Grothendieck’s inequality and completely correlation preserving functions - a summary of recent results and an indication of related research problems

Frank Oertel

Philosophy, Logic & Scientific Method
Centre for Philosophy of Natural and Social Sciences (CPNSS)
London School of Economics and Political Science
Houghton Street, London WC2A 2AE, UK
f.oertel@email.de

Abstract. As part of the search for the value of the smallest upper bound of the best constant for the famous Grothendieck inequality, the so-called Grothendieck constant (a hard open problem - unsolved since 1953), we provide a further approach, primarily built on functions which map correlation matrices entrywise to correlation matrices by means of the Schur product, multivariate Gaussian analysis, copulas and inversion of suitable Taylor series. We summarise first results and point towards related open problems and topics for future research.

1. Introduction

Despite its emergence more than six decades ago, the techniques and results of the actually pathbreaking work of A. Grothendieck in the metric theory of tensor products are still not widely known nor appreciated. Very likely this is due to the fact that Grothendieck included virtually no proofs, and that he used the (duality) theory of the rather abstract (yet very powerful) notion of tensor products of Banach spaces (cf. [14, 10, 11]). The fundamental idea exploited in [10] is a one-to-one correspondence between Grothendieck’s finitely generated tensor norms and maximal Banach operator ideals (in the sense of Pietsch - cf. [32]) via trace duality. Theory and applications of operator ideals are widely known (not by functional analysts only), as opposed to the tensor norm theory of Grothendieck so that also [10] (such as [11]) is a very valuable source which strongly helps to make Grothendieck’s approach accessible to a wider community.

In particular, the famous Grothendieck inequality (also known as the fundamental theorem...
of the metric theory of tensor products), published in Grothendieck’s famous paper [14] had a profound influence on the geometry of Banach spaces and operator theory in the 1970s and 1980s. Meanwhile, in addition to this impact, Grothendieck’s inequality exhibits deep applications in different directions (including theoretical computer science, computational complexity, analysis of Boolean functions, random graphs (including the mathematics of the systemic risk in financial networks, analysis of nearest-neighbour interactions in a crystal structure (Ising model), correlation clustering and image segmentation in the field of computer vision), NP-hard combinatorial optimisation, non-convex optimisation and semidefinite programming (cf. [15]), foundations and philosophy of quantum mechanics, quantum information theory, quantum correlations, quantum cryptography, communication complexity protocols and even high-dimensional private data analysis (cf. [12])! Also in these fields it offers many challenging related open questions.

The interest in Grothendieck’s work revived when J. Lindenstrauss and A. Pełczyński recast its main results in the more traditional language of operators and matrices (see [23] and [11, Theorem A.3.1]) which is also the basis of our own research. A slightly bit modified version of this rewritten version of Grothendieck’s inequality reads as follows (cf. [13, Lemma 2.2]):

**Grothendieck’s Inequality (Lindenstrauss-Pełczyński style).** Let $F \in \{\mathbb{R}, \mathbb{C}\}$. There is an absolute constant $K > 0$ such that for any $m, n \in \mathbb{N}$, for any $m \times n$ matrix $(a_{ij})$ with entries in $F$, any $F$-Hilbert space $H$ and any vectors $u_1, \ldots, u_m, v_1, \ldots, v_n \in H$ of norm $1$ the following inequality is satisfied:

$$\left| \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} \langle u_i, v_j \rangle_H \right| \leq K \sup \left\{ \left| \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} p_i q_j \right| : |p_i| = |q_j| \forall i, j \right\}.$$

The smallest possible value of the corresponding constant $K$ is called the **Grothendieck constant** $K^G$. The superscripts $\mathbb{R}$ and $\mathbb{C}$ are used to indicate the different values in the real and complex case. The complex constant is smaller than the real one, since (cf. [22, 33]):

**Theorem.**

$$K^C_G \leq e^{1-\gamma} < \frac{\pi}{2} < K^R_G \leq \sqrt{2} K^C_G,$$

where $\gamma := \sum_{n=2}^{\infty} (-1)^n \frac{\zeta(n)}{n} = -\Gamma'(1) \approx 0.577215664901533 \ldots$ denotes the Euler-Mascheroni constant.

Computing the exact numerical value of the constants $K^R_G$ and $K^C_G$ is still an open problem (unsolved since 1953). Here, our own research activities are attached. We look for a general framework (primarily build on methods originating from (block) matrix analysis (cf. [19]), multivariate statistics with real and complex Gaussian random vectors, theory of special functions, modelling of statistical dependence with copulas and combinatorics, whose complexity increases rapidly in dimension, though) which allows us either to give the value of $K^R_G$, respectively $K^C_G$ explicitly or to approximate these values from above and from below at least. Surprisingly, our approach - which in particular allows a short proof of the real Grothendieck inequality, even with Krivine’s upper bound of $K^R_G$ - confronts us strongly with the question whether the seemingly non-avoidable combinatoric complexity actually allows us to determine the values of $K^R_G$, respectively $K^C_G$ explicitly, or not (cf. research problem 7.1 below).
As usual, \( \mathbb{N}_0 := \mathbb{N} \cup \{0\} \) denotes the set of all non-negative integers. Additionally, for any \( k \in \mathbb{N} \), we put \( \mathbb{N}_k := \{n : n \in \mathbb{N} \text{ and } n \geq k\} \). In the case of finite-dimensional Hilbert spaces Grothendieck’s inequality in matrix form is given by the following well-known result:

**Theorem.** Let \( \mathbb{F} \in \{\mathbb{R}, \mathbb{C}\} \). Then for any \( d \in \mathbb{N} \) there is a constant \( K(d) > 0 \) such that

\[
\left| \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} \langle u_i, v_j \rangle \right| \leq K(d) \sup \left\{ \left| \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} p_i q_j \right| : |p_i| = |q_j| \forall i, j \right\},
\]

for any \( m, n \in \mathbb{N} \), for any matrix \((a_{ij}) \in \mathbb{M}(m \times n ; \mathbb{F})\), for any vectors \( u_1, \ldots, u_m, v_1, \ldots, v_n \in \mathbb{S}^{d-1} \). Here, \( \mathbb{S}^{d-1} := \{w : w \in l_2^d \text{ and } \|w\|_2 = 1\} \) denotes the unit sphere of \( l_2^d \equiv l_2^d(\mathbb{F}) \).

**Remark.** Note that we may include the case \( d = 1 \) here, since if \( d = 1 \), \( \|w\| = |w| \) and \( u^* v = v^* u \) for all \( u, v, w \in \mathbb{F} \), implying that by our definition \( \mathbb{S}^0 = \{z \in \mathbb{F} : |z| = 1\} \).

Let \( K^F_G(d) \) denote the smallest possible value of the corresponding constant \( K(d) \). Since the sequence \((K^F_G(d))_{d \in \mathbb{N}} \) obviously is non-decreasing it follows that \( K^F_G = \lim_{d \to \infty} K^F_G(d) = \sup \{K^F_G(d) : d \in \mathbb{N}\} \). Moreover, we may add:

**Proposition.** Let \( d \in \mathbb{N} \). Then

\[
K^F_G(2d) \leq \sqrt{2} K^C_G(d).
\]

In particular, by taking the limit \( d \to \infty \), we reobtain \( K^F_G \leq \sqrt{2} K^C_G \).

An important special case of Grothendieck’s inequality (known as little Grothendieck inequality) appears if just positive semidefinite matrices \( A \) are considered. Let \( k^F_G \) denote the Grothendieck constant, derived from Grothendieck’s inequality restricted to the set of all positive semidefinite \( n \times n \) matrices over \( \mathbb{F} \). Then (cf. [27]):

**Theorem** (A. Grothendieck, 1953; H. Niemi, 1983). Let \( \mathbb{F} \in \{\mathbb{R}, \mathbb{C}\} \) and \( H \) be an arbitrary Hilbert space over \( \mathbb{F} \). Let \( n \in \mathbb{N} \). Then

• \( k^F_G = \frac{\pi}{2} \) \hspace{1em} (A. Grothendieck)

and

• \( k^C_G = \frac{4}{\pi} \) \hspace{1em} (H. Niemi) .

In particular, \( \frac{\pi}{2} \leq K^F_G \) and \( \frac{4}{\pi} \leq K^C_G \).

Until present the following encapsulation of \( K^F_G \) holds (cf. [6] and the related references therein (including [22])):

\[
1,676 < K^F_G \overset{(!)}{=} \frac{\pi}{2 \ln(1 + \sqrt{2})} \approx 1,782.
\]
2. A correlation matrix version of Grothendieck’s inequality

Regarding our approach, the following equivalent reformulation of the Grothendieck inequality (in the following abbreviated by “GT”) which discloses a link to correlation matrices (and hence to multivariate statistics and Gaussian analysis) is of crucial importance. Recall that for fixed \( k \in \mathbb{N} \), the non-negligible set inclusion

\[
\text{C}_1(k; \mathbb{F}) \subseteq \text{acx} \left( \left\{ \sigma_{ij} \mid i,j \in [k] \in \mathcal{M}(k \times k; \mathbb{F}) \right\} \right)
\]

can be shown that \( \sigma_{ii} = 1 \) for all \( i \in [k] \) (i.e., the diagonal of \( \Sigma \) is filled with 1’s only). Of particular relevance is the set \( \text{C}_1(k; \mathbb{F}) \) of all \( k \times k \) correlation matrices of rank 1 and the (Hermitian) block matrix \( J(A) := \frac{1}{2} \begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix} \), where \( m, n \in \mathbb{N} \) and \( A \in \mathcal{M}(m \times n; \mathbb{F}) \). Observe that in the following equivalent reformulation of GT - seemingly - no Hilbert space \( H \) is needed!

**Proposition (correlation matrix version of GT and little GT).** Let \( \mathbb{F} \in \{ \mathbb{R}, \mathbb{C} \} \) and \( m, n \in \mathbb{N} \). Let \( \Sigma \) be an arbitrary \( (m+n) \times (m+n) \) correlation matrix with entries in \( \mathbb{F} \) and \( A \in \mathcal{M}(m \times n; \mathbb{F}) \). Viewing \( A \) as bounded linear operator from \( l^\infty_k \) into \( l^1_{\mathbb{F}} \), we have

\[
|\text{tr}(J(A) \Sigma)| \leq K_G^\mathbb{F} \max_{\Theta \in \Theta_1(m+n;\mathbb{F})} |\text{tr}(J(A) \Theta)| = K_G^\mathbb{F}\|A\|_{2,\infty,1}.
\]

If in addition \( A \) is positive semidefinite then the little GT is equivalent to

\[
|\text{tr}(A^* \Sigma)| \leq K_G^\mathbb{F} \max_{\Theta \in \Theta_1(m+n;\mathbb{F})} |\text{tr}(A^* \Theta)|.
\]

**Observation.** Let \( k \in \mathbb{N} \). As we just have seen the little GT can be equivalently written as

\[
|\text{tr}(B^* \Sigma)| \leq K_G^\mathbb{F} \max_{\Theta \in \Theta_1(k;\mathbb{F})} |\text{tr}(B^* \Theta)| = K_G^\mathbb{F}\|B\|_{2,\infty,1},
\]

where \( B \in \mathcal{M}(k \times k; \mathbb{F}) \) is an arbitrary positive semidefinite matrix and \( \Sigma \) an arbitrary \( k \times k \) correlation matrix with entries in \( \mathbb{F} \). However, we don’t know whether we also may substitute in GT itself the block matrix \( J(A) \) through an arbitrary matrix \( B \in \mathcal{M}(k \times k; \mathbb{F}) \). If this were the case an application of the bipolar theorem shows that the latter would be equivalent to the non-negligible set inclusion

\[
\text{C}(k; \mathbb{F}) \subseteq K_G^\mathbb{F} \text{acx} \left( \left\{ B^* \mid (B^* \Sigma) \subseteq \text{C}_1(k; \mathbb{F}) \right\} \right)
\]

for all \( k \in \mathbb{N} \), where \( \text{C}(k; \mathbb{F}) \) denotes the set of all \( k \times k \) correlation matrices with entries in \( \mathbb{F} \) and \( \text{acx} \) the absolute convex hull (of a set). It can be shown that

\[
\text{C}(k; \mathbb{F}) \subseteq K_G^\mathbb{F} \text{acx} \left( \left\{ xy^\top : (x, y) \in (S^0)^k \times (S^0)^k \right\} \right) = K_G^\mathbb{F} \text{B}_N(l_1^k, l_\infty^k)
\]

though, where \( \text{B}_N(l_1^k, l_\infty^k) \) denotes the unit ball of the Banach space of nuclear operators between \( l_1^k \) and \( l_\infty^k \), equipped with the nuclear norm (which should not be mixed up with \( B_N(l_1^k, l_2^k) = cx(\{xy^\top : \|x\|_2 \|y\|_2 = 1\}) \) (cf. https://convexoptimization.com/T00LS/0976401304.pdf, Example 2.3.2.0.2, equation (97))). This non-trivial functional analytic result (whose proof involves the structure of the set of all quantum correlation matrices (described by B. S. Tsirelson - cf. [31] and cited references therein) and a description of the extreme points of \( B_N(l_1^k, l_\infty^k) \) is not subject of discussion in this document, though.
In fact, if we allow the implementation of a possibly strictly larger absolute constant than $K^\mathbb{R}_G$ it is possible to deduce a further non-trivial inequality - which even implies GT as a corollary! Namely,

**Theorem.** Let $F \in \{\mathbb{R}, \mathbb{C}\}$. Then there exists an absolute constant $K^F_\ast > 1$ such that

$$|\text{tr}(B^* \Sigma)| \leq K^F_\ast \max_{\Theta \in C_1(k;F)} |\text{tr}(B^* \Theta)|,$$

for any $k \in \mathbb{N}$, any $\Sigma \in C(k;F)$ and any $B \in M(k \times k;F)$. Moreover,

$$C(k;F) \subseteq K^F_\ast \acx(C_1(k;F))$$

for all $k \in \mathbb{N}$,

\begin{align*}
K^\mathbb{R}_G \in [K^\mathbb{R}_G, \sinh \left(\frac{\pi}{2}\right)] \quad \text{and} \quad K^\mathbb{C}_G \in [K^\mathbb{C}_G, \frac{2}{\pi} - 1].
\end{align*}

3. **Grothendieck’s identity and Haagerup’s idendity: a common source**

The main ingredients of the proof of GT are two *equalities*, namely Grothendieck’s identity (if $F = \mathbb{R}$ - cf. e.g. the proof of [11, Prop. 4.4.2]) and Haagerup’s identity (if $F = \mathbb{C}$ - see [17]). Rewritten in terms of real Gaussian random vectors (if $F = \mathbb{R}$) and complex proper Gaussian random vectors (if $F = \mathbb{C}$) they imply the following two results, revealing a common underlying structure for both fields, $\mathbb{R}$ and $\mathbb{C}$. To this end, recall (e.g. from [1]) that for any $a, b \in \mathbb{C}$, any $c \in \mathbb{C} \setminus \{-n : n \in \mathbb{N}_0\}$ and any $z \in \mathbb{D} = \{z \in \mathbb{C} : |z| < 1\}$ the well-defined power series

$$2F_1(a, b, c; z) := \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)} \frac{z^n}{n!}$$

denotes the *Gaussian hypergeometric function*. If in addition $\Re(c) > \Re(a+b)$ then the series converges absolutely on $\partial \mathbb{D} = \{z \in \mathbb{C} : |z| = 1\}$ and satisfies $2F_1(a, b, c; 1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}$ (Gauss’ Summation Theorem).

**Grothendieck’s Identity.** Let $n \in \mathbb{N}$, $u, v \in \mathbb{R}^n$ such that $\|u\| = 1$ and $\|v\| = 1$ and $X \sim N_n(0, I_n)$ be a standard-normally distributed real Gaussian random vector. Then

$$\int_{\mathbb{S}^{n-1}} \sgn(u^\top x)\sgn(v^\top x) s^{n-1} \, dx = \mathbb{E}[\sgn(u^\top X)\sgn(v^\top X)] = \frac{2}{\pi} \arcsin (u^\top v)$$

$$= \mathbb{E}[\|X_\perp\|^2] u^\top v 2F_1 \left(1; \frac{1}{2}, \frac{3}{2}; |u^\top v|^2\right),$$

where $s^{n-1} := \frac{\Gamma(n/2)}{2\pi^{n/2}} s^{n-1}$ denotes the normalised (“uniform”) surface area probability measure on the unit sphere $\mathbb{S}^{n-1}$ and $\mathbb{P}(X_\perp \cdot) = \gamma_n$ the Gaussian probability measure on $\mathbb{R}^n$.

**Remark.** If $n = 1$, we put $\sigma^0(\mathbb{S}^0) = \sigma^0(\{-1, 1\}) := 2.$

**Haagerup’s Identity.** Let $n \in \mathbb{N}$, $u, v \in \mathbb{C}^n$ such that $\|u\| = 1$ and $\|v\| = 1$. Let $Z \sim \mathbb{C}N_n(0, I_n)$ be a standard-normally distributed complex proper Gaussian random vector. Then
\[
\int_{C^n} \text{sign}(u^*z) \text{sign}(v^*z) \gamma_n^{(C)}(dz) = \mathbb{E}[\text{sign}(u^*Z)\text{sign}(v^*Z)] = \text{sign}(u^*v) \frac{1}{4} \int_0^{2\pi} \arcsin(|u^*v| \cos(t)) \cos(t) \, dt
\]
\[
= \frac{\pi}{4} u^*v F_1 \left( \frac{1}{2}, \frac{1}{2}; 2; |u^*v|^2 \right) = \mathbb{E}[|Z_1|^2] u^*v F_1 \left( \frac{1}{2}, \frac{1}{2}; 2; |u^*v|^2 \right),
\]

where \( \gamma_n^{(C)}(B) := \gamma_n^{(R)} \left( \{ (\sqrt{2} R(z)^\top, \sqrt{2} S(z)^\top) : z \in B \} \right) \) \((B \in B(C^n))\) denotes the Gaussian probability measure on \(C^n\).

**Observation.** If in addition \( u^*v \neq 0 \), we may add the following real spherical integral representation in Haagerup’s identity:

\[
\int_{C^n} \text{sign}(u^*z) \text{sign}(v^*z) \gamma_n^{(C)}(dz) = \text{sign}(u^*v) \mathbb{E}[f_{u,v}(Z)] = \text{sign}(u^*v) \int_{S^{2n-1}} \mathbb{R}(f_{u,v}(x+iy)) \gamma_{2n-1}(d(x, y)),
\]

where \( C^n \ni z \mapsto f_{u,v}(z) := \frac{1}{\text{sign}(u^*v)} \text{sign}(u^*z) \text{sign}(v^*z) \).

It can be shown that both identities arise as a special case of the following result, where we explicitly describe all non-negative integer powers of an expectation of inner products of suitably correlated - real - Gaussian random vectors. Here, we possibly should point to the so-called kernel trick, used also for the computation of inner products in high-dimensional feature spaces using simple functions defined on pairs of input patterns which is a crucial ingredient of support vector machines in statistical learning theory; i.e., learning machines that construct decision functions of sign type. This trick allows the formulation of nonlinear variants of any algorithm that can be cast in terms of inner products (cf. [41, Chapter 5.6]).

To this end, let us consider the real correlation matrices

\[
\Sigma_{2d}(\rho) := \left( \begin{array}{cc}
I_d & \rho I_d \\
\rho I_d & I_d
\end{array} \right) =
\begin{pmatrix}
1 & 0 & \ldots & 0 & \rho & 0 & \ldots & 0 \\
0 & 1 & \ldots & 0 & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & 1 & 0 & \ldots & \rho \\
\rho & 0 & \ldots & 0 & 1 & \ldots & 0 \\
0 & \rho & \ldots & 0 & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & \rho & 0 & \ldots & 0 & 1
\end{pmatrix},
\]

where \(-1 \leq \rho \leq 1\) and \(d \in \mathbb{N}\).

**Theorem.** Let \(d, m \in \mathbb{N}, \rho \in (-1, 1)\) and \((X^\top, Y^\top) \sim (X_1, \ldots, X_d, Y_1, \ldots, Y_d)^\top \sim N_{2d}(0, \Sigma_{2d}(\rho))\).

(i) If \(m\) is odd then

\[-1 \leq \mathbb{E}\left[ \frac{X}{\|X\|_{t_1^2}} \frac{Y}{\|Y\|_{t_1^2}} \right]^{m} = c_m(d, m)(1-\rho^2)^{\frac{d}{2}} \rho \frac{\Gamma\left(\frac{d+1}{2}\right) \Gamma\left(\frac{m+2}{2}\right)}{2 \Gamma\left(\frac{m+4}{2}\right)} \leq 1,
\]

where

\[c_m(d, m) := \frac{2}{\sqrt{\pi}} \frac{\Gamma\left(\frac{d+1}{2}\right) \Gamma\left(\frac{m+2}{2}\right)}{\Gamma\left(\frac{m+4}{2}\right)}.
\]
(ii) If \( m \) is even then
\[
-1 \leq \mathbb{E} \left[ \left\langle \frac{X}{\|X\|_{l_2^d}}, \frac{Y}{\|Y\|_{l_2^d}} \right\rangle^m \right] = c_+(d, m) \left( 1 - \rho^2 \right)^{\frac{m}{2}} 3F_2 \left( \frac{d}{2}, \frac{d}{2}, \frac{m+1}{2}, \frac{m+d}{2}; \rho^2 \right) \leq 1,
\]
where
\[
c_+(d, m) := \frac{1}{\sqrt{\pi}} \frac{\Gamma \left( \frac{d}{2} \right) \Gamma \left( \frac{m+1}{2} \right)}{\Gamma \left( \frac{m+2}{2} \right)}.
\]
If we apply the latter result to \( m = 1 \) (and \( d \in \mathbb{N} \)), we obtain a result which contains [7], Lemma 2.1 as a special case if \( \rho \in (-1, 1) \). Clearly, that result also holds for \( \rho \in \{-1, 1\} \).

Corollary. Let \( d \in \mathbb{N}, \rho \in [-1, 1] \) and \( (X^\top, Y^\top) \equiv (X_1, \ldots, X_d, Y_1, \ldots, Y_d)^\top \sim N_{2d}(0, \Sigma_{2d}(\rho)) \). Then
\[
-1 \leq \mathbb{E} \left[ \left\langle \frac{X}{\|X\|_{l_2^d}}, \frac{Y}{\|Y\|_{l_2^d}} \right\rangle^2 \right] = c_d \rho \, 2F_1 \left( \frac{1}{2}, \frac{1}{2}, \frac{1+d}{2}; \rho^2 \right) \leq 1,
\]
where
\[
c_d := \frac{1}{2} 2F_1 \left( \frac{1}{2}, \frac{1}{2}, \frac{2+d}{2}; 1 \right) = \frac{2 \Gamma \left( \frac{d+1}{2} \right)^2}{d \Gamma \left( \frac{d}{2} \right)^2} = \frac{1}{\sqrt{\mathbb{E}[\|X\|_{l_2^d}^2]}}.
\]

Observation. This result (respectively [7, Lemma 2.1]) shows why in the real case as well as the complex case the function sign works so smoothly. Since if we choose sign then we obtain in both cases an inner product (where \( \langle x, y \rangle_{l_2^d} := x \cdot y \) for all \( x, y \in \mathbb{R} \equiv l_2^d \), of course). In particular, observe that for all \( m \in \mathbb{N} \) \( c_-(1, m) = \frac{2}{\pi}, c_+(1, m) = 1 \) and \( 2F_1 \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{2}; \rho^2 \right) = \arcsin'(\rho) = \frac{1}{\sqrt{1-\rho^2}} \) for all \( \rho \in (-1, 1) \). Another observation which actually leads to a straightforward and short proof is the fact that in our calculation of the related multiple integral we also implement the probability space \( (\Omega_d, \mathcal{B}(\Omega_d), \mathbb{P}_d) \), where
\[
\Omega_d := S^{d-1} \times S^{d-1}, \mathbb{P}_d := \sigma_d \otimes \sigma_d
\]
and \( \mathcal{B}(\Omega_d) \) denotes the Borel sigma-algebra on \( \Omega_d \).

However, in [6] the authors show that in fact \( K^{\mathbb{R}}_G < \frac{\pi}{2 \ln(1+\sqrt{2})} \), implying that in the real case sign is not the “optimal” function to choose (answering a question of H. König to the negative (see [21])!

## 4. Completely correlation preserving functions and their impact on the upper bound of the Grothendieck constant

Already while looking for the smallest upper bound of both, \( K^{\mathbb{R}}_G \) and \( K^{\mathbb{C}}_G \), we are lead to a deep interplay of different subfields of mathematics (both, pure and applied) including Gaussian harmonic analysis and Malliavin calculus (Mehler kernel, Ornstein-Uhlenbeck semigroup, Hermite polynomials, Gegenbauer polynomials*, integration over spheres in \( \mathbb{R}^n \)), complex

---

*also known as ultraspherical polynomials
analysis (analytic continuation and biholomorphic mappings, special functions), combinatorial analysis (inversion of Taylor series and ordinary partial Bell polynomials), matrix analysis (positive semidefinite matrices, block matrices) and multivariate statistics and high-dimensional Gaussian dependence modelling (correlation matrices, real and complex Gaussian random vectors, Gaussian measure).

In particular, we have to look for those functions which map correlation matrices of any size and any rank entrywise into a correlation matrix of the same size again, by means of the so-called Schur product (also known as Hadamard product) of matrices:

**Definition** (Schur product). Let $m, n \in \mathbb{N}$. Let $A = (a_{ij}) \in \mathbb{M}(m \times n; \mathbb{F})$ and $B = (b_{ij}) \in \mathbb{M}(m \times n; \mathbb{F})$. The Schur product $A \ast B \in \mathbb{M}(m \times n; \mathbb{F})$ is defined as

$$(A \ast B)_{ij} := a_{ij} b_{ij} \quad ((i, j) \in [m] \times [n]).$$

The usefulness of the Schur product structure is reflected in the Schur product theorem which states that the (closed and convex) cone of all positive semidefinite matrices is stable under Schur multiplication:

**Theorem** (Schur, 1911). Let $m, n \in \mathbb{N}$. Let $A = (a_{ij}) \in \mathbb{M}(m \times n; \mathbb{F})$ and $B = (b_{ij}) \in \mathbb{M}(m \times n; \mathbb{F})$. If both, $A$ and $B$ are positive semidefinite then also $A \ast B$ is positive semidefinite.

In particular, for any $k \in \mathbb{N}$ the Schur product of two $k \times k$ correlation matrices of the same size again is a $k \times k$ correlation matrix.

**Definition.** Let $m, n \in \mathbb{N}$. Given $\emptyset \neq U \subseteq \mathbb{F}$, a function $f : U \rightarrow \mathbb{F}$ and a matrix $A = (a_{ij}) \in \mathbb{M}(m \times n; U)$ put

$$f[A] := (f(a_{ij})) \quad ((i, j) \in [m] \times [n]).$$

In particular, if $f(x) = \sum_{n=0}^{\infty} c_n x^n$, $x \in U$, where $c_n \in \mathbb{F}$ for all $n \in \mathbb{N}$, we have

$$f[A]_{ij} = \sum_{n=1}^{\infty} c_n a_{ij}^n \quad \text{for all} \quad (i, j) \in [m] \times [n].$$

Functions of the latter type, where $c_n \geq 0$ for all $n \in \mathbb{N}$ play a significant role, also with respect to an analysis of $K^G_F$. This is due to the following (cf. [4, Theorem 2.1])

**Theorem** (Schoenberg, 1942; Rudin, 1959). Let $f : [-1, 1] \rightarrow \mathbb{R}$ be a function. Then the following statements are equivalent:

(i) $f$ is continuous and $f[A]$ is positive semidefinite for all positive semidefinite matrices $A$ with entries in $[-1, 1]$ and of any size.

(ii) $f[A]$ is positive semidefinite for all positive semidefinite matrices $A$ with entries in $[-1, 1]$ and of any size.

(iii) $f(x) = \sum_{n=0}^{\infty} a_n x^n$ for all $x \in [-1, 1]$, where $a_n \geq 0$ for all $n \in \mathbb{N}_0$ and $(a_n)_{n \in \mathbb{N}_0} \in l_1$. 

8
Corollary. Built on these facts, Grothendieck’s identity implies the following theorem.

Let $f$ be a function. Then the following statements are equivalent:

(i) Given $n \in \mathbb{N}$, $g$ is $n$-correlation-preserving (short: $n$-CP) if for any $n \times n$ correlation matrix $\Sigma \in C(n; \mathbb{F})$ also $g[\Sigma] \in C(n; \mathbb{F})$ is an $n \times n$ correlation matrix.

(ii) $g$ is called completely correlation-preserving (short: CCP) if $g$ is $n$-correlation-preserving for all $n \in \mathbb{N}$.

Obviously, every CCP function $g$ satisfies $g(\mathbb{D}_d) \subseteq \mathbb{D}_d$. Since any positive semidefinite matrix factors through a correlation matrix (with respect to the standard matrix product), we obtain the following result, given that $\mathbb{F}_1 = \mathbb{R}$:

**Theorem.** Let $g : [-1, 1] \rightarrow \mathbb{R}$ be a function. Then the following statements are equivalent:

(i) $g$ is CCP.

(ii) $g(1) = 1$ and $g[A]$ is positive semidefinite for all positive semidefinite matrices $A$ with entries in $[-1, 1]$ and of any size.

(iii) $g(\rho) = \sum_{n=0}^{\infty} a_n \rho^n$ for all $\rho \in [-1, 1]$, where $a_n \geq 0$ for all $n \in \mathbb{N}_0$ and $(a_n)_{n \in \mathbb{N}_0} \in S_1$.

(iv) $g(\rho) = \mathbb{E}_{\mathbb{P}}[\rho^X] = \sum_{n=0}^{\infty} \mathbb{P}(X = k) \rho^k$ is the probability generating function of some discrete random variable $X : \Omega \rightarrow \mathbb{N}_0$, defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$.

Built on these facts, Grothendieck’s identity implies the following

**Corollary** (Grothendieck’s identity as entrywise matrix equality). Let $k \in \mathbb{N}$ and $\Sigma \in C(k; \mathbb{R})$ be an arbitrarily given $k \times k$ correlation matrix. Then also $\frac{2}{\pi} \arcsin[\Sigma] \in C(k; \mathbb{R})$ is a $k \times k$ correlation matrix. There exist column vectors $u_1, u_2, \ldots, u_k \in \mathbb{S}^{k-1}$ such that for any $X \equiv (X_1, \ldots, X_k) \sim N_k(0, I_k)$

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

where the random matrix $\Theta(u) \equiv \Theta(\text{vec}(u_1, \ldots, u_k))$ is given as

$$\Theta(u)_{ij} := \text{sign}(\langle X, u_i \rangle) \text{sign}(\langle X, u_j \rangle)$$

for all $i, j \in [k]$. $\Theta(u) = \text{sign}\left[\left(\bigoplus_{i=1}^{k} X^\top\right)u\right] \text{sign}\left[\left(\bigoplus_{i=1}^{k} X^\top\right)u\right] \sim$ is a random correlation matrix of rank 1.
Let $d \in \{1, 2\}$ and put $\mathbb{T}_d := \partial \mathbb{D}_d := \{ z \in \mathbb{F}_d : |z| = 1 \}$. Another important estimation (even with upper bound 1) which might support our search for a “suitable” CCP function which is different from the CCP function $\frac{2}{\pi} \arcsin$ is the following one

**Proposition.** Let $d \in \{1, 2\}$, $z \in \overline{\mathbb{D}_d}$ and $b: \mathbb{F}_d \to \mathbb{T}_d$. Let $h_b: \overline{\mathbb{D}_d} \to \overline{\mathbb{D}_d}$ be a function such that

$$h_b(z) = \mathbb{E}[b(Z) b(W)]$$

for any $z \in \overline{\mathbb{D}_d}$ and any $(Z, W)^\top \sim \mathbb{F}_d \mathcal{N}_2(0, \Sigma_2(z))$. Then

(i) For all $k \in \mathbb{N}$ and $\Sigma \in C(k; \mathbb{F}_d)$,

$$h_b[\Sigma] \in C(k; \mathbb{F}_d).$$

(ii) For all $k \in \mathbb{N}$, $\Sigma \in C(k; \mathbb{F}_d)$ and $A \in \mathbb{M}(k \times k; \mathbb{F}_d)$,

$$|\text{tr}(A^* h_b[\Sigma])| \leq \max_{\Theta \in G_{1}(k; \mathbb{F}_d)} |\text{tr}(A^* \Theta)|.$$ 

Moreover, $h_b(1) = 1$ and $h_b(0) = |\mathbb{E}[b(Z)]|^2$ for any $Z \in \mathbb{F}_d \mathcal{N}_1(0, 1)$.

**Observation.** In the statistical learning community in artificial intelligence a function $b: \mathbb{R}^k \to \{-1, 1\}, k \in \mathbb{N}$ is called “concept” (cf. e.g. [37]). We adopt this name. If the function $h_b$ were invertible, for some $b$ then $h_b^{-1}$ cannot be a CCP function (else $K_{G}^F \leq 1$ (!) - a contradiction). In particular, $h_b^{-1}$ cannot be represented as a power series with non-negative coefficients, such as e.g. $h_{\text{sign}}^{-1}(y) = \sin \left( \frac{\pi}{2} y \right) = \sum_{n=0}^{\infty} (-1)^n \frac{\pi^{2n+1}}{2^{2n+1}(2n+1)!} y^{2n+1}$, $y \in [-1, 1]$ if we consider $h_{\text{sign}}(x) = \frac{2}{\pi} \arcsin(x)$, $x \in [-1, 1]$.

However, we will see that inversion of CCP functions plays the key role regarding the search for the lowest upper bound of the Grothendieck constant $K_{G}^F$. Unfortunately, a closed form representation of the coefficients of the inverse of a Taylor series runs against a well-known combinatorial complexity issue (due to the presence of ordinary partial Bell polynomials as building blocks of these coefficients - cf. research problem 7.1 below for details), which in general does not allow a closed form representation of these coefficients, such as is the case with the inverse of Haagerup’s function $\overline{\mathbb{D}} \ni z \mapsto \frac{\pi}{4} z^2 \mathcal{F}_1 \left( \frac{1}{2}, \frac{1}{2}; 2; |z|^2 \right)$ in the complex case (cf. [17], Remark on page 216), as opposed to Grothendieck’s function $[-1, 1] \ni \rho \mapsto \frac{2}{\pi} \rho^2 \mathcal{F}_1 \left( \frac{1}{2}, \frac{1}{2}, \frac{3}{2}; \rho^2 \right) = \frac{2}{\pi} \arcsin(\rho)$ in the real case. Clearly, further research is here required (as indicated below).

Keeping inversion of CCP functions in mind we now are going to present two key results of our research.

**Theorem.** Let $d \in \{1, 2\}$ and $m, n \in \mathbb{N}$. Let $A \in \mathbb{M}(m \times m; \mathbb{F}_d)$ and $B \in \mathbb{M}(n \times n; \mathbb{F}_d)$ be positive semidefinite and $Z \in \mathbb{M}(m \times n; \mathbb{F}_d)$. Let $f: \overline{\mathbb{D}_d} \to \mathbb{F}_d$ and $g: \overline{\mathbb{D}_d} \to \mathbb{F}_d$ be functions. Suppose that $f$ can be represented as $f(z) = \sum_{n=1}^{\infty} a_n z^n$ for all $z \in \overline{\mathbb{D}_d}$, where $a_n \geq 0$ for all $n \in \mathbb{N}$. Assume that $g$ can be represented as $g_b(z) = \sum_{n=1}^{\infty} b_n z^n$ for all $z \in \overline{\mathbb{D}_d}$, where $b_n \in \mathbb{F}_d$ for all $n \in \mathbb{N}$. Assume further that

$$|b_n| \leq a_n \text{ for all } n \in \mathbb{N}.$$
If the block matrix
\[ \Sigma := \begin{pmatrix} A & Z \\ Z^* & B \end{pmatrix} \]
is positive semidefinite, and if all matrices \(A, B\) and \(Z\) have entries in \(\mathbb{D}_d\) then also the block matrix
\[ \Sigma_{f,g} := \begin{pmatrix} f[A] & g[Z] \\ g[Z]^* & f[B] \end{pmatrix} \]
is positive semidefinite. If in addition \(f(r) = 1\) for some \(0 < r \leq 1\), and if \(\Sigma \in C(m+n, \mathbb{F}_d)\) is a correlation matrix then also \((r\Sigma)_{f,g} \in C(m+n, \mathbb{F}_d)\) is a correlation matrix.

To prepare the underlying ideas of our next result, we carefully list the single steps and assumptions, possibly leading to an algorithmic approach regarding the implementation of an approximation to the lowest upper bound of the Grothendieck constant \(K_{FG}\). All of these conditions are satisfied for the Grothendieck function and the Haagerup function and were used to construct a “small” upper bound of the respective Grothendieck constant. However, if we wish to apply these steps to a “better fitting function” \(b\) which is different from both, the Grothendieck function and the Haagerup function, we are strongly confronted with non-trivial persistent combinatorial issues; described in Section 5 below.

So, fix \(d \in \{1, 2\}\) and consider the following workflow step by step.

(SIGN) Choose a function \(b : \mathbb{F}_d^k \rightarrow \mathbb{T}_d\) for some “suitable” \(k \in \mathbb{N}\) and consider its allocated CCP function \(h_b\), constructed according to the lines of the above Proposition (such as e.g. the Grothendieck function, respectively the Haagerup function \(h_{sign}\)).

(H) Assume that \(h_b(0) = 0\) and that \(h_b : \mathbb{D}_d \rightarrow \mathbb{D}_d\) is a homeomorphism.

(RA) Assume that \(g_b := h_b^{-1} : \mathbb{D}_d \rightarrow \mathbb{D}_d\) can be represented as \(g_b(z) = \sum_{n=1}^{\infty} \beta_n z^n\) for all \(z \in \mathbb{D}_d\), where \(\beta_n \in \mathbb{R}\) (!) for all \(n \in \mathbb{N}\) and \(\beta \equiv (\beta_n)_{n \in \mathbb{N}} \in \ell_1\); i.e., \(\|\beta\|_1 \equiv \sum_{n=1}^{\infty} |\beta_n| < \infty\).

(ABS) Put \(f_b(z) := \sum_{n=1}^{\infty} |\beta_n| z^n\) (\(z \in \mathbb{D}_d\)).

(PI(1)) Assume that \(f_b(r) = 1\) for some \(0 < r < 1\).

Clearly, we have \(1 = g_b(1) = \sum_{n=1}^{\infty} \beta_n \leq \|\beta\|_1 = f_b(1)\). Moreover, \(|f_b(rz)| \leq f_b(r) = 1\) for any \(z \in \mathbb{D}_d\), implying that \(\mathbb{D}_d \ni h_b \circ f_b(rz) = h_b(f_b(rz))\) is well-defined if \(z \in \mathbb{D}_d\). Note that \(r\) depends on the choice of \(b\).

Let \(k \in \mathbb{N}\). Fix an arbitrary correlation matrix
\[ \Sigma = \begin{pmatrix} A & Z \\ Z^* & B \end{pmatrix} \in C(2k, \mathbb{F}_d) . \]
Combining the previous two results and since \( g_b(z) = g_b(z) \) it therefore follows that

\[
\Sigma_b(r) := \begin{pmatrix} h_b \circ f_b[r A] & r Z \\ r Z^* & h_b \circ f_b[r B] \end{pmatrix} = h_b \left[ \begin{pmatrix} f_b[r A] & g_b[r Z] \\ (g_b[r Z])^* & f_b[r B] \end{pmatrix} \right] \in C(2k, \mathbb{F}_d)
\]

again is a correlation matrix. Consequently, we have

\[
 r |\text{tr}(J(A) \Sigma)| = |\text{tr}(J(A) (r \Sigma))| = |\text{tr}(J(A) \Sigma_b(r))| \leq K_G^r \|A\|_{\infty,1},
\]

and hence

**Theorem.** Let \( k \in \mathbb{N}, d \in \{1, 2\}, b : \mathbb{F}_d^k \rightarrow \mathbb{T}_d \) and \( h_b : \mathbb{D}_d \rightarrow \mathbb{D}_d \) the allocated CCP function. Assume that the assumptions (H) and (RA) of the workflow hold. Let \( f_b : \mathbb{D}_d \rightarrow \mathbb{F}_d \) be constructed as above and assume that \( f_b \) satisfies the condition (PI(1)) for some \( 0 < r^* < 1 \). Then

\[
K_G^r \leq \frac{r^*}{r^*}.
\]

**Example** (Krivine’s upper bound reproduced). Let \( \mathbb{F} = \mathbb{R} \). Consider \( b := \text{sign} \). Due to Grothendieck’s identity we know that

\[
h_b(\rho) = \frac{2}{\pi} \arcsin(\rho) \text{ for all } \rho \in [-1, 1].
\]

The continuous function \( h_b : [-1, 1] \rightarrow [-1, 1] \) is strictly increasing and hence invertible, with continuous inverse

\[
g_b(\tau) := h_b^{-1}(\tau) = \sin \left( \frac{\pi}{2} \tau \right) = \sum_{n=0}^{\infty} (-1)^n \frac{\pi^{2n+1}}{2^{2n+1} (2n + 1)!} \tau^{2n+1} \quad (\tau \in [-1, 1]).
\]

Hence,

\[
f_b(\tau) = \sum_{n=0}^{\infty} \frac{\pi^{2n+1}}{2^{2n+1} (2n + 1)!} \tau^{2n+1} = \frac{1}{i} \sin \left( \frac{\pi}{2} i \tau \right) = \sinh \left( \frac{\pi}{2} \tau \right) \quad (\tau \in [-1, 1]).
\]

Since \( f_b \left( \frac{2 \ln(1 + \sqrt{2})}{\pi} \right) = 1 \) it follows that

\[
K_G^r = \frac{\pi}{2 \ln(1 + \sqrt{2})}.
\]

5. **Emerging research problems**

Not very surprisingly, the long-standing, intensive and technically quite demanding attempts to detect the - still not available - value of the both Grothendieck constants (open since 1953) leads to further challenging tasks and open problems, such as the following ones; addressed in particular to highly motivated students who also wish to get a better understanding of the reasons underlying these difficulties.
5.1. Research problem 1: Grothendieck’s constant versus Taylor series inversion

Only between 2011 and 2013 it was shown (cf. [6]) that $K_G^\mathbb{R}$ is strictly smaller than Krivine’s upper bound, stating that $K_G^\mathbb{R} < \frac{\pi}{2\ln(1+\sqrt{2})}$. Consequently, in the real case sign is not the “optimal” function to choose (answering a question of H. König to the negative - cf. [21]). So, if we wish to reduce the value of the upper bound of the real Grothendieck constant we have to look for functions $b : \mathbb{R}^k \to \{-1, 1\}$ which are different from sign : $\mathbb{R} \to \{-1, 1\}$. However, these functions should satisfy all of the conditions in the listed workflow above.

In particular, we have to look for both, the coefficients of the Taylor series of $h_b$ and the coefficients of the Taylor series of the inverse function $g_b := h_b^{-1}$. It is well-known that the latter task increases strongly in computational complexity if we want to calculate such Taylor coefficients of a higher degree, leading to the involvement of non-trivial combinatorial facts, reflected in the use of partitions of positive integers and partial exponential Bell polynomials as part of the Taylor coefficients of the inverse Taylor series (a thorough introduction to this framework including the related Lagrange-Bürmann inversion formula is given in [20, 8]).

To reveal the origin of these difficulties let us focus on the real case, with $k = 1$. First note that

$$h_b(\rho) = \sum_{n=1}^{\infty} \langle b, H_n \rangle^2_{\gamma_1} \rho^n$$

for all $\rho \in [-1, 1]$, where for $n \in \mathbb{N}$ and $x \in \mathbb{R}$

$$H_n(x) := \frac{1}{\sqrt{n!}} (-1)^n \exp \left( \frac{x^2}{2} \right) \frac{d^n}{dx^n} \exp \left( -\frac{x^2}{2} \right)$$

denotes the (probabilistic version of the) $n$-th Hermite polynomial and $\gamma_1$ the Gaussian measure on $\mathbb{R}$ (cf. e.g. [5]). Put $0 \leq \alpha_0 := \langle b, H_n \rangle^2_{\gamma_1}$. If $h_b'(0) \neq 0$ we know that at least the real-analytic function $h_b | (-1, 1)$ is invertible around $0 = h_b(0)$. Its inverse is also expressible as a power series there; i.e., around $0$, $(h_b | (-1, 1))^{-1}$ is real-analytic, too. Hence, given the assumption (RA) it follows that $h_b^{-1}(y) = g_b(y) = \sum_{n=1}^{\infty} \beta_n y^n$ for all $y \in [-1, 1]$, where $\beta_1 = \frac{1}{\alpha_1}$ and

$$\beta_n = \frac{1}{n} \sum_{k=1}^{n-1} \frac{1}{\alpha_1^{n+k}} (-1)^k \binom{n-1+k}{k} B_{n-1,k}^\circ (\alpha_2, \alpha_3, \ldots, \alpha_{n-k+1})$$

$$= \frac{1}{n} \sum_{k=1}^{n-1} (-1)^k \binom{n-1+k}{k} B_{n-1,k}^\circ (\alpha_2, \alpha_3 \alpha_1, \alpha_4 \alpha_1^2, \ldots, \alpha_{n-k+1} \alpha_1^{n-k})$$

for all $n \in \mathbb{N}_2$. Thereby,

$$B_{n,k}^\circ (x_1, x_2, \ldots, x_{n+1-k}) := \sum_{\nu \in P(n,k)} \frac{k!}{\prod_{i=1}^{n+1-k} \nu_i !} \prod_{i=1}^{n+1-k} x_i^{\nu_i}$$

denotes the ordinary partial Bell polynomial and $P(n,k)$ indicates the set of all multi-indices $\nu = (\nu_1, \nu_2, \ldots, \nu_{n+1-k}) \in \mathbb{N}_0^{n+1-k}$ ($k \leq n$) which satisfy the Diophantine equations $\sum_{i=1}^{n+1-k} \nu_i = k$ and $\sum_{i=1}^{n+1-k} i \nu_i = n$; i.e., summation is extended over all partitions of the
number $n$ into exactly $k$ summands (cf. e.g. [8, 9, 25]). We explicitly list $\beta_2, \beta_3, \beta_4, \beta_5, \beta_6$ and $\beta_7$:

$$
\beta_2 \alpha_1^3 = -\alpha_2, \\
\beta_3 \alpha_1^5 = -\alpha_1 \alpha_3 + 2 \alpha_2^2, \\
\beta_4 \alpha_1^7 = -\alpha_1^2 \alpha_4 + 5 \alpha_1 \alpha_2 \alpha_3 - 5 \alpha_2^3, \\
\beta_5 \alpha_1^9 = -\alpha_1^3 \alpha_5 + 6 \alpha_1^2 \alpha_2 \alpha_4 + 3 \alpha_1^2 \alpha_3^2 - 21 \alpha_1 \alpha_2^2 \alpha_3 + 14 \alpha_4^2, \\
\beta_6 \alpha_1^{11} = -\alpha_1^4 \alpha_6 + 7 \alpha_1^3 \alpha_2 \alpha_5 + 7 \alpha_1^3 \alpha_3 \alpha_4 - 28 \alpha_1^2 \alpha_2 \alpha_3^2 - 28 \alpha_1 \alpha_2^2 \alpha_4 + 84 \alpha_1 \alpha_2^2 \alpha_3 - 42 \alpha_2^5, \\
\beta_7 \alpha_1^{13} = -\alpha_1^5 \alpha_7 + 8 \alpha_1^4 \alpha_2 \alpha_6 + 8 \alpha_1^4 \alpha_3 \alpha_5 + 4 \alpha_1^4 \alpha_4^2 - 36 \alpha_1^3 \alpha_2^2 \alpha_5 - 72 \alpha_1^3 \alpha_2 \alpha_3 \alpha_4 \\
-12 \alpha_1^3 \alpha_3^3 + 120 \alpha_1^3 \alpha_2^2 \alpha_4 + 180 \alpha_1^2 \alpha_2 \alpha_3 \alpha_5 - 330 \alpha_1 \alpha_2^2 \alpha_3^2 + 132 \alpha_2^6.
$$

It appears to us that there is a general pattern in these formulas which might lead to an expression of the following type:

$$
n \beta_n \alpha_1^{2n-1} = -\alpha_1^{n-2} \alpha_n + \sum_{k=2}^{n-2} (-1)^k m_k \binom{2n-1}{k} \alpha_1^{(n-1)-k} p_k(\alpha_2, \alpha_3, \ldots, \alpha_n) + (-1)^{n-1} \frac{2n-1}{n-1},
$$

where $m_k \in [k]$, $p_k(\alpha_2, \alpha_3, \ldots, \alpha_n) := \sum_{(\nu_2, \ldots, \nu_n) \in \mathbb{A}_k} \prod_{l=2}^{n} \alpha_l^{\nu_l}$ and $\mathbb{A}_k \subset \{ \mu \in \mathbb{N}^{n-1}: \sum_{l=2}^{n} l \mu_{l-1} = n - 1 + k \}$.

The strong difficulties are twofold: already in the one-dimensional case we need to know the explicit value of all of the Fourier coefficients

$$
\langle b, H_n \rangle_{\gamma_1} = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} b(x) H_n(x) \exp \left( -\frac{1}{2} x^2 \right) \, dx = \mathbb{E}[b(X) H_n(X)] = \frac{d^n}{dt^n} \mathbb{E}[b(X + t)] \big|_{t=0},
$$

where $X \sim N_1(0, 1)$, together with a closed form expression (if available at all) of all of the coefficients $\beta_n$, where the latter involves (in general, unknown values of) ordinary partial Bell polynomials. It appears to us that in general one cannot use proofs by standard induction on $n \in \mathbb{N}$ to verify statements about Bell polynomials. Here, the Noetherian Induction Principle seems to be more appropriate (cf [30]).

At least in the case of Grothendieck’s $b := \text{sign} = 2\mathbf{1}_{(0, \infty)} - 1$ we can show that for all $n \in \mathbb{N}$,

$$
\alpha_{2(n-1)} = 0, \alpha_1 = \frac{2}{\pi} \text{ and } \alpha_{2n+1} = \frac{2}{\pi} \frac{((2n - 1)!!)^2}{(2n + 1)!}.
$$

Consequently, if $n \in \mathbb{N}$, the (best-known) power series representation of $g_b(y) = \sin \left( \frac{y}{2} \right)$ leads to the following interesting identity:

$$
(-1)^n \frac{(\pi/2)^{2n+1}}{(2n+1)!} = \beta_{2n+1} \\
= \frac{(\pi/2)^{2n+1}}{(2n+1)!} \sum_{k=1}^{2n} (-1)^k \frac{(2n + k)!}{k!} B_{2n,k} \left( \frac{0}{6}, \frac{0}{40}, \frac{3}{140}, \frac{5}{112}, \ldots, \frac{1 + (-1)^{k+1}}{2} \frac{(2n - k)!!}{(2n - k + 2)!} \right).
$$
However, already in this case we don’t know a closed form expression for the numbers 
\[ B_{2n,k}(0, \frac{1}{6}, 0, \frac{3}{20}, 0, \frac{5}{12}, \ldots, \frac{1+(-1)^{k+1}((2n-k)!!)^2}{2((2n-k+2)!!)}}. \] An even stronger problem appears in the complex case, since already a closed-form formula for the coefficients of the Taylor series of the inverse of the Haagerup function is still unknown (cf. [17]). Here, we would like to list the very recent paper [34], where the authors point to similar difficulties including the formulation of related - open - problems. Moreover, the solved examples in [34] show the large barriers which we have to resolve while working with (partial) Bell polynomials. Here, [30] will disclose further surprising properties of these polynomials. In particular, we will provide a closed form sum representation of the polynomials underlying a very useful - recursive - construction of T. M. Apostol (see [2]) of the coefficients of the Taylor series of inverse functions.

Therefore, given the intrinsic combinatoric and computational complexity regarding the determination of the Taylor series coefficients of the Taylor series of the non-CCP function \( g_b \) (via the Faà-di Bruno formula), related research problems (which actually do not require any knowledge of the Grothendieck inequality) could be the following ones:

**(1-RP1)** Let \( n \in \mathbb{N}_4 \) and \( k \in \{2, 3, \ldots, n-2\} \). Recall that

\[
n\beta_{n} a_{k}^{n-1} = -n a_{1}^{-2} a_{n} \sum_{k=2}^{n-2} (-1)^{k} m_{k} \binom{n-1+k}{k} a_{1}^{n-1-k} p_{k}(\alpha_{2}, \alpha_{3}, \ldots, \alpha_{n}) + (-1)^{n-1} \binom{2(n-1)}{n-1} a_{2}^{n-1}.
\]

Prove this representation and determine \( A_{kk} \) and the numbers \( m_{k} \) therein explicitly (if feasible at all)!

**(1-RP2)** Continue to investigate the structure of partial Bell polynomials; possibly with the aid of high-performance computers and related (algebraic) software tools.

### 5.2. Research problem 2: Grothendieck’s inequality and copulas

If we thoroughly overhaul the CCP function \([-1,1] \ni \rho \mapsto \frac{2}{\pi} \arcsin(\rho)\) we recognise that some knowledge of Gaussian copulas (i.e., finite-dimensional multivariate distribution functions of univariate marginals generated by the distribution function of Gaussian random vectors - cf. e.g. [35, 26, 40] and [28]) and (the probabilistic version) of the Hermite polynomials might become very fruitful regarding our indicated search for different “suitable” CCP functions. \([-1,1] \ni \rho \mapsto \psi(\frac{1}{2}, \frac{1}{2}; t) = \frac{2}{\pi} \arcsin(\rho)\) namely reveals as a special case of the CCP function

\[-1,1] \ni \rho \mapsto \psi(p, p; \rho) = \frac{1}{c(p)} \sum_{n=1}^{\infty} \frac{1}{n} H_{n-1}^{2}(\Phi^{-1}(p)) \rho^{n} = \frac{1}{2\pi p(1-p)} \exp \left( -\left( \Phi^{-1}(p) \right)^{2} \right) \rho \sum_{n=0}^{\infty} \frac{1}{n+1} H_{n}^{2}(\Phi^{-1}(p)) \rho^{n},\]

where \(0 < p < 1\) and

\[
c(p) := \frac{p(1-p)}{\Phi^{2}(\Phi^{-1}(p))} = 2\pi p(1-p) \exp \left( \left( \Phi^{-1}(p) \right)^{2} \right) = \sum_{n=0}^{\infty} \frac{1}{n+1} H_{n}^{2}(\Phi^{-1}(p)) \cdot
\]

If we put \( b_{p} := 2I_{\Phi^{-1}(p), \infty} - 1 = 1 - 2I_{(\infty, \Phi^{-1}(p))} \in \{-1,1\}\), then the tetrachoric series expansion of the bivariate Gaussian copula (cf. [16, 24, 3]) implies the following generalisation
of Grothendieck’s identity:

\[ h_p(\rho) := h_p(\rho) : = \mathbb{E}[b_p(X) b_p(Y)] = (2p - 1)^2 + \frac{2}{\pi} \exp \left( - (\Phi^{-1}(p))^2 \right) \sum_{n=1}^{\infty} \frac{1}{n} H_{n-1}^2(\Phi^{-1}(p)) \rho^n \]

Due to our construction of \( \psi(p, p; \cdot) \) the latter is clearly equivalent to

\[ \rho(b_p(X), b_p(Y)) = \psi(p, p; \rho) \]

for all \( p \in (0, 1) \) and \( \rho \in [-1, 1] \) and \( (X, Y) \sim N_2(0, \Sigma_2(\rho)) \), where \( \rho(b_p(X), b_p(Y)) \) denotes Pearson’s correlation coefficient between the random variables \( b_p(X) \) and \( b_p(Y) \). Unfortunately,

\[ h_p(\rho) = \psi(p, p; \rho) \text{ for all } \rho \in [-1, 1] \text{ iff } p = \frac{1}{2}. \]

These facts imply the following research problems at least:

(2-RP1) Prove whether there are \( p \in (-1, 1) \setminus \{\frac{1}{2}\} \) and functions \( \chi_p : \mathbb{R} \to \{-1, 1\} \) such that

\[ \psi(p, p; \rho) = h_{\chi_p}(\rho) = \mathbb{E}[\chi_p(X) \chi_p(Y)] \]

for all \( \rho \in [-1, 1] \) and \( (X, Y) \sim N_2(0, \Sigma_2(\rho)) \), so that the condition (SIGN) of our workflow is satisfied for \( h_{\chi_p} \).

(2-RP2) Generalise the above approach (which is built on the tetrachoric series of the bivariate Gaussian copula) to the \( n \)-variate case, where \( n \in \mathbb{N}_3 \) and adapt problem (2-RP1) accordingly.

(2-RP3) Verify whether the above approach can be transferred to the complex case. Could we then similarly generalise the Haagerup identity?

(2-RP4) If (2-RP1), respectively (2-RP2) holds, prove whether the remaining conditions (H), (RA), (ABS) and (PI1) of the workflow hold. If this were the case calculate (respectively approximate numerically) the related upper bound of \( K_G^R \). Include high-performance computers and computer algebra systems if necessary.

### 5.3. Research problem 3: Grothendieck’s inequality and non-commutative dependence structures in quantum mechanics

Even a mathematical modelling of non-commutative dependence in quantum theory and its applications to quantum information and quantum computation is strongly linked with the existence of the real Grothendieck constant \( K_G^R \).

The latter can be very roughly adumbrated as follows: the experimentally proven non-Kolmogorovian (non-commutative) nature of the underlying probability theory of quantum physics leads to the well-known fact that in general a normal state of a composite quantum system cannot be represented as a convex combination of a product of normal states of the subsystems. This phenomenon is known as entanglement or quantum correlation. The Einstein-Podolsky-Rosen paradox, the violation of Bell’s inequalities (limiting spatial
correlation) and the Leggett-Garg inequalities (limiting temporal correlation) in quantum mechanics and related theoretical and experimental research implied a particular focus on a deeper understanding of this type of correlation - and hence to the *modelling of a specific type of dependence* of two (or more) quantum observables in a composite quantum system, measured by two (or more) space-like separated instruments, each one having a classical parameter (such as the orientation of an instrument which measures the spin of a particle). The transition probability function, i.e., the *joint* probability distribution of observables in some fixed state of the system (considered as a function of the above-mentioned parameters) may violate Bell’s inequalities and is therefore not realisable in “classical” (commutative) physics. The surprising fact, firstly recognised by B.S. Tsirelson (cf. [38, 39] and [31]), is that also this - experimentally verified - gap is an implication of the existence of the real Grothendieck constant $K_G^R > 1$. In other words, $K_G^R$ indicates “how non-local quantum mechanics can be at most”.

Already in the classical Kolmogorovian model, i.e., in the framework of probability space triples $(\Omega, \mathcal{F}, \mathbb{P})$, a rigorous description of tail dependence - which *exceeds* the standard dependence measure, given by Pearson’s correlation coefficient, is a challenging task. To disclose (and simulate) the geometry of dependence one has to determine finite-dimensional multivariate distribution functions of univariate marginals, hence *copulas*. In the description of research problem 2 we have seen that Gaussian copulas are lurking in Grothendieck’s identity. More precisely, we have (cf. [36]):

**Example** (Stieltjes, 1889). Let $\rho \in [-1, 1]$. Let $X,Y \sim N_1(0,1)$ such that $\mathbb{E}[XY] = \rho$. Then

$$\mathbb{E}[\text{sign}(X)\text{sign}(Y)] = 4C\left(\frac{1}{2}, \frac{1}{2}; \rho\right) - 1 = \frac{2}{\pi} \arcsin(\rho) = \frac{2}{\pi} \arcsin(\mathbb{E}[XY]),$$

where $[-1, 1] \ni \rho \mapsto C\left(\frac{1}{2}, \frac{1}{2}; \rho\right)$ denotes the bivariate Gaussian copula with Pearson’s correlation coefficient $\rho$ as parameter, evaluated at $(\frac{1}{2}, \frac{1}{2})$.

Keeping a *non-commutative* version of Grothendieck’s inequality at the back of our mind (cf. [33, 38, 39]) these facts might lead to problems of the following type:

(3-RP1) Look for objects like “non-commutative copulas”, leading to a search for “non-commutative distribution functions”.

(3-RP2) Create a “multivariate” spectral theory of *non-commuting* normal operator tuples and introduce non-commutative tail dependency measures in non-commutative $C^*$-algebras and operator spaces.

We finish this research list with a few completely open questions and a conclusion:

Can we remove the underlying Gaussian structure in Grothendieck’s inequality (for both fields, $\mathbb{R}$ and $\mathbb{C}$) and implement tail dependent distribution functions instead (such as the generalized extreme value (GEV) distribution) and maintain the inequality? If this were the case, could that approach also be used to improve the lower and the upper bound of the Grothendieck constant? What about infinitely divisible probability distributions in general? It is very likely that just the use of correlation matrices in the trace inequality version of GT would then no longer suffice.

†also known as *Tsirelson bound*
5.4. Conclusion

Apart from its comprehensive mathematical fascination and richness the highly fascinating open problem of determining the value of the both Grothendieck constants $K^R_G$ and $K^C_G$ meanwhile is deeply linked with different fields, even including applications in computer science, high-dimensional data analysis and quantum mechanics. Therefore, related research very likely would lead to a very fruitful exchange of related information and collaboration with experts from different fields, working in theory and in practice.

Any comments, remarks, questions, ideas, corrections and suggestions are highly welcome!

Acknowledgments. I would like to thank Feng Qi for very helpful comments including the correction of a hidden typo in Section 5.1.

References

[1] G. E. Andrews, R. Askey, and R. Roy. Special functions. Cambridge University Press (1999).
[2] T. M. Apostol. Calculating higher derivatives of inverses. Am. Math. Mon. 107, No. 8, 738-741 (2000).
[3] A.F. Atiya., and H.A. Fayed. A novel series expansion for the multivariate normal probability integrals based on Fourier series. Math. Comput. 83, No. 289, 2385-2402 (2014).
[4] A. Belton, D. Guillot, A. Khare, and M. Putinar. Matrix positivity preservers in fixed dimension. I. Adv. Math. 298, 325-368 (2016).
[5] V. I. Bogachev. Gaussian measures. Transl. from the Russian by the author. Mathematical Surveys and Monographs. 62. Providence, RI: American Mathematical Society (AMS). xii (1998).
[6] M. Braverman, K. Makarychev, Y. Makarychev, and A. Naor. The Grothendieck constant is strictly smaller than Krivine’s bound. Forum Math. Pi 1, Paper No. e4, 42 p. (2013). https://arxiv.org/abs/1103.6161 (2011).
[7] J. Briët, F. de Oliveira, M. Fernando, and F. Vallentin. Grothendieck inequalities for semidefinite programs with rank constraint. Theory Comput. 10, Paper No. 4, 77-105 (2014).
[8] L. Comtet. Advanced combinatorics. The art of finite and infinite expansions. Translated from the French by J. W. Nienhuys. Rev. and enlarged ed. Dordrecht, Holland - Boston, U.S.A.: D. Reidel Publishing Company (1974).
[9] D. Cvijović. New identities for the partial Bell polynomials. Appl. Math. Lett. 24, No. 9, 1544-1547 (2011).
[10] A. Defant, and K. Floret. *Tensor norms and operator ideals*. North-Holland Mathematics Studies 176. North-Holland, Amsterdam (1993).

[11] J. Diestel, J. Fourie, and J. Swart. *The metric theory of tensor products. Grothendieck’s résumé revisited*. American Mathematical Society (AMS), Providence, RI (2008).

[12] C. Dwork, A. Nikolov, and K. Talwar. Efficient Algorithms for Privately Releasing Marginals via Convex Relaxations. *Discrete Comput. Geom.*, 53:650-673 (2015).

[13] S. Friedland, L.-H. Lim, and J. Zhang. An elementary and unified proof of Grothendieck’s inequality. *Enseign. Math. (2)* 64, No. 3-4, 327-351 (2018).

[14] A. Grothendieck. Résumé de la Théorie Métrique des Produit Tensoriels Topologiques. *Bol. Mat. Sao Paulo*, 8, 1-79 (1953).

[15] M.X. Goemans and D.P. Williamson. Improved Approximation Algorithms for Maximum Cut and Satisfiability Problems Using Semidefinite Programming. *J. Assoc. Comp. Machinery.*, Vol. 42, No. 6, 1115-1145 (1995).

[16] S. S. Gupta. Probability integrals of multivariate normal and multivariate $t$. *Ann. Math. Stat.* 34, 792-828 (1963).

[17] U. Haagerup. A new upper bound for the complex Grothendieck constant. *Isr. J. Math.* 60, No. 2, 199-224 (1987).

[18] B. Harris, A. P. Soms. The use of the tetrachoric series for evaluating multivariate normal probabilities. *J. Multivariate Anal.* 10, 252-267 (1980).

[19] R. A. Horn, and C. R. Johnson. *Matrix analysis. 2nd ed*. Cambridge University Press (2013).

[20] K. Knopp. *Theory and application of infinite series*. Transl. from the 2nd ed. and revised in accordance with the Fourth by R. C. H. Young. London-Glasgow: Blackie & Son, Ltd. XII (1951).

[21] H. König. On an extremal problem originating in questions of unconditional convergence. *Recent progress in multivariate approximation (Witten-Bommerholz, 2000)*, ser. Internat. Ser. Numer. Math. Basel: Birkhäuser, vol. 137, pp. 185-192 (2001).

[22] J.L. Krivine. Sur la constante de Grothendieck. *C. R. Acad. Sci. Paris Ser. A* 284, 445-446 (1977).

[23] J. Lindenstrauss, and A. Pełczyński. Absolutely summing operators in $L_p$-spaces and their applications. *Stud. Math.* 29, 275-326 (1968).

[24] C. Meyer. The bivariate normal copula. *Commun. Stat., Theory Methods* 42, No. 13, 2402-2422 (2013).

[25] M. Masjed-Jamei, Z. Moalemi, W. Koepf, and H.M. Srivastava. An extension of the Taylor series expansion by using the Bell polynomials. *Rev. R. Acad. Cienc. Exactas Fís. Nat., Ser. A Mat., RACSAM* 113, No. 2, 1445-1461 (2019).
[26] R. B. Nelsen. *An introduction to copulas. 2nd ed.* Springer Series in Statistics. Springer, New York (2006).

[27] H. Niemi. Grothendieck’s inequality and minimal orthogonally scattered dilations. *Probability theory on vector spaces III, Proc. Conf., Lublin/Pol. 1983, Lect. Notes Math. 1080, 175-187* (1984).

[28] F. Oertel. An analysis of the Rüschendorf transform - with a view towards Sklar’s Theorem. *Depend. Model., Vol. 3, No. 1, 113-125* (2015).

[29] F. Oertel. Grothendieck’s inequality and mappings between correlation matrices: towards an improved upper bound of the Grothendieck constant (*NB: title on an interim basis*). *Work in progress.*

[30] F. Oertel. A convolution approach to ordinary partial Bell polynomials: Apostol’s approach revisited (*NB: title on an interim basis*). *Work in progress.*

[31] C. Palazuelos. Random constructions in Bell inequalities: a survey. *Found. Phys. 48, No. 8, 857-885* (2018).

[32] A. Pietsch. *Operator ideals.* North-Holland Mathematical Library 20. North-Holland, Amsterdam (1980).

[33] G. Pisier. Grothendieck’s theorem, past and present. *Bull. Am. Math. Soc., New Ser. 49, No. 2, 237-323* (2012). Cf. also: [http://www.math.tamu.edu/~pisier/grothendieck.UNCUT.pdf](http://www.math.tamu.edu/~pisier/grothendieck.UNCUT.pdf).

[34] F. Qi, D.-W. Niu, D. Lim, and Y.-H. Yao. Special values of the Bell polynomials of the second kind for some sequences and functions. *J. Math. Anal. Appl. 491*, no. 2 (2020).

[35] A. Sklar. Fonctions de répartition à n dimensions et leurs marges. *Publications de l’Institut Statistique de l’Université de Paris 8*, 229-231 (1959).

[36] T.S. Stieltjes. Extrait d’une lettre adressé à M. Hermite. *Bull. Sci. Math. Ser. 2 13:170* (1889).

[37] B. Szörényi. Characterizing Statistical Query Learning: Simplified Notions and Proofs. *R. Gavaldà et al (Eds.): Algorithmic Learning Theory. 20th international conference, ALT 2009, Porto, Portugal, October 3–5, 2009. Lecture Notes in Artificial Intelligence 5809, 186-200. Springer Berlin* (2009).

[38] B.S. Tsirelson. Quantum generalizations of Bell’s inequality. *Lett. Math. Phys. 4*, no. 2, 93-100 (1980).

[39] B.S. Tsirelson. Some results and problems on quantum Bell-type inequalities. *Hadronic J. Suppl. 8*, no. 4, 329-345 (1993).

[40] M. Úbeda Flores, E. de Amo Artero, F. Durante, and J. Fernández-Sánchez (editors). *Copulas and Dependence Models with Applications. Contributions in Honor of Roger B. Nelsen.* Springer (2017).
[41] V. N. Vapnik. *The nature of statistical learning theory. 2nd ed.* Statistics for Engineering and Information Science. Springer, New York (2000).