

A statistical interpretation of Grothendieck's inequality and its relation to the size of non-locality of quantum mechanics

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CPNSS, LSE

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Sigma Club



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A portrait of A. Grothendieck





A. Grothendieck lecturing at IHES (1958-1970)





Excerpt from A. Grothendieck's handwritten lecture notes I

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Excerpt from A. Grothendieck's handwritten lecture notes II

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Excerpt from A. Grothendieck's handwritten lecture notes III

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Grothendieck's inequality in matrix form I

Theorem (Lindenstrauss-Pelczyński (1968))

Let $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$ and $m, n \in \mathbb{N}$. Let . Then there exists a universal constant K > 0 - not depending on m and n - such that for all matrices $A = (a_{ij}) \in \mathbb{M}(m \times n; \mathbb{F})$, all \mathbb{F} -Hilbert spaces H, all unit vectors $u_1, \ldots, u_m, v_1, \ldots, v_n \in H$ the following inequality is satisfied:

$$\sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} \langle u_i, v_j \rangle_H \Big| \le K \max \left\{ \Big| \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} p_i q_j \Big| : p_i, q_j \in \{-1, 1\} \right\}.$$



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The smallest possible value of the corresponding constant *K* is denoted by $K_G^{\mathbb{F}}$. It is called Grothendieck's constant.



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Grothendieck's inequality in matrix form II

An easy exercise shows that GT is equivalent to





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$$\max\left\{ \left| \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} p_i q_j \right| : p_i, q_j \in \{-1, 1\} \right\} \le 1$$

then

$$\Big|\sum_{i=1}^m\sum_{j=1}^n a_{ij}\langle u_i,v_j\rangle_H\Big|\leq K.$$

for all Hilbert spaces over \mathbb{F} and all unit vectors u_1, \ldots, u_m , $v_1, \ldots, v_n \in H$.



Grothendieck's inequality in matrix form III

Thanks to a strong use of vector measures, representing kernel Hilbert spaces (RKHS's) and Hilbert space-valued stochastic processes, all applied by members of probability schools we may list a sharp value for $K_G^{\mathbb{F}}$ in the following particular case:



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$$K_G^{\mathbb{R}} = rac{\pi}{2}$$
 and $K_G^{\mathbb{C}} = rac{4}{\pi}$.

From now on are going to consider the real case (i. e., $\mathbb{F} = \mathbb{R}$) only. Nevertheless, we allow an unrestricted use of all matrices $A \in \mathbb{M}(m \times n; \mathbb{R})$ for any $m, n \in \mathbb{N}$.



Grothendieck's inequality in matrix form IV

Until present the following encapsulation of $K_G^{\mathbb{R}}$ holds, primarily due to R. E. Rietz (1974), J. L. Krivine (1977), and most recently, M. Braverman, K. Makarychev, Y. Makarychev, and A. Naor (4-author paper from 2011, available on the arXiv):



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$$1,676 < K_G^{\mathbb{R}} < \frac{\pi}{2\ln(1+\sqrt{2})} \approx 1,782.$$



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Conjecture Is $K_G^{\mathbb{R}} = \sqrt{\pi} \approx 1,772$?



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Grothendieck's inequality rewritten I

By transforming Grothendieck's inequality into an equivalent inequality between traces of matrix products (respectively Hilbert-Schmidt inner products) we are lead to a surprising interpretation which reveals deep links to combinatorial (binary) optimisation, semidefinite programming (SDP) and multivariate statistics, built on suitable non-linear transformations of correlation matrices.



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We will sketch this approach which might lead to a constructive improvement of Krivine's upper bound $\frac{\pi}{2\ln(1+\sqrt{2})}$. At least it also can be reproduced in this approach.



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We will sketch this approach which might lead to a constructive improvement of Krivine's upper bound $\frac{\pi}{2\ln(1+\sqrt{2})}$. At least it also can be reproduced in this approach.

When the context is clear we suppress the Hilbert space symbol "*H*" and use the notation " $\langle \cdot, \cdot \rangle$ " instead of " $\langle \cdot, \cdot \rangle_H$ ".



Grothendieck's inequality rewritten II

Let $m, n \in \mathbb{N}, A \in \mathbb{M}(m \times n; \mathbb{R}), u := (u_1, \dots, u_m)^\top \in S_H^m$ and $v := (v_1, \dots, v_n)^\top \in S_H^n$ be given, where $S_H := \{w \in H : ||w|| = 1\}$ denotes the unit sphere in H.



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Firstly, note that

$$\sum_{i=1}^{m}\sum_{j=1}^{n}a_{ij}\langle u_{i},v_{j}\rangle_{H}=$$



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is precisely the Hilbert-Schmidt inner product (or the Frobenius inner product) of the matrices $A \in \mathbb{M}(m \times n; \mathbb{R})$ and $\Gamma_H(u, v) \in \mathbb{M}(m \times n; \mathbb{R})$, where



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$$\Gamma_{H}(u,v) := \begin{pmatrix} \langle u_{1}, v_{1} \rangle_{H} & \langle u_{1}, v_{2} \rangle_{H} & \dots & \langle u_{1}, v_{n} \rangle_{H} \\ \langle u_{2}, v_{1} \rangle_{H} & \langle u_{2}, v_{2} \rangle_{H} & \dots & \langle u_{2}, v_{n} \rangle_{H} \\ \vdots & \vdots & \vdots & \vdots \\ \langle u_{m}, v_{1} \rangle_{H} & \langle u_{m}, v_{2} \rangle_{H} & \dots & \langle u_{m}, v_{n} \rangle_{H} \end{pmatrix}$$



Grothendieck's inequality rewritten: Bell is lurking

Let $m, n \in \mathbb{N}, A \in \mathbb{M}(m \times n; \mathbb{R}), u := (p_1, \dots, p_m)^\top \in (\mathbb{S}^0)^m$ and $q := (q_1, \dots, q_n)^\top \in (\mathbb{S}^0)^n$ be given, where $\mathbb{S}^0 := \{-1, 1\}$ denotes the unit "sphere" in $\mathbb{R} = \mathbb{R}^{0+1}$.



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Similarly as before, we obtain

$$\sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} p_i q_j = \operatorname{tr} \left(A^{\top} \, \Gamma_{\mathbb{R}}(p,q) \right) = \langle A, \Gamma_{\mathbb{R}}(p,q) \rangle,$$

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$$\Gamma_{\mathbb{R}}(p,q) := pq^{\top} = \begin{pmatrix} p_1q_1 & p_1q_2 & \dots & p_1q_n \\ p_2q_1 & p_2q_2 & \dots & p_2q_n \\ \vdots & \vdots & \vdots & \vdots \\ p_mq_1 & p_mq_2 & \dots & p_mq_n \end{pmatrix}$$





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Full matrix representation of the Hilbert space vectors

Pick all m + n Hilbert space unit vectors $u_1, u_2, \ldots, u_m, v_1, v_2, \ldots, v_n \in H$ and represent them as



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$\langle u_2, v_1 \rangle$	$\langle u_2, v_2 \rangle$	• • •	$\langle u_2, v_n \rangle$
÷	1	1	÷
$\langle u_m, v_1 \rangle$	$\langle u_m, v_2 \rangle$		$\langle u_m, v_n \rangle$



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$$\begin{pmatrix} \langle u_1, v_1 \rangle & \langle u_1, v_2 \rangle & \dots & \langle u_1, v_n \rangle \\ \langle u_2, v_1 \rangle & \langle u_2, v_2 \rangle & \dots & \langle u_2, v_n \rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle u_m, v_1 \rangle & \langle u_m, v_2 \rangle & \dots & \langle u_m, v_n \rangle \end{pmatrix}$$

Does this matrix look familiar to you?



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Does this matrix look familiar to you? It is a part of something larger...



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Does this matrix look familiar to you? It is a part of something larger... Namely:



Block matrix representation I





Block matrix representation I

$$\begin{pmatrix} \langle u_1, v_1 \rangle & \langle u_1, v_2 \rangle & \dots & \langle u_1, v_n \rangle \\ \langle u_2, v_1 \rangle & \langle u_2, v_2 \rangle & \dots & \langle u_2, v_n \rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle u_m, v_1 \rangle & \langle u_2, v_1 \rangle & \dots & \langle u_m, v_1 \rangle \\ \langle u_1, v_2 \rangle & \langle u_2, v_2 \rangle & \dots & \langle u_m, v_2 \rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle u_1, v_n \rangle & \langle u_2, v_n \rangle & \dots & \langle u_m, v_n \rangle \end{pmatrix}$$

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Block matrix representation I

$$\begin{pmatrix} \langle u_1, v_1 \rangle & \langle u_1, v_2 \rangle & \dots & \langle u_1, v_n \rangle \\ \langle u_2, v_1 \rangle & \langle u_2, v_2 \rangle & \dots & \langle u_2, v_n \rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle u_m, v_1 \rangle & \langle u_m, v_2 \rangle & \dots & \langle u_m, v_n \rangle \\ \langle v_1, u_1 \rangle & \langle v_1, u_2 \rangle & \dots & \langle v_1, u_m \rangle \\ \langle v_2, u_1 \rangle & \langle v_2, u_2 \rangle & \dots & \langle v_2, u_m \rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle v_n, u_1 \rangle & \langle v_n, u_2 \rangle & \dots & \langle v_n, u_m \rangle \end{pmatrix}$$



Block matrix representation II

$\langle u_1, u_1 \rangle$	$\langle u_1, u_2 \rangle$		$\langle u_1, u_m \rangle$	$\langle u_1, v_1 \rangle$	$\langle u_1, v_2 \rangle$		$\langle u_1, v_n \rangle$
$\langle u_2, u_1 \rangle$	$\langle u_2, u_2 \rangle$		$\langle u_2, u_m \rangle$	$\langle u_2, v_1 \rangle$	$\langle u_2, v_2 \rangle$		$\langle u_2, v_n \rangle$
÷	1	γ_{i_1}	1	1	1	γ_{i_1}	
$\langle u_m, u_1 \rangle$	$\langle u_m, u_2 \rangle$		$\langle u_m, u_m \rangle$	$\langle u_m, v_1 \rangle$	$\langle u_m, v_2 \rangle$		$\langle u_m, v_n \rangle$
$\langle v_1, u_1 \rangle$	$\langle v_1, u_2 \rangle$		$\langle v_1, u_m \rangle$	$\langle v_1, v_1 \rangle$	$\langle v_1, v_2 \rangle$		$\langle v_1, v_n \rangle$
$\langle v_2, u_1 \rangle$	$\langle v_2, u_2 \rangle$	• • •	$\langle v_2, u_m \rangle$	$\langle v_2, v_1 \rangle$	$\langle v_2, v_2 \rangle$		$\langle v_2, v_n \rangle$
	1	1	1		1	$\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}_{\mathcal{T}}}}}}}}}}$	
$\langle v_n, u_1 \rangle$	$\langle v_n, u_2 \rangle$		$\langle v_n, u_m \rangle$	$\langle v_n, v_1 \rangle$	$\langle v_m, v_2 \rangle$		$\langle v_n, v_n \rangle$

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Block matrix representation III

(1	$\langle u_1, u_2 \rangle$		$\langle u_1, u_m \rangle$	$\langle u_1, v_1 \rangle$	$\langle u_1, v_2 \rangle$		$\langle u_1, v_n \rangle$
$\langle u_2, u_1 \rangle$	1		$\langle u_2, u_m \rangle$	$\langle u_2, v_1 \rangle$	$\langle u_2, v_2 \rangle$		$\langle u_2, v_n \rangle$
:		\mathbb{P}_{2}				$\mathcal{T}_{\mathcal{T}_{\mathcal{T}}}$	
$\langle u_m, u_1 \rangle$	$\langle u_m, u_2 \rangle$		1	$\langle u_m, v_1 \rangle$	$\langle u_m, v_2 \rangle$		$\langle u_m, v_n \rangle$
$\langle v_1, u_1 \rangle$	$\langle v_1, u_2 \rangle$		$\langle v_1, u_m \rangle$	1	$\langle v_1, v_2 \rangle$		$\langle v_1, v_n \rangle$
$\langle v_2, u_1 \rangle$	$\langle v_2, u_2 \rangle$		$\langle v_2, u_m \rangle$	$\langle v_2, v_1 \rangle$	1		$\langle v_2, v_n \rangle$
		1	1			$\mathcal{T}_{\mathcal{T}_{\mathcal{T}}}$	
$\langle v_n, u_1 \rangle$	$\langle v_n, u_2 \rangle$		$\langle v_n, u_m \rangle$	$\langle v_n, v_1 \rangle$	$\langle v_m, v_2 \rangle$		1 /

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 $PSD(n; \mathbb{R}) := \{S : S^{\top} = S \in \mathbb{M}(n \times n; \mathbb{R}), S \text{ is positive semidefinite} \}.$





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Recall that $PSD(n; \mathbb{R})$ is a closed convex cone.





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Recall that $PSD(n; \mathbb{R})$ is a closed convex cone. Moreover, we consider the set

 $C(n;\mathbb{R}) := \{ S \in PSD(n;\mathbb{R}) \text{ such that } S_{ii} = 1 \text{ for all } i \in [n] \}.$





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A refresher of a few definitions I Let $n \in \mathbb{N}$. We put

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The following statement (resulting from spectral decomposition/SVD) is of utmost importance:



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The following statement (resulting from spectral decomposition/SVD) is of utmost importance:

Theorem (Square roots in $PSD(n; \mathbb{R})$)

Let $n \in \mathbb{N}$ and $S \in \mathbb{M}(n \times n; \mathbb{R})$. TFAE:

(i)
$$S \in PSD(n; \mathbb{R})$$
.

(ii) $S = B^2$ for some $B \in PSD(n; \mathbb{R})$.

This $B \in PSD(n; \mathbb{R})$ is unique and called the square root of S: $S^{1/2} := B$.



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A refresher of a few definitions II

Let $d, k \in \mathbb{N}$ and $(H, \langle \cdot, \cdot \rangle)$ be an arbitrary *d*-dimensional Hilbert space (i. e, $H = l_2^d$). Let $w_1, w_2, \ldots, w_k \in H$. Put $w := (w_1, \ldots, w_k)^\top \in H^k$ and $S := (w_1 | w_2 | \ldots | w_k) \in \mathbb{M}(d \times k; \mathbb{R})$. The matrix $\Gamma_H(w, w) \in PSD(k; \mathbb{R})$, defined as

$$\Gamma_H(w,w)_{ij} := \langle w_i, w_j \rangle = \left(S^\top S \right)_{ij} \quad \left(i, j \in [k] := \{1, 2, \dots, k\} \right)$$

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is called Gram matrix of the vectors $w_1, \ldots, w_k \in H$. Observe that

$$\begin{pmatrix} \langle u_1, v_1 \rangle & \langle u_1, v_2 \rangle & \dots & \langle u_1, v_n \rangle \\ \langle u_2, v_1 \rangle & \langle u_2, v_2 \rangle & \dots & \langle u_2, v_n \rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle u_m, v_1 \rangle & \langle u_m, v_2 \rangle & \dots & \langle u_m, v_n \rangle \end{pmatrix}$$

is not a Gram matrix!



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Let $n \in \mathbb{N}$. Fix a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and let $\xi := (\xi_1, \xi_2, \dots, \xi_n)^\top : \Omega \longrightarrow \mathbb{R}^n$ be a random vector. Let $\mu := (\mu_1, \mu_2, \dots, \mu_n)^\top \in \mathbb{R}^n$ and $C \in PSD(n; \mathbb{R})$.



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Recall that ξ is an *n*-dimensional Gaussian random vector with respect to the "parameters" μ and *C* (short: $\xi \sim N_n(\mu, C)$) if and only if for all $a \in \mathbb{R}^n$ there exists $\eta_a \sim N_1(0, 1)$ such that

$$\langle a,\xi\rangle = \sum_{i=1}^n a_i\xi_i = \langle a,\mu\rangle + \sqrt{\langle a,Ca\rangle}\eta_a = \langle a,\mu\rangle + \|C^{1/2}a\|\eta_a.$$



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Note that we don't require here that *C* is invertible! Following Feller, the matrix $\mathbb{V}(\xi)$ defined as

$$\mathbb{V}(\xi)_{ij} := \mathbb{E}[\xi_i \xi_j] - \mathbb{E}[\xi_i] \mathbb{E}[\xi_j] \stackrel{(!)}{=} C_{ij} \quad (i, j \in [n])$$

is known as the variance matrix of the Gaussian random vector ξ .



Characterisation of $PSD(n; \mathbb{R})$ |

Proposition Let $n \in \mathbb{N}$ and $S \in \mathbb{M}(n \times n; \mathbb{R})$. TFAE:





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Characterisation of $PSD(n; \mathbb{R})$ |

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- (i) *S* is the variance matrix of some Gaussian random vector.
- (ii) $S = \mathbb{E}[\xi\xi^{\top}]$ for some Gaussian random vector $\xi \sim N_n(0, C)$.



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Proposition

Let $n \in \mathbb{N}$ and $S \in \mathbb{M}(n \times n; \mathbb{R})$. TFAE:

(i) S is the variance matrix of some Gaussian random vector.

(ii) S = E[ξξ^T] for some Gaussian random vector ξ ~ N_n(0, C).
(iii) S ∈ PSD(n; ℝ).

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- (i) *S* is the variance matrix of some Gaussian random vector.
- (ii) $S = \mathbb{E}[\xi\xi^{\top}]$ for some Gaussian random vector $\xi \sim N_n(0, C)$.
- (iii) $S \in PSD(n; \mathbb{R})$.
- (iv) There exists a Hilbert space *L* and vectors z_1, \ldots, z_n in *L* such that

$$S = \Gamma_L(z, z) = \sum_{l=1}^n z_l z_l^\top = \sum_{l=1}^n \operatorname{diag}(z_l) J \operatorname{diag}(z_l)$$

where $z := (z_1, z_2, ..., z_n)^{\top} \in L^n$ and $J_{kl} := 1$ for all $k, l \in [n]$.



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Characterisation of $PSD(n; \mathbb{R})$ II

This leads us straightforwardly to the following important block matrix representation of positive semidefinite matrices:

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This leads us straightforwardly to the following important block matrix representation of positive semidefinite matrices:

Corollary

Let $m, n \in \mathbb{N}$ and $S \in PSD(m + n; \mathbb{R})$ Then there is a (finite-dimensional) Hilbert space *H* and vectors $u_1, u_2, \ldots, u_m, v_1, v_2, \ldots, v_n \in H$ such that

$$S = \Gamma_H(w, w) = \begin{pmatrix} \Gamma_H(u, u) & \Gamma_H(u, v) \\ \Gamma_H(u, v)^\top & \Gamma_H(v, v) \end{pmatrix} = \begin{pmatrix} \mathbb{E}[\xi\xi^\top] & \mathbb{E}[\xi\eta^\top] \\ \mathbb{E}[\xi\eta^\top]^\top & \mathbb{E}[\eta\eta^\top] \end{pmatrix}$$

where $w_i := u_i$ if $1 \le i \le m$ and $w_i := v_{i-m}$ if $m + 1 \le i \le m + n$ and $(\xi_1, ..., \xi_m, \eta_1, ..., \eta_n)^\top \sim N_{m+n}(0, S)$.

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Geometry of correlation matrices

Observation Let $n \in \mathbb{N}$ and $\Sigma = (\sigma_{ij}) \in \mathbb{M}(n \times n; \mathbb{R})$. TFAE:



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(iii) $\Sigma = \Gamma_{l_2^n}(x, x) = \sum_{i=1}^n x_i x_i^\top = \sum_{i=1}^n diag(x_i) J diag(x_i)$ for
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(iv) Σ is a correlation matrix, induced by some *n*-dimensional Gaussian random vector.

In particular, condition (i) implies that $\sigma_{ij} \in [-1, 1]$ for all $i, j \in [n]$.



Lurking correlation matrices in GT I

Let $u := (u_1, u_2, \dots, u_m)^\top \in S_H^m$ and $v := (v_1, v_2, \dots, v_n)^\top \in S_H^n$. Consider $\Gamma_H(u, v) \in \mathbb{M}(m \times n; \mathbb{R})$, defined as





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$$\Gamma_H(u,v)_{ij} := \langle u_i, v_j \rangle_H \quad ((i,j) \in [m] \times [n]).$$

Put $w := (u^{\top}, v^{\top})^{\top} \equiv (u_1, u_2, \dots, u_m, v_1, v_2, \dots, v_n)^{\top}$. Then $w \in S_H^{m+n}$.



Lurking correlation matrices in GT I

Let $u := (u_1, u_2, \dots, u_m)^\top \in S_H^m$ and $v := (v_1, v_2, \dots, v_n)^\top \in S_H^n$. Consider $\Gamma_H(u, v) \in \mathbb{M}(m \times n; \mathbb{R})$, defined as

$$\Gamma_H(u,v)_{ij} := \langle u_i, v_j \rangle_H \quad ((i,j) \in [m] \times [n]).$$

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$$\Gamma_{H}(w,w) = \begin{pmatrix} \Gamma_{H}(u,u) & \Gamma_{H}(u,v) \\ \Gamma_{H}(u,v)^{\top} & \Gamma_{H}(v,v) \end{pmatrix}$$



Lurking correlation matrices in GT II

Moreover,

$$\Gamma_{\mathbb{R}}(p,q) = pq^{ op}$$
 for all $p \in \mathbb{R}^m, q \in \mathbb{R}^n$

and





Lurking correlation matrices in GT II

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and

$$\Gamma_{\mathbb{R}}(x,x) = xx^{\top} = \begin{pmatrix} pp^{\top} & pq^{\top} \\ qp^{\top} & qq^{\top} \end{pmatrix} \text{ for all } x := (p^{\top},q^{\top})^{\top} \in \mathbb{R}^{m+n}.$$

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Geometry of correlation matrices II

Exercise Let $k \in \mathbb{N}$. Then the sets $\{S : S = xx^{\top} \text{ for some } x \in \{-1, 1\}^k\}$ and $\{\Sigma : \Sigma \in C(k; \mathbb{R}) \text{ and } rk(\Sigma) = 1\}$ coincide.





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Geometry of correlation matrices III

Proposition (K. R. Parthasarathy (2002)) Let $k \in \mathbb{N}$. $C(k; \mathbb{R})$ is a compact and convex subset of the k^2 -dimensional vector space $\mathbb{M}(k \times k; \mathbb{R})$. Any $k \times k$ -correlation matrix of rank 1 is an extremal point of the set $C(k; \mathbb{R})$.



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In particular, the (finite) set of all $k \times k$ -correlation matrices of rank 1 is not convex.

Let $k \in \mathbb{N}$. Put

 $C_1(k;\mathbb{R}) := \big\{ \Sigma : \Sigma \in C(k;\mathbb{R}) \text{ and } \mathsf{rk}(\Sigma) = 1 \big\}.$



Canonical block injection of A I

A naturally appearing question is the following:



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Having gained - important - additional structure by "enlarging" the $m \times n$ -matrix $\Gamma_H(u, v)$ to a $(m + n) \times (m + n)$ -correlation matrix, how could this gained information be used to rewrite Grothendieck's inequality accordingly?



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Definition

Let $m, n \in \mathbb{N}$ and $A \in \mathbb{M}(m \times n; \mathbb{R})$ arbitrary. Put

$$\widehat{A} := \frac{1}{2} \begin{pmatrix} \mathbf{0} & A \\ A^\top & \mathbf{0} \end{pmatrix}$$

Let us call $\mathbb{M}(m \times n; \mathbb{R}) \ni \widehat{A}$ the canonical block injection of *A*.



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Let us call $\mathbb{M}(m \times n; \mathbb{R}) \ni \widehat{A}$ the canonical block injection of *A*. Observe that \widehat{A} is symmetric, implying that $\widehat{A} = \widehat{A}^{\top}$.



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A further equivalent rewriting of GT I

Proposition Let $m, n \in \mathbb{N}$ and $A = (a_{ij}) \in \mathbb{M}(m \times n; \mathbb{R})$. Let K > 0. TFAE:





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$$\sup_{(u,v)\in S_{H}^{m}\times S_{H}^{n}}\left|\sum_{i=1}^{m}\sum_{j=1}^{n}a_{ij}\langle u_{i},v_{j}\rangle_{H}\right| \leq K \max_{(p,q)\in\{-1,1\}^{m}\times\{-1,1\}^{n}}\left|\sum_{i=1}^{m}\sum_{j=1}^{n}a_{ij}p_{i}q_{j}\right|$$

for all Hilbert spaces H over \mathbb{R} .



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(ii) sup $|\langle \widehat{A}, \Gamma \rangle| \le K$ max $|\langle \widehat{A}, \Gamma \rangle| \le K$

$$\sup_{\Gamma \in C(m+n;\mathbb{R})} |\langle \widehat{A}, \Gamma \rangle| \le K \max_{\substack{\Sigma \in C(m+n;\mathbb{R})\\ rk(\Sigma) = 1}} |\langle \widehat{A}, \Sigma \rangle|.$$



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A further equivalent rewriting of GT II

Proposition Let $m, n \in \mathbb{N}$ and $A = (a_{ij}) \in \mathbb{M}(m \times n; \mathbb{R})$. Let K > 0. TFAE: (i)

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for all Hilbert spaces H over \mathbb{R} . (ii) $\max_{k \in \mathbb{R}} |\langle \widehat{A}, \Gamma \rangle| \le K \quad \max_{k \in \mathbb{R}} |\langle \widehat{A}, \Gamma \rangle| \le K$

$$\max_{\Gamma \in C(m+n;\mathbb{R})} |\langle \widehat{A}, \Gamma \rangle| \le K \max_{\Sigma \in C_1(m+n;\mathbb{R})} |\langle \widehat{A}, \Sigma \rangle|$$



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We don't know whether condition (ii) holds for all matrices in $\mathbb{M}((m+n) \times (m+n); \mathbb{R})$.

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GT versus NP-hard optimisation

Observation On the left side of GT: a convex conic optimisation problem (since it is SDP) and hence of polynomial worst-case complexity (P)):

 $\max_{\Gamma \in C(m+n;\mathbb{R})} |\langle \widehat{A}, \Gamma \rangle|$



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Thus, Grothendieck's constant $K_G^{\mathbb{R}}$ is precisely the "integrality gap"; i. e., the maximum ratio between the solution quality of the NP-hard Boolean optimisation on the right side of GT and of its SDP relaxation on the left side!



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Schur product and the matrix f[A]

Definition Let $\emptyset \neq I \subseteq \mathbb{R}$ and $f : I \longrightarrow \mathbb{R}$ a function. Let $A = (a_{ij}) \in \mathbb{M}(m \times n; \mathbb{R})$ such that $a_{ij} \in I$ for all $(i, j) \in [m] \times [n]$.



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Guiding Example The Schur product (or Hadamard product)

 $(a_{ij}) \ast (b_{ij}) := (a_{ij}b_{ij})$

of matrices (a_{ij}) and (b_{ij}) leads to f[A], where $f(x) := x^2$.



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Remark

The notation "f[A]" is used to highlight the difference between the matrix f(A) originating from the spectral representation of A(for normal matrices A) and the matrix f[A], defined as above !



Grothendieck's identity I

How can we link an NP-hard non-convex Boolean optimisation problem and its convex SDP relaxation?



Grothendieck's identity I

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Theorem (Grothendieck's identity - T. S. Stieltjes (1889)) Let $-1 \le \rho \le 1$ and $(\xi, \eta)^{\top} \sim N_2(0, \Theta_{\rho})$, where

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Grothendieck's identity II

Corollary Let $k \in \mathbb{N}$. Let $\Theta \in C(k; \mathbb{R})$ an arbitrarily given correlation matrix. Then there exists a Gaussian random vector $\xi \sim N_k(0, \Theta)$ such that

$$\frac{2}{\pi} \arcsin[\Theta] = \mathbb{E}[\Sigma(\xi)],$$

where

$$\Sigma(\xi(\omega))_{ij} := sign(\xi_i(\omega))sign(\xi_j(\omega))$$

for all $\omega \in \Omega$, and for all $i, j \in [k]$.



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Grothendieck's identity II

Corollary

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$$\frac{2}{\pi} \arcsin[\Theta] = \mathbb{E}\big[\Sigma(\boldsymbol{\xi})\big] \,,$$

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for all $\omega \in \Omega$, and for all $i, j \in [k]$. $\Sigma(\xi(\omega))$ is a correlation matrix of rank 1 for all $\omega \in \Omega$, and we have

$$\max_{\substack{\Sigma \in C(k;\mathbb{R}) \\ rank(\Sigma) = 1}} |\langle \widehat{A}, \Sigma \rangle| \geq \mathbb{E} \left[|\langle \widehat{A}, \Sigma(\xi) \rangle| \right]$$
$$\geq |\langle \widehat{A}, \mathbb{E} \left[\Sigma(\xi) \right] \rangle| = \frac{2}{\pi} |\langle \widehat{A}, \arcsin[\Theta] \rangle|.$$



Grothendieck's identity III

Corollary

Let $m, n \in \mathbb{N}$ and H be an arbitrary Hilbert space. Let $u \in S_H^m$ and $v \in S_H^n$. Then

$$\Theta_{u,v} := \frac{2}{\pi} \arcsin[\Gamma_H(u,v)] = \mathbb{E} \left[sign(\xi) sign(\eta)^\top \right]$$

for some Gaussian random vectors $\xi \sim N_m(0, \Theta_{u,u})$ and $\eta \sim N_n(0, \Theta_{v,v})$.



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More generally, we have

Proposition (Schoenberg (1942))

Let $k \in \mathbb{N}$ and $0 < r \le \infty$. Let Θ be an arbitrary $(k \times k)$ -correlation matrix. Let f be a function that admits a power series representation $f(x) = \sum_{n=0}^{\infty} a_n x^n$ for some sequence $(a_n) \subseteq [0, \infty)$ on (-r, r). Let 0 < f(1) and put $f^{[1]} := \frac{1}{f(1)}f$. Then $f^{[1]}[\Theta]$ again is a $(k \times k)$ -correlation matrix.



Grothendieck's identity IV

Since for all $\rho \in [-1, 1]$

$$\arcsin(\rho) = \sum_{n=0}^{\infty} \frac{1}{4^n} \binom{2n}{n} \frac{\rho^{2n+1}}{(2n+1)!} = \rho + \sum_{n=1}^{\infty} \frac{1}{4^n} \binom{2n}{n} \frac{\rho^{2n+1}}{(2n+1)!}$$

it follows that (in general)





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it follows that (in general)

$$\begin{aligned} \max_{\substack{\Sigma \in C(k;\mathbb{R}) \\ rank(\Sigma) = 1}} |\langle \widehat{A}, \Sigma \rangle| &\geq \frac{2}{\pi} |\langle \widehat{A}, \arcsin[\Theta] \rangle| \\ &= \frac{2}{\pi} |\langle \widehat{A}, \Theta \rangle + \sum_{n=1}^{\infty} \frac{1}{4^n (2n+1)!} {2n \choose n} \langle \widehat{A}, [\Theta]^{2n+1} \rangle |. \end{aligned}$$



Exercise Let $k \in \mathbb{N}$ and $M \in PSD(k; \mathbb{R})$.

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Exercise Let $k \in \mathbb{N}$ and $M \in PSD(k; \mathbb{R})$. Show that

$\operatorname{arcsin}[M] - M \in PSD(k; \mathbb{R})$.





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Exercise Let $k \in \mathbb{N}$ and $M \in PSD(k; \mathbb{R})$. Show that $\arcsin[M] - M \in PSD(k; \mathbb{R})$.

How can we treat the difficult handling of the remaining part

$$\sum_{n=1}^{\infty} \frac{1}{4^n (2n+1)!} \binom{2n}{n} \langle \widehat{A}, [\Theta]^{2n+1} \rangle$$

(which unfortunately "sits inside" an absolute value)?



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Grothendieck's identity V

A seemingly fruitful and different approach is the following:

Grothendieck's identity V

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A seemingly fruitful and different approach is the following:

 (i) Transform an arbitrarily given correlation matrix Θ₀ non-linearly - and entrywise - to another correlation matrix Θ₁ := Φ[Θ₀] for some Φ : C(k; ℝ) → C(k; ℝ) such that this non-linear transformation Φ strongly reduces the impact of the arcsin function (up to a given small error).

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- (ii) Apply Grothendieck's identity to the so obtained correlation matrix Θ_1 and apply the estimation above to $\arcsin[\Theta_1]$.

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- (ii) Apply Grothendieck's identity to the so obtained correlation matrix Θ_1 and apply the estimation above to $\arcsin[\Theta_1]$.
- (iii) A reiteration of the steps (i) and (ii) could lead to an iterative algorithm which might converge to a "suitable" upper bound of $K_G^{\mathbb{R}}$.



- A very short glimpse at A. Grothendieck's work in functional analysis
- 2 Grothendieck's inequality in matrix formulation
- **3** Grothendieck's inequality rewritten
- 4 Grothendieck's inequality and correlation matrices
- **5** Towards a calculation of Grothendieck's constant $K_G^{\mathbb{R}}$
- 6 Grothendieck's inequality and its relation to non-locality in quantum mechanics



Modelling quantum correlation I

Following Tsirelson's thoughts we consider two sets, the set of all "classical" (local) $(m \times n)$ -cross-correlation matrices and the set of all $(m \times n)$ -quantum correlation matrices:



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Modelling quantum correlation I

Following Tsirelson's thoughts we consider two sets, the set of all "classical" (local) $(m \times n)$ -cross-correlation matrices and the set of all $(m \times n)$ -quantum correlation matrices:

(i) Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a ("classical" Kolmogorovian) probability space. Let $A = (a_{ij}) \in \mathbb{M}(m \times n; \mathbb{R})$. $A \in C_{\mathsf{loc}}(m \times n; \mathbb{R})$ iff $a_{ij} = \mathbb{E}_{\mathbb{P}}[X_i Y_j]$, where $X_i, Y_j : \Omega \longrightarrow [-1, 1]$ are random variables - all defined on the same given probability space $(\Omega, \mathcal{F}, \mathbb{P})$.



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- (ii) Let $A = (a_{ij}) \in \mathbb{M}(m \times n; \mathbb{R})$. $A \in QC(m \times n; \mathbb{R})$ iff there are $k, l \in \mathbb{N}$, a density matrix ρ on $\mathcal{B}(H_{k,l})$, where $H_{k,l} := \mathbb{C}^k \otimes \mathbb{C}^l$, and linear operators $A_i \in \mathcal{B}(\mathbb{C}^k)$, $B_j \in \mathcal{B}(\mathbb{C}^l)$ such that $||A_i|| \leq 1$, $||B_j|| \leq 1$ and

$$a_{ij} = \langle \rho, A_i \otimes B_j \rangle = \mathsf{tr}\big(\rho(A_i \otimes B_j)\big) = \mathsf{tr}\big(\rho(A_i \otimes E_l)(E_k \otimes B_j)\big)$$

for all $(i,j) \in [m] \times [n]$.



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Modelling quantum correlation II

Does $QC(m \times n; \mathbb{R})$ relate to our previous investigation of the left side of GT?



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In fact! Tsirelson unrevealed the following characterisation:

Theorem (Tsirelson (1987, 1993))
Let
$$A = (a_{ij}) \in \mathbb{M}(m \times n; \mathbb{R})$$
. TFAE:
(i) $A \in QC(m \times n; \mathbb{R})$.
(ii) $A = \Gamma_{l_2^k}(u, v)$ for some $k \in \mathbb{N}$ and some $u \in (S^{k-1})^m$ and $v \in (S^{k-1})^n$.



Modelling quantum correlation III

$$\Gamma_{l_2^k}(u,v) = \begin{pmatrix} \langle u_1, v_1 \rangle & \langle u_1, v_2 \rangle & \dots & \langle u_1, v_n \rangle \\ \langle u_2, v_1 \rangle & \langle u_2, v_2 \rangle & \dots & \langle u_2, v_n \rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle u_m, v_1 \rangle & \langle u_m, v_2 \rangle & \dots & \langle u_m, v_n \rangle \end{pmatrix}$$

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Modelling quantum correlation III

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 $\Gamma_{l_2^k}(u,v) = UV$ is the product of the matrices $U: l_2^k \longrightarrow l_{\infty}^m$ and $V: l_1^n \longrightarrow l_2^k$, where

$$V := (v_1 | v_2 | \dots | v_n) \text{ and } U := \begin{pmatrix} u_1^\top \\ u_2^\top \\ \vdots \\ u_m^\top \end{pmatrix}.$$



Modelling quantum correlation IV

Hence, we see that if $u \in S_H^m$ and $v \in S_H^n$ one can canonically associate a linear operator to the $(m \times n)$ -matrix $\Gamma_H(u, v)$ which factors through the Hilbert space $H := l_2^k$ such that $\Gamma_H(u, v) = UV$ for some $(m \times k)$ -matrix U and some $(k \times n)$ -matrix V, satisfying

 $\gamma_2(\Gamma_H(u,v)) \le \|U\|_{2,\infty} \cdot \|V\|_{1,2} \le 1$:



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Modelling quantum correlation V

Theorem (Grothendieck (1953), Pisier (2001), Tsirelson (1987))

Let *H* be a separable Hilbert space and $m, n \in \mathbb{N}$. Let $u := (u_1, \ldots, u_m)^\top \in S_H^m$ and $v := (v_1, \ldots, v_n)^\top \in S_H^n$. Then

$$\Gamma_{H}(u,v) \in K_{G}^{\mathbb{R}} \operatorname{cx}(\{pq^{\top} : p \in \{-1,1\}^{m}, q \in \{-1,1\}^{n}\})$$

= $K_{G}^{\mathbb{R}} \operatorname{C}_{loc}(m \times n; \mathbb{R}).$



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$$\begin{split} \Gamma_H(u,v) &\in K_G^{\mathbb{R}} \operatorname{cx}(\{pq^{\top} : p \in \{-1,1\}^m, q \in \{-1,1\}^n\}) \\ &= K_G^{\mathbb{R}} \operatorname{C}_{\operatorname{loc}}(m \times n; \mathbb{R}) \,. \end{split}$$

Corollary (Tsirelson (1987, 1993)) Let $m, n \in \mathbb{N}$. Then

$$QC(m \times n; \mathbb{R}) \subseteq K_G^{\mathbb{R}} C_{loc}(m \times n; \mathbb{R}).$$

Moreover, $C_{loc}(m \times n; \mathbb{R}) \subseteq QC(m \times n; \mathbb{R})$. The latter set inclusion is strict.



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Bell's inequalities and GT I

It is well-known that it is also experimentally verified that entangled composite quantum systems violate certain relations between correlations - known as *Bell's inequalities*.

Bell's inequalities and GT I



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Purely in terms of of a very elementary application of classical Kolmogorovian probability theory - and completely independent of any modelling assumptions in physics - Bell's inequalities can be represented in form of an inequality originating from *J. F. Clauser, M. A. Horne, A. Shimony* and *R. A. Holt* in 1969.


Bell's inequalities and GT II

Lemma (BCHSH Inequality)

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be an arbitrary probability space. Let X_1, X_2, X_3 and X_4 be arbitrary random variables with values in $[-1, 1] \mathbb{P}$ -a.s., all defined on Ω . Then

$$|\mathbb{E}_{\mathbb{P}}[X_1X_2] - \mathbb{E}_{\mathbb{P}}[X_1X_3]| \le 1 - \mathbb{E}_{\mathbb{P}}[X_2X_3]$$





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In particular,

$$|\mathbb{E}_{\mathbb{P}}[X_1X_2] + \mathbb{E}_{\mathbb{P}}[X_1X_3] + \mathbb{E}_{\mathbb{P}}[X_4X_2] - \mathbb{E}_{\mathbb{P}}[X_4X_3]| \le 2$$
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Notice that this result holds independently of the choice of the joint distribution of the rv's X_1, X_2, X_3, X_4 .



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Bell's inequalities and GT II

How is the BCHSH inequality linked with GT?



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In other words:



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Bell's inequalities and GT III

Observation (BCHSH Inequality in matrix form) Let $(\Omega, \mathcal{F}, \mathbb{P})$ be an arbitrary probability space (in the sense of Kolmogorov).



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$$A^{Had} := \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$
 (Hadamard matrix \rightsquigarrow "quantum gate")



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Then

$$|\langle A^{\textit{Had}}, \Gamma \rangle| = |\textit{tr}(A^{\textit{Had}}\Gamma)| \le 2 \text{ for all } \Gamma \in C_{\textit{loc}}(2 \times 2; \mathbb{R}).$$



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Bell's inequalities and GT IV

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Bell's inequalities and GT IV

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$$|\langle A^{Had}, \Gamma_H(u, v) \rangle| = |tr(A^{Had}\Gamma_H(u, v))| \le 2\sqrt{2}$$

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Even more holds!

To this end, we recall the main ideas underlying the EPR/Bell-CHSH experiment.

Bell's inequalities and GT V

A source emits in opposite directions two spin $\frac{1}{2}$ particles created from one particle of spin 0. By rotating magnets perpendicular to the directions of the two spin $\frac{1}{2}$ particles, both, Alice and Bob measure the spin in 2 different directions, leading to angles $-\frac{\pi}{2} \leq \alpha_1, \alpha_2 < \frac{\pi}{2}$ for Alice and $-\frac{\pi}{2} \leq \beta_1, \beta_2 < \frac{\pi}{2}$ for Bob. Only one angle per measurement can be chosen on both sides. The outcome of this experiment is a "random" pair of observables belonging to the set

$$\{(A_1, B_1), (A_1, B_2), (A_2, B_1), (A_2, B_2)\}.$$

Any of these observables takes its values in $\{-1, +1\}$.



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Describing this experiment purely in terms of mathematics we immediately recognise that the Bell-Tsirelson constant $2\sqrt{2}$ is attained by the Hadamard matrix, since:



Bell's inequalities and GT VI

Theorem (EPR/Bell-CHSH violates Bell and attains $2\sqrt{2}$) Consider the Hilbert space $H := \mathbb{C}^2 \otimes \mathbb{C}^2$. Let $H \ni x := \frac{1}{\sqrt{2}} (e_1 \otimes e_1 + e_2 \otimes e_2)$ ("entangled Bell state").



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$$\Gamma^{EPR} := \begin{pmatrix} \langle x, (A_1 \otimes B_1)x \rangle_H & \langle x, (A_1 \otimes B_2)x \rangle_H \\ \langle x, (A_2 \otimes B_1)x \rangle_H & \langle x, (A_2 \otimes B_2)x \rangle_H \end{pmatrix}$$

where $A_i := R(\alpha_i)$, $B_j := R(\beta_j)$ and

$$\mathbb{M}(2 \times 2; \mathbb{C}) \ni R(\varphi) := \begin{pmatrix} \cos(\varphi) & \sin(\varphi) \\ \sin(\varphi) & -\cos(\varphi) \end{pmatrix},$$



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Then $\Gamma^{EPR} \in QC(2 \times 2; \mathbb{R})$ and $|\langle A^{Had}, \Gamma^{EPR} \rangle| = |tr(A^{Had} \Gamma^{EPR})| = 2\sqrt{2} > 2.$