{Tr}(\rho_{BC}^2) \geq 0.$$

$k = 4$: For all tripartite states,

$$1 - \frac{1}{20}[15\,\mathrm{Tr}(\rho_{AB}^2) - 3\,\mathrm{Tr}(\rho_{AB}^4) + 15\,\mathrm{Tr}(\rho_{AC}^2) - 3\,\mathrm{Tr}(\rho_{AC}^4) + 9\,\mathrm{Tr}(\rho_{BC}^2) - 16\,\mathrm{Tr}(\rho_{BC}^3) + 3\,\mathrm{Tr}(\rho_{BC}^4)] \geq 0.$$

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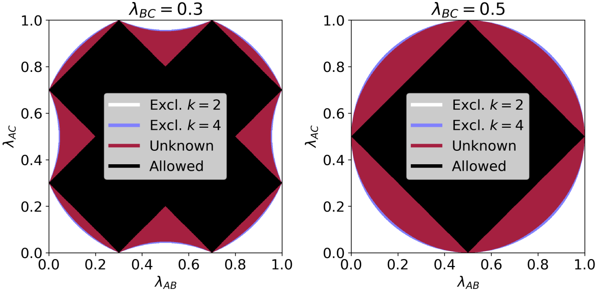

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Summary/Outlook

- Checking spectral compatibility of marginals is hard, but important (entropic inequalities, bounds on local unitary invariants...).
- Complete SDP hierarchy allows to check it numerically.
- Sometimes, analytical results are possible using the dual representation.

- In some cases, enough information to completely fix X_k: Compatibility problem $\Leftrightarrow$ Entanglement problem.

Thank you for your attention!

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arXiv:2211.06349

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Backup: Symmetries

Problem: SDP is too big.

Identify symmetries!

Single system

$$\mathrm{Tr}\left[(1\dots\ell)\rho^{\otimes k}\right] = \mathrm{Tr}\left[(1\dots\ell)U^{\otimes k}\rho^{\otimes k}{U^{\otimes k}}^{\dagger}\right]$$

n-partite system

$$\mathrm{Tr}\left[(1\dots\ell)_A\,\rho^{\otimes k}\right]$$
$$= \mathrm{Tr}\left[(1\dots\ell)_A\,(U_1\otimes\cdots\otimes U_n)^{\otimes k}\rho^{\otimes k}{(U_1\otimes\cdots\otimes U_n)^{\otimes k}}^{\dagger}\right]$$

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$$[U^{\otimes k}, \sigma] = 0 \qquad \forall \sigma \in S_k\,, U \in \mathcal{U}(d)\,.$$

k copies of single system

$$(\mathbb{C}^d)^{\otimes k} \simeq \bigoplus_{\substack{\lambda \vdash k \\ \text{height}(\lambda) \leq d}} \mathcal{U}_\lambda \otimes \mathcal{S}_\lambda\,.$$

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This allows to check positivity of the dual variable in the irreps only!

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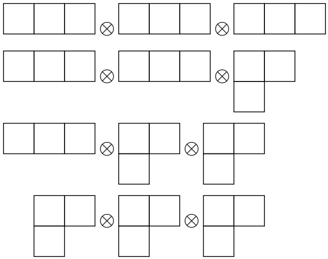
Backup: In practice

- Sagemath for irreducible representations.
- Choose unitary representation. $R(\sigma^{-1}) = R(\sigma)^T$
- Take every combination of irreps. E.g. 3 copies of 3-qubit state

Irreducible Representation	dimension
	$1 \cdot 1 \cdot 1 = 1$ $1 \cdot 1 \cdot 2 = 2$ $1 \cdot 2 \cdot 2 = 4$ $2 \cdot 2 \cdot 2 = 8$

Backup: Effects

1. Reduces SDP size massively
2. Incompatibility witnesses can certify incompatibility in all dimensions (*"dimension-free"*) if $k \leq d$.
3. Incompatibility witnesses are purity / moment inequalities.

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