Improved local models and new Bell inequalities via Frank-Wolfe algorithms

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Discrete Optimization x Machine Learning

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Berlin Mathematics Research Center

What is this talk about?

Introduction

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truly quantum (non-local) or just classical (local) in complicated form?

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Today:

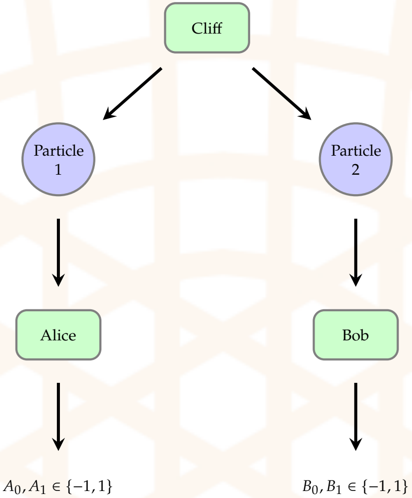
- An optimization perspective on the non-locality problem
- Frank–Wolfe approach (what else did you expect?)
- Myriad of new non-locality thresholds
- Improvement of the Grothendieck constant of order 3

(Hyperlinked) References are not exhaustive; check references contained therein.

Let's play a game

Bell Experiment - Classical Setup

- Cliff prepares pair of particles with properties $a_0, a_1 \in \{-1, 1\}$ for Particle 1 and properties $b_0, b_1 \in \{-1, 1\}$ for Particle 2, sends one to Alice and one to Bob.



Assumptions.
Realism: Properties exist irrespective of observation.
Locality: Alice's and Bob's measurements do not influence each other.

[Bell, 1964, Nielsen and Chuang, 2001]

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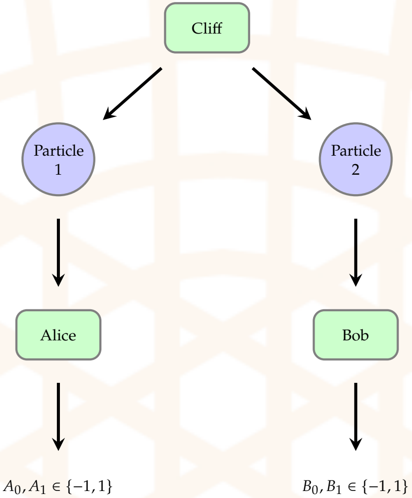

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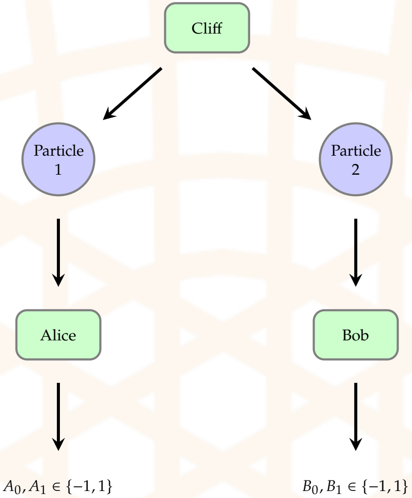
- Alice and Bob pick one of their measurements randomly, results in 4 combinations: $(A_0, B_0), (A_0, B_1), (A_1, B_0), (A_1, B_1)$



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as either $b_0 = b_1$ or $b_0 = -b_1$.

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Note.
For the initiated: corresponds to a facet of the corresponding cut/correlation polytope.
For the uninitiated: don't ask.

Quantum Mechanics = Linear algebra on steroids: Quick Recap

- Ket and Bra. Elements in a Hilbert space, e.g., $|\phi\rangle$, can be represented as $|\phi\rangle = \sum_{i=0}^{N-1} \alpha_i |i\rangle$, with associated bra as $\langle\phi| = (\alpha_0^*, \ldots, \alpha_{N-1}^*)^T$.
- Representation. $|\phi\rangle = \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_{N-1} \end{pmatrix}$ and $\langle\phi| = (\alpha_0^*, \ldots, \alpha_{N-1}^*)$.
- Linearity. $|a\phi + b\gamma\rangle = a|\phi\rangle + b|\gamma\rangle$ and $\langle a\phi + b\gamma| = a^* \langle\phi| + b^* \langle\gamma|$.
- Inner Product: $\langle i \mid j\rangle = \delta_{ij}$ and $\langle\psi \mid \phi\rangle = (\beta_0^*, \ldots, \beta_{N-1}^*)^T \cdot \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_{N-1} \end{pmatrix} = \sum_{i=0}^{N-1} \beta_i^* \alpha_i$.
- Density Matrix: $|\phi\rangle\langle\phi|$ for a state $|\phi\rangle$.
- Observable M: Orthogonal projection matrices P_i with $I = \sum_i P_i$ and $P_i^2 = P_i$ and $M = \sum_i \lambda_i P_i$ with $\lambda_i \in \mathbb{R}$ (distinct) outcomes.
- Expected value of measurement with M: $\mathrm{tr}(M|\phi\rangle\langle\phi|)$.

[See my blog for a short overview]

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- Cliff prepares bipartite quantum state:

$$|\phi\rangle \doteq \frac{1}{\sqrt{2}}(|0\rangle\,|1\rangle - |1\rangle\,|0\rangle),$$

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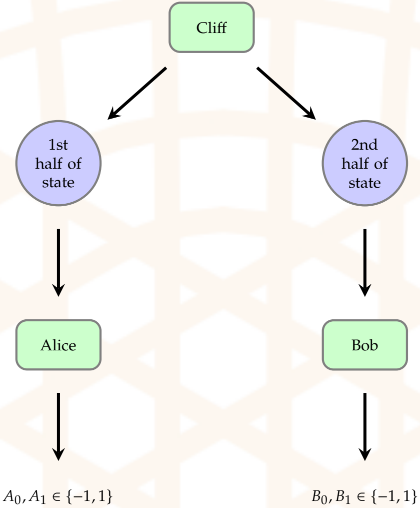

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$$A_0 \doteq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad A_1 \doteq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

  and

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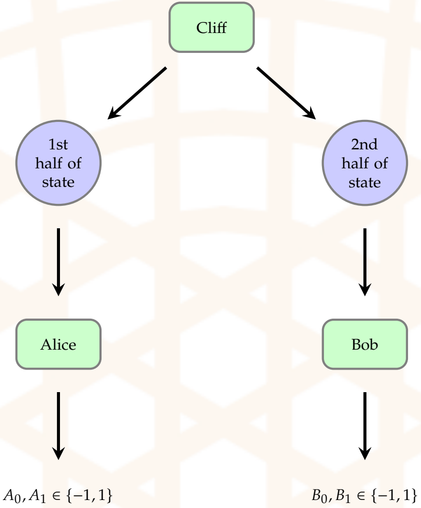

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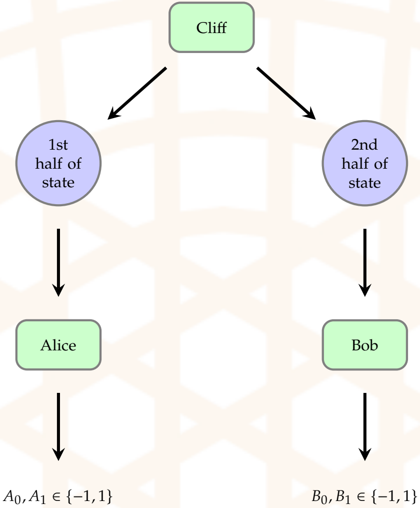

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Bell's Theorem - Quantum Correlations

Observe. Expected values of measurements:

$$\operatorname{tr}(A_0 \otimes B_0 \left|\phi\right\rangle \left\langle\phi\right|) = \frac{1}{\sqrt{2}} \qquad \operatorname{tr}(A_0 \otimes B_1 \left|\phi\right\rangle \left\langle\phi\right|) = \frac{1}{\sqrt{2}}$$

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Same linear combination of expected values as before:

$$\begin{aligned} &\mathrm{tr}(A_0 \otimes B_0 \left|\phi\right\rangle \left\langle\phi\right|) + \mathrm{tr}(A_0 \otimes B_1 \left|\phi\right\rangle \left\langle\phi\right|) \\ &+ \mathrm{tr}(A_1 \otimes B_0 \left|\phi\right\rangle \left\langle\phi\right|) - \mathrm{tr}(A_1 \otimes B_1 \left|\phi\right\rangle \left\langle\phi\right|) = 2\sqrt{2} \end{aligned}$$

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$\Rightarrow$ Quantum violation of CHSH(!!). This is **non-locality**.

Bell's Theorem - Geometry

After two seconds of meditation. Define the Local Polytope for m measurements

$$\mathcal{L}_m \doteq \mathrm{conv}(ab^T \mid a, b \in \{-1, 1\}^m).$$

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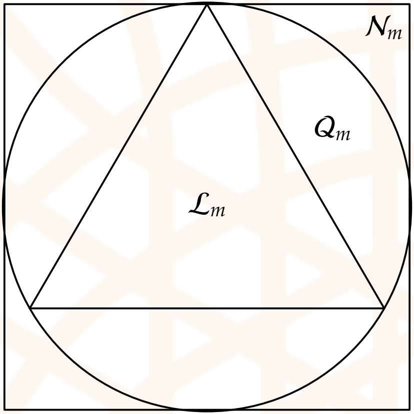
What we did is to test whether the "correlation matrix"associated with the density $|\phi\rangle\langle\phi|$ is contained in $\mathcal{L}_m$ (here with $m = 2$) via the separating hyperplane:

$$a_0 b_0 + a_1 b_0 + a_0 b_1 - a_1 b_1 \leq 2,$$

which is the CHSH inequality.

$\Rightarrow$ Our game today: Membership problem over $\mathcal{L}_m$.

Bell's Theorem - Geometry



Where does your correlation matrix lie? (m = # measurements)

- $\mathcal{L}_m$: Local polytope ($\equiv$ cut polytope on bipartite graph $K_{m,m}$) = classical correlations
- $\mathcal{Q}_m$: Approximable by sequence of SDPs = quantum correlations
- $\mathcal{N}_m$: No-signaling polytope ($\equiv$ rooted semimetric polytope) = no-signaling

for more background see [Avis and Ito, 2006]

Short detour:
The Approximate Carathéodory Problem

The Approximate Carathéodory Problem

Problem and Guarantee

Problem. Find $x \in \text{conv}(\mathcal{V})$ with low cardinality satisfying $\|x - x^*\|_p \leq \epsilon$.

Theorem (Approximate Carathéodory guarantee)

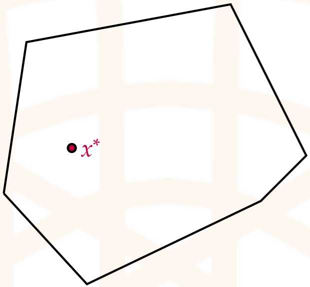
Let $p \geq 2$. Then there exists $x \in \text{conv}(\mathcal{V})$ with cardinality $\mathcal{O}(pD_p^2/\epsilon^2)$ satisfying $\|x - x^*\|_p \leq \epsilon$, where $D_p = \sup_{v,w \in \mathcal{V}} \|w - v\|_p$.

- This result is independent of the space dimension n
- The bound is tight [Mirrokni et al., 2017]
- Probabilistic proof [Pisier, 1981, Barman, 2015]
  (not 'implementable' b/c exact convex combination as input)
- Deterministic proof [Mirrokni et al., 2017]
  (via variant of Mirror Descent)
- Algorithmic proof with many additional configurations [Combettes and Pokutta, 2023]
  (via Frank–Wolfe algorithm)

$$f(x) = \|x - x^*\|_2^2$$

Algorithm Frank-Wolfe Algorithm (FW)

1: $x_0 \in \mathcal{V}$
2: **for** $t = 0$ **to** $T - 1$ **do**
3: $\quad v_t \leftarrow \arg\min_{v \in \mathcal{V}} \langle \nabla f(x_t), v \rangle$
4: $\quad x_{t+1} \leftarrow x_t + \gamma_t (v_t - x_t)$



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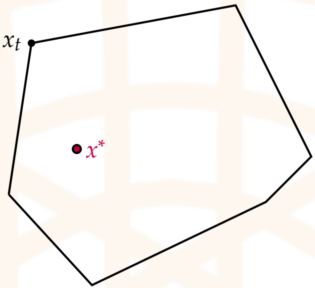

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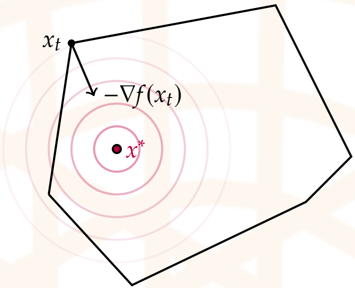

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Solving the Approximate Carathéodory via Conditional Gradients

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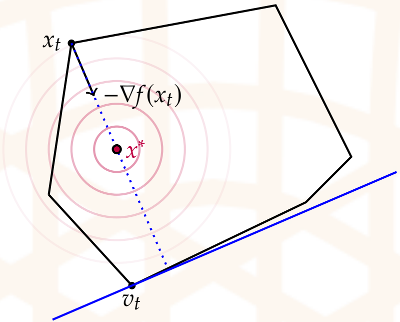

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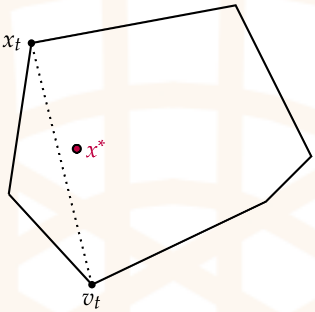

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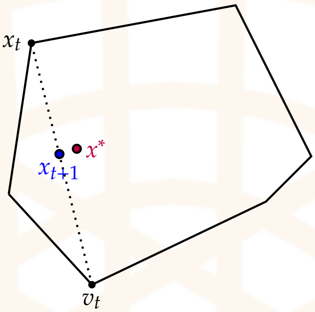

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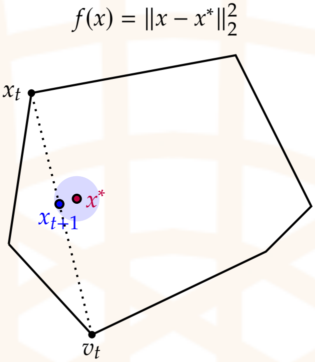

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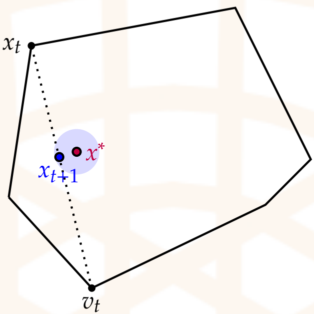

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- FW minimizes f over $\mathrm{conv}(\mathcal{V})$ by sequentially picking up vertices
- Only accesses $\mathrm{conv}(\mathcal{V})$ via linear minimization
- The final iterate x_T has cardinality at most $T + 1$
- For membership: provides convex combination decomposition of x^*
- For non-membership: provides separating hyperplane with normal $\nabla f(x_t)$

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Back to our problem...

Our task

Given state $|\phi\rangle$ decide whether its correlations are local or non-local.

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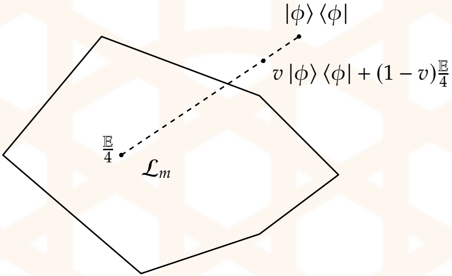
Slightly refined question. At which visibility v do the (correlations of the) mixed state

$$\rho_v \doteq v\,|\phi\rangle\langle\phi| + (1-v)\frac{\mathbb{E}}{4}$$

become non-local, where $\mathbb{E}$ is the all-1 matrix (i.e., trivial correlation).



Our task—mathematically

Given density ρ_v:

- **Non-locality.** Find an appropriate m, compute correlation matrix $p \in \mathbb{R}^{m \times m}$ from ρ_v, and show that there exist a separating hyperplane M, so that

$$\operatorname{tr}(Md) \leq 1 \quad \forall d \in \mathcal{L}_m \qquad \text{and} \qquad \operatorname{tr}(Mp) > 1 \qquad \text{which implies} \qquad v_\rho \leq \frac{1}{\operatorname{tr}(Mp)}.$$

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- **Non-locality.** Find an appropriate m, compute correlation matrix $p \in \mathbb{R}^{m \times m}$ from ρ_v, and show that there exist a separating hyperplane M, so that

$$\mathrm{tr}(Md) \leq 1 \quad \forall d \in \mathcal{L}_m \qquad \text{and} \qquad \mathrm{tr}(Mp) > 1 \qquad \text{which implies} \qquad v_\rho \leq \frac{1}{\mathrm{tr}(Mp)}.$$

- **Locality.** Harder as we would need to show for $m = \infty$. Solution: use approximation with finite measurements m and work-in approximation factor $\alpha < 1$. Solve approximate Carathéodory for p over $\mathcal{L}_m$ to obtain convex decomposition (= deterministic strategy). Provides lower bound on $\alpha^2 v \leq v_\rho$.

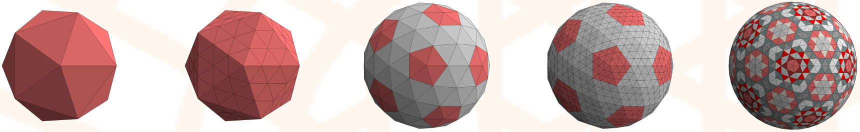

Figure: Polyhedral approximations of Bloch sphere (measurements). Right-most polyhedron has a shrinking factor (also called inradius) of 0.9968.

[Images via Sébastien's polyhedronisme].

Some more technicalities...

Non-locality (upper bounds).

- The LMO over $\mathcal{L}_m$ is NP-hard $\Rightarrow$ FW (even advanced variants) too slow.
- Thus use approximation / heuristic as LMO $\Rightarrow Q \subseteq \mathcal{L}_m$.
- Obtained hyperplane $\operatorname{tr}(Mx) \leq 1$ might not be valid for $\mathcal{L}_m$.
- Can be fixed by "pushing out" M via *one* optimization over $\mathcal{L}_m$ $\Rightarrow$ solve QUBO problem.
- Pushed out inequality might not be separating. Didn't happen and can be easily checked.

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Locality (lower bounds).

- We need a rational decomposition of p into deterministic strategies.
- Require a rational approximation of the convex multipliers.
- (Usually) does not degrade visibility bound.

Results

After several months of computation...

Werner state visibility v_c^{Wer}.

<table>
<tr><th></th><th>v_c^{Wer}</th><th>Reference</th><th>#Inputs</th><th>Year</th></tr>
<tr><td rowspan="6">Upper bounds</td><td>0.7071</td><td>Clauser et al. [1969a]</td><td>2</td><td>1969</td></tr>
<tr><td>0.7056</td><td>Vértesi [2008]</td><td>465</td><td>2008</td></tr>
<tr><td>0.7054</td><td>Hua et al. [2015]</td><td>∞</td><td>2015</td></tr>
<tr><td>0.7012</td><td>Brierley et al. [2016]</td><td>42</td><td>2016</td></tr>
<tr><td>0.6964</td><td>Diviánszky et al. [2017]</td><td>90</td><td>2017</td></tr>
<tr><td>0.6955</td><td rowspan="2">This work: Designolle et al. [2023]</td><td>97</td><td rowspan="2">2023</td></tr>
<tr><td rowspan="4">Lower bounds</td><td>0.6875</td><td>$406 \sim \infty$</td></tr>
<tr><td>0.6829</td><td>Hirsch et al. [2017]</td><td>$625 \sim \infty$</td><td>2017</td></tr>
<tr><td>0.6595</td><td>Acín et al. [2006]
using Krivine [1979]</td><td>∞</td><td>2006
1979</td></tr>
<tr><td>0.5</td><td>Werner [1989]</td><td>∞</td><td>1989</td></tr>
</table>

Table: Successive refinements of the bounds on v_c^{Wer}, the nonlocality threshold of the two-qubit Werner states under projective measurements. Using m measurements to simulate all projective ones is denoted by $m \sim \infty$.

Results

After several months of computation...

Bonus. Grothendieck constant of order 3 satisfies

$$K_G(3) = \frac{1}{v_c^{\mathrm{Wer}}}.$$

Thus. Currently tightest bounds

$$1.4376 \approx \frac{1}{v_{\mathrm{up}}} \leq K_G(3) \leq \frac{1}{v_{\mathrm{low}}} \approx 1.4546.$$

[see also Grothendick inequality on Wikipedia]

Results

After several months of computation...

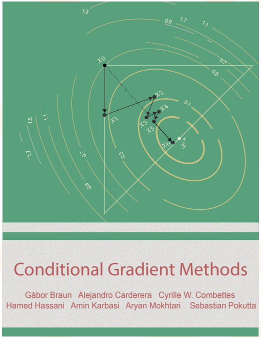
First strong non-locality bounds for tripartite W and GHZ state.

<table>
<tr><th></th><th>v_c^{GHZ}</th><th>Reference</th><th>#Inputs</th><th>Year</th></tr>
<tr><td rowspan="4">Upper</td><td>0.5</td><td>Greenberger et al. [1989]</td><td>2</td><td>1989</td></tr>
<tr><td>0.4961</td><td>Vértesi and Pál [2011]</td><td>5</td><td>2011</td></tr>
<tr><td>0.4932</td><td>Brierley et al. [2016]</td><td>16</td><td>2016</td></tr>
<tr><td>0.4916</td><td rowspan="2">This work</td><td>16</td><td rowspan="2">2023</td></tr>
<tr><td rowspan="3">Lower</td><td>0.4688</td><td>$61 \sim \infty$</td></tr>
<tr><td>0.232</td><td>Cavalcanti et al. [2016]</td><td>$12 \sim \infty$</td><td>2016</td></tr>
<tr><td>0.2</td><td>Dür and Cirac [2000]</td><td>Entnglmnt threshold</td><td>2000</td></tr>
</table>

<table>
<tr><th></th><th>v_c^{W}</th><th>Reference</th><th>#Inputs</th><th>Year</th></tr>
<tr><td rowspan="4">Upper</td><td>0.6442</td><td>Sen [De]</td><td>2</td><td>2003</td></tr>
<tr><td>0.6007</td><td>Gruca et al. [2010]</td><td>5</td><td>2010</td></tr>
<tr><td>0.5956</td><td>Pandit et al. [2022]</td><td>6</td><td>2022</td></tr>
<tr><td>0.5482</td><td rowspan="2">This work</td><td>16</td><td rowspan="2">2023</td></tr>
<tr><td rowspan="3">Lower</td><td>0.4861</td><td>$46 \sim \infty$</td></tr>
<tr><td>0.228</td><td>Cavalcanti et al. [2016]</td><td>$12 \sim \infty$</td><td>2016</td></tr>
<tr><td>0.2096</td><td>Szalay [2011]</td><td>Entnglmnt threshold</td><td>2011</td></tr>
</table>

Shameless plug...

Thank you!



Conditional Gradient Methods

Gábor Braun, Alejandro Carderera, Cyrille W Combettes, Hamed Hassani, Amin Karbasi, Aryan Mokhtari, and Sebastian Pokutta

`https://conditional-gradients.org/`
`https://arxiv.org/abs/2211.14103`

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