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The realization problem for tail correlation functions

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Abstract For a stochastic process $\{X_t\}_{t\in T}$ with identical one-dimensional margins and upper endpoint τ_{up} its tail correlation function (TCF) is defined through $\chi^{(X)}(s,t) = \lim_{\tau\to\tau_{\mathrm{up}}} P(X_s > \tau \mid X_t > \tau)$. It is a popular bivariate summary measure that has been frequently used in the literature in order to assess tail dependence. In this article, we study its realization problem. We show that the set of all TCFs on $T\times T$ coincides with the set of TCFs stemming from a subclass of max-stable processes and can be completely characterized by a system of affine inequalities. Basic closure properties of the set of TCFs and regularity implications of the continuity of χ are derived. If T is finite, the set of TCFs on $T \times T$ forms a convex polytope of $|T| \times |T|$ matrices. Several general results reveal its complex geometric structure. Up to $|T| = 6$ a reduced system of necessary and sufficient conditions for being a TCF is determined. None of these conditions will become obsolete as $|T| \geq 3$ grows.

Keywords convex polytope · extremal coefficient · max-stable process · tail correlation matrix · tail dependence matrix · Tawn-Molchanov model

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Introduction

The study of the existence of stochastic models with some prescribed distributional properties has a long tradition in the theory of probability and various fields of application. Let $\{X_t\}_{t\in T}$ be a stochastic process on some index set T (which may be finite or infinite with some topological structure). Typically, a real-valued summary statistic $\kappa^{(X)}(s,t)$ of the distribution of (X_s, X_t) is of particular interest for all pairs $(s,t) \in T \times T$. The question is whether for some prescribed function κ on $T \times T$ a stochastic model $\{X_t\}_{t\in T}$ exists that *realizes* κ, i.e. if $\kappa^{(X)} = \kappa$. Recent accounts and surveys on such *realization problems* with an emphasis on $\{0,1\}$-valued processes (or random sets, two-phased media, binary processes) include Torquato (2002), Quintanilla (2008), Emery (2010), Lachieze-Rey and Molchanov (2015) and Lachièze-Rey (2015). Also from a statistical point of view realization problems are important, namely for consistent inference.

As pointed out by Lachieze-Rey and Molchanov (2015), the question of realizability usually leads to a (possibly infinite and even in finite setups huge) set of positivity conditions for the quantity of interest, and secondly, to a set of regularity conditions if the topology of the underlying space is of interest as well. These positivity conditions are needed in statistical applications to correct estimators $\widehat{\kappa}^{(X)}$ for $\kappa^{(X)}$ to an admissible function.

Let us consider a classical example. Assuming that the second moments of a real-valued stochastic process $\{X_t\}_{t\in T}$ exist at each locaction $t \in T$, the process possesses a covariance function $C^{(X)}(s,t) = \mathrm{Cov}(X_s, X_t)$. It is well-known that $C = C^{(X)}$ must be *positive semi-definite*, i.e. $C(s,t) = C(t,s)$ and

$$\sum_{i=1}^{m}\sum_{j=1}^{m} a_i a_j C(t_i,t_j) \geq 0 \quad \forall\, (t_1,\ldots,t_m) \in T^m,\ (a_1,\ldots,a_m) \in \mathbb{R}^m,\ m \in \mathbb{N}. \tag{1}$$

Conversely, for any such function C, there exists a stochastic process $\{X_t\}_{t\in T}$ with covariance function $C^{(X)} = C$. The stochastic process $\{X_t\}_{t\in T}$ is not unique, but it may be chosen to be a centered Gaussian process as can be easily checked by Kolmogorov's extension theorem. Such a process on the space T (if additionally equipped with some topology), may have very uncomfortable regularity properties. Several authors have established connections between the regularity of the covariance function C and the existence of a corresponding stochastic process with a certain sample path regularity, cf. e.g. Adler (1990) for an overview in case of continuity. In statistical applications, the development of efficient non-parametric estimators for the covariance function that ensure positive semi-definiteness can be a challenging task, cf. e.g. Hall et al (1994) and Politis (2011).

When it comes to the extreme values in the upper quantile regions of a real-valued stochastic process $\{X_t\}_{t\in T}$, summary measures like the covariance function often do not exist and would be genuinely inappropriate to characterize dependence. Instead, among several other summary statistics that have emerged in an extreme value context (cf. for instance Beirlant et al (2004) Section 8.2.7), the following bivariate quantity

$$\chi^{(X)}(s,t) := \lim_{\tau \to \tau_{\mathrm{up}}} \mathbb{P}(X_s > \tau \,|\, X_t > \tau), \qquad s,t \in T,$$

which we call *tail correlation function* (TCF) (Strokorb et al, 2015), has received particular attention. As commonly done and in accordance with stationarity assumptions, we assume here and hereafter that $\{X_t\}_{t\in T}$ has identical one-dimensional marginal distributions with upper endpoint τ_{up} (which may be ∞).

Dating back to Geffroy (1958/1959), Sibuya (1960) and Tiago de Oliveira (1962/63), the TCF enjoys steady popularity among practitioners and scholars in order to account for tail dependence, albeit frequently reported under different names. The insurance, finance, economics and risk management literature knows it mainly as *(upper) tail dependence coefficient* (Frahm et al, 2005), *coefficient of (upper) tail dependence* (McNeil et al, 2003) or simply as *(upper) tail dependence* (Patton, 2006). In environmental contexts it has been additionally addressed as χ*-measure* (Coles et al, 1999). Spatial environmental applications tend to prefer the equivalent quantity $2-\chi$, referred to as *extremal coefficient function*. Among many others, the references Blanchet and Davison (2011), Engelke et al (2015) and Thibaud and Opitz (2015) use it as an exploratory tool for testing the goodness of fit. In the context of stationary time series, the TCF constitutes a special case of the *extremogram* (Davis and Mikosch, 2009). Moreover, the standard classification of the random pair (X_s, X_t) as exhibiting either *asymptotic/extremal independence* (when $\chi^{(X)}(s,t) = 0$) or *asymptotical/extremal dependence* (when $\chi^{(X)}(s,t) \in (0,1]$) is based on the TCF χ.

Even though the TCF is a ubiquitous quantity within the extremes literature, surprisingly little is known about the class of TCFs and even less when it comes to the interplay of TCFs and their realizing models. This is the central theme of the present text. That is, we are aiming at giving at least partial answers to the following questions:

(A) Can we decide if a given real-valued function $\chi : T \times T \to \mathbb{R}$ is the TCF of a stochastic process $\{X_t\}_{t\in T}$?
(B) If this is the case, can we find a specific stochastic process $\{X_t\}_{t\in T}$ with $\chi^{(X)} = \chi$?

We also address the following regularity question.

(C) Does the continuity of a TCF χ imply the existence of a stochastic process realizing χ that additionally satisfies some regularity property?

A satisfactory answer to Question (A) is desirable in a statistical context in order to decide whether estimators of the TCF produce admissible TCFs as an outcome. This concerns specifically spatial applications where one is bound to encounter very high-dimensional observations and therefore only partial low-dimensional information (such as the TCF) can be taken into account for inference. A first attempt to include properties of the class of TCFs to improve statistical inference can be found in Schlather and Tawn (2003). The TCF $\chi = \chi^{(X)}$ is a *non-negative correlation function*. That is, χ is positive semi-definite in the sense of (1) with $\chi(s,t) \geq 0$ and $\chi(t,t) = 1$ for all $s,t \in T$ (cf. e.g. Schlather and Tawn (2003), Davis and Mikosch (2009) and Fasen et al (2010)). However, even though TCFs are non-negative correlation functions, not all such functions are TCFs. For instance, $\eta := 1 - \chi$ has to satisfy the *triangle inequality*

$$\eta(s,t) \leq \eta(s,r) + \eta(r,t) \qquad r,s,t \in T \tag{2}$$

(Schlather and Tawn, 2003). In the context of $\{0,1\}$-valued stochastic processes, it is well-known that the respective covariance functions obey this triangle inequality and implications are addressed e.g. in Matheron (1988), Markov (1995) and Jiao et al (2007). If $T = \mathbb{R}^d$ and the underlying process is stationary, then the function $h \mapsto \chi(o,h)$ (with $o \in \mathbb{R}^d$ being the origin) cannot be differentiable unless it is constant.

The simplest TCFs are the constant function $\chi(s,t) = 1$ realized by a process of identical random variables, and the function $\chi(s,t) = \delta_{st} := \mathbb{1}_{s=t}$ realized by a process of independent random variables. Another example for $\chi^{(X)}(s,t) = \delta_{st}$ is a Gaussian process X on T, whose correlation function ρ on $T \times T$ attains the value 1 only on the diagonal $\{(t,t) : t \in T\}$ (Sibuya, 1960, Theorem 3). While Gaussian processes do not exhibit tail dependence, the class of *max-stable processes* naturally provides rich classes of non-trivial TCFs. For instance, any function of the form $\chi(s,t) = \int_{[0,\infty)} \exp\left(-\lambda \|s-t\|\right) \Lambda(d\lambda)$ will be the TCF of a max-stable process on $T = \mathbb{R}^d$, if Λ is a probability measure on $[0,\infty)$ (Strokorb et al, 2015). Beyond the realizability question, Kabluchko and Schlather (2010) and Wang et al (2013) establish some connections between mixing properties of X and decay properties of its TCF $\chi^{(X)}$ when $T = \mathbb{R}^d$ and $X = \{X_t\}_{t \in \mathbb{R}^d}$ is stationary and max-stable. It is natural to ask whether even further TCFs will arise if we do not restrict ourselves to the max-stable class, since an affirmative answer would imply a first important reduction for the questions (A)-(C).

(D) Is the set of TCFs stemming from max-stable processes properly contained in the set of all TCFs or do these sets coincide?

Finally, realization problems are usually intimately connected with the question of admissible operations on the quantities of interest. To illustrate this again by means of covariance funcions, note that the product and convex combination of two covariance functions and the pointwise limit of a sequence of covariance functions is again a covariance function. We ask the same question for TCFs.

(E) Is the set of TCFs closed under basic operations such as taking (pointwise) products, convex combinations and limits?

In order to deal with the questions above, we establish close connections with $\{0,1\}$-valued processes, polytopes, partitions of sets and combinatorics. Recent developments indicate that such tools may appear more frequently in the analysis of extremes, cf. Molchanov (2008), Yuen and Stoev (2014), Wang and Stoev (2011), Embrechts et al (2015) and Thibaud et al (2015).

We divide the text into two parts.

Part I deals with the realization problem of TCFs of stochastic processes $\{X_t\}_{t\in T}$ on arbitrary base spaces T. Close connections with $\{0,1\}$-valued processes will be established and enter the subsequent considerations. We give answers to Questions (D) and (E), partial answers to the Questions (A), (B) and (C) and reduce Question (A) to infinitely (countably) many finite-dimensional problems (in case our base space T is countable).

Part II deals with these finite-dimensional problems, that is, the realization problem of TCFs of random vectors $\{X_t\}_{t\in T}$ on finite base spaces T with $|T| = n$ for some $n \in \mathbb{N}$. We are aiming at establishing a (reduced) system of necessary and sufficient conditions for deciding whether a given function is a TCF or not and study the geometry of the set of TCFs. Arguments used in this part will be related to the study of polytopes, are often of combinatorial nature or are based on additional software computations. The latter is a typical phenomenon for realization problems of this kind.

More detailed descriptions are given at the beginning of each part. Finally, we end with a discussion of our results. The appendix contains all tables.

Part I

The realization problem for TCFs on arbitrary sets T

To start with, Section 1 reviews some preparatory results on max-stable processes, extremal coefficient functions and a particular subclass of max-stable processes, which we called Tawn-Molchanov (TM) processes (Strokorb and Schlather, 2015). These processes are important for our analysis, since it turns out that any TCF can be realized by (at least one) TM process, our main result in Section 2 and a substantial reduction of the realization problem of TCFs. Section 2 also reveals a close connection between the class of TCFs and the class of correlation functions of $\{0,1\}$-valued stochastic processes and addresses the existence of stochastic processes for a prescribed TCF χ with some minimal regularity properties if χ is at least continuous. Subsequently, Section 3 collects some immediate consequences concerning closure properties of the set of TCFs and the characterization of the set of TCFs by means of finite-dimensional inequalities, our starting point for Part II.

1 Max-stable processes, extremal coefficients and TM processes

A stochastic process $X = \{X_t\}_{t\in T}$ is *simple max-stable*, if it has unit Fréchet margins (meaning $\mathbb{P}(X_t \le x) = \exp(-1/x)$ for all $t \in T$ and $x > 0$), and if the maximum process $\bigvee_{i=1}^n X^{(i)}$ of independent copies of X has the same finite dimensional distributions (f.d.d.) as the process nX for each $n \in \mathbb{N}$. The crucial point in the realization problem for TCFs will be the close connection of the TCF $\chi^{(X)}$ of a simple max-stable process $X = \{X_t\}_{t\in T}$ to the *extremal coefficient function (ECF)* $\theta^{(X)}$ of the respective process X. Therefore, let $\mathcal{F}(T)$ denote the *set of finite subsets* of the space T. The ECF $\theta^{(X)}$ of a simple max-stable process X on T is a function on $\mathcal{F}(T)$ that is given by $\theta^{(X)}(\emptyset) := 0$ and

$$\theta^{(X)}(A) := -\tau \log \mathbb{P}\Big(\bigvee_{t\in A} X_t \le \tau\Big), \qquad \tau > 0,$$

in case $A \neq \emptyset$. The r.h.s. is indeed independent of $\tau > 0$ and lies in the interval $[1, |A|]$, where $|A|$ denotes the number of elements in A. In fact, the value $\theta^{(X)}(A)$ can be interpreted as the effective number of independent random variables in the collection $\{X_t\}_{t\in A}$ (cf. Smith (1990); Schlather and Tawn (2002)). We call the set of all possible ECFs of simple max-stable processes

$$\Theta(T) = \Big\{\, \theta^{(X)} : \mathcal{F}(T) \to \mathbb{R} \,:\, X \text{ a simple max-stable process on } T \,\Big\}. \tag{3}$$

The bounded ECFs will be denoted

$$\Theta_b(T) = \{\, \theta \in \Theta(T) \,:\, \theta \text{ is bounded} \,\}. \tag{4}$$

In fact, the set of ECFs $\Theta(T)$ can be completely characterized by a property called *complete alternation* (cf. Theorem 5 below). Using the notation and definition from Molchanov (2005), we set for a function $f : \mathcal{F}(T) \to \mathbb{R}$ and elements $K, L \in \mathcal{F}(T)$

$$(\Delta_K f)(L) := f(L) - f(L \cup K).$$

Then a function $f : \mathcal{F}(T) \to \mathbb{R}$ is called *completely alternating* on $\mathcal{F}(T)$ if for all $n \ge 1$, $\{K_1, \ldots, K_n\} \subset \mathcal{F}(T)$ and $K \in \mathcal{F}(T)$

$$(\Delta_{K_1}\Delta_{K_2}\ldots\Delta_{K_n} f)(K) = \sum_{I\subset\{1,\ldots,n\}} (-1)^{|I|} f\left(K \cup \bigcup_{i\in I} K_i\right) \le 0. \tag{5}$$

This condition can be slightly weakened as in Lemma 2 below. Its proof uses the following auxiliary argument.

Lemma 1 *Let M be a finite set and $f : \mathcal{F}(M) \to \mathbb{R}$ be a function on the subsets of M. Let $K, L \subset M$ with $K \cap L = \emptyset$. Then*

$$\sum_{I\subset L} (-1)^{|I|+1} f(K \cup I) = \sum_{J\subset (K\cup L)^c} \Big(\sum_{I\subset L\cup J} (-1)^{|I|+1} f((L\cup J)^c \cup I) \Big). \tag{6}$$

Proof Each set $(L \cup J)^c \cup I$ occuring on the r.h.s. can be written as a disjoint union $K \cup A \cup B$, with $A \subset L, B \subset (K \cup L)^c$. Let us consider the terms on the r.h.s. with fixed $A \subset L$ and fixed $B \subset (K \cup L)^c$. If $B = \emptyset$, the only possible I and J leading to such a situation are $I = A$ and $J = (K \cup L)^c$, i.e., one obtains the term on the l.h.s. with $I = A$. If $B \neq \emptyset$, the possibilities can be listed as $I = A \cup (B \setminus C)$ and $J = (K \cup L \cup C)^c$ for some $C \subset B$. Summing these terms over all $C \subset B$ yields $\sum_{C \subset B} (-1)^{|A|+|B \setminus C|+1} f(K \cup A \cup B) = (-1)^{|A|+1}(1-1)^{|B|} f(K \cup A \cup B) = 0$.

It follows that for finite sets M (instead of arbitrary T) complete alternation can be formulated by bounding the value $f(M)$ by lower order values $f(L)$ for $L \subset M$ as follows (cf. also Schlather and Tawn (2002), Ineq. (12)).

Lemma 2 *a) A function $f : \mathcal{F}(T) \to \mathbb{R}$ is completely alternating on $\mathcal{F}(T)$ if and only if for all $\emptyset \neq L \in \mathcal{F}(T)$ and $K \in \mathcal{F}(T)$ with $K \cap L = \emptyset$*

$$\sum_{I \subset L} (-1)^{|I|+1} f(K \cup I) \geq 0. \tag{7}$$

b) Let M be a non-empty finite set. Then $f : \mathcal{F}(M) \to \mathbb{R}$ is completely alternating if and only if (7) holds for all $\emptyset \neq L \subset M$ and $K = L^c$, which is equivalent to

$$\bigvee_{\substack{L \subset M \\ |L| \text{ odd}}} \sum_{\substack{I \subset L \\ I \neq L}} (-1)^{|I|} f(L^c \cup I) \leq f(M) \leq \bigwedge_{\substack{\emptyset \neq L \subset M \\ |L| \text{ even}}} \sum_{\substack{I \subset L \\ I \neq L}} (-1)^{|I|+1} f(L^c \cup I). \tag{8}$$

Proof a) Note that $\mathcal{F}(T)$ forms an abelian semigroup w.r.t. the union operation that is generated already by the singletons $\{t\}$ for $t \in T$ and that $\Delta_{\{t\}}\Delta_{\{t\}} = \Delta_{\{t\}}$. Therefore, it suffices already to require (5) only for $K_i = \{t_i\}$ for pairwise distinct elements $t_i \in T$ $(i = 1, \ldots, n)$ (cf. Berg et al (1984), Proposition 4.6.6). Set $L = \{t_1, \ldots, t_n\}$. Hence f is completely alternating on $\mathcal{F}(T)$ if and only if for all $\emptyset \neq L \in \mathcal{F}(T)$ and $K \in \mathcal{F}(T)$ the inequality (7) holds. Secondly, the expression on the l.h.s. of (7) equals automatically 0 if $K \cap L \neq \emptyset$.

b) Because of (6), it suffices to check (7) for $\emptyset \neq L \subset M$ and $K = L^c$. Separating $f(M)$ and summarizing the cases where $|L|$ is odd and where $|L|$ is even yields the second equivalence.

The following example shows that the concept of complete alternation is closely linked to the distributions of $\{0, 1\}$-valued processes.

Example 3 (Molchanov (2005), p. 52) Let $Y = \{Y_t\}_{t \in T}$ be a stochastic process with values in $\{0, 1\}$ and let the function $C^{(Y)} : \mathcal{F}(T) \to [0, 1]$ be given by $C^{(Y)}(\emptyset) = 0$ and $C^{(Y)}(A) = \mathbb{P}(\exists\, t \in A \text{ such that } Y_t = 1)$. Then $C^{(Y)}$ is completely alternating. Conversely, if $C : \mathcal{F}(T) \to [0, 1]$ is completely alternating with $C(\emptyset) = 0$, then C determines the f.d.d. of a stochastic process $Y = \{Y_t\}_{t \in T}$ with values in $\{0, 1\}$, such that $C^{(Y)} = C$.

Remark 4 (Molchanov (2005), p. 10) From the perspective of the theory of random sets it is more natural to define a functional $C^{\Xi}(K) = \mathbb{P}(\Xi \cap K \neq \emptyset)$ for a random closed set Ξ on compact sets K. In this case, C^{Ξ} will be termed the *capacity functional* of the random closed set Ξ and is not only completely alternating on compact sets, but also upper semi-continuous in the sense that $C^{\Xi}(K_n) \downarrow C^{\Xi}(K)$ for $K_n \downarrow K$. These properties ensure that Ξ can be defined on a sufficiently regular probability space. A priori our considerations below do not include any regularity constraints. However, we will come back to Question (C) in Corollary 11 and Remark 12.

Theorem 5 (Strokorb and Schlather (2015), Theorem 8)
Let $\theta : \mathcal{F}(T) \to \mathbb{R}$ be a function on the finite subsets of T. Then

$$\theta \in \Theta(T) \qquad \Longleftrightarrow \qquad \begin{cases} \theta \textit{ is completely alternating,} \\ \theta(\emptyset) = 0, \\ \theta(\{t\}) = 1 \textit{ for } t \in T. \end{cases}$$

If $\theta \in \Theta(T)$, then there exists a simple max-stable process $X = \{X_t\}_{t \in T}$ on T with ECF $\theta^{(X)} = \theta$, whose f.d.d. are given by

$$-\log \mathbb{P}\left(X_{t_i} \leq x_i \,,\, i = 1, \ldots, m\right) =$$
$$\sum_{k=1}^{m} \sum_{1 \leq i_1 < \cdots < i_k \leq m} -\Delta_{\{t_{i_1}\}} \ldots \Delta_{\{t_{i_k}\}} \theta\left(\{t_1, \ldots, t_m\} \setminus \{t_{i_1}, \ldots, t_{i_k}\}\right) \bigvee_{j \in \{i_1, \ldots, i_k\}} x_j^{-1}.$$

If a process $\{X_t\}_{t \in T}$ has the f.d.d. stated in Theorem 5, then it is called *Tawn-Molchanov process (TM process) associated with the ECF θ* henceforth. Note that this convention and the notation from Molchanov and Strokorb (2015) differ in the sense that Molchanov and Strokorb (2015) consider TM processes with at least upper-semi continuous sample paths. By construction, the class of f.d.d.'s of TM processes on a space T is in a one-to-one correspondence with the set of ECFs $\Theta(T)$. In fact, if $\theta \in \Theta(T)$ and X is an associated TM process, the process X takes a unique role among simple max-stable processes sharing the same ECF θ in that it provides a sharp lower bound for the f.d.d. (Strokorb and Schlather, 2015, Corollary 33).

Corollary 6 (Strokorb and Schlather (2015), Corollaries 13 and 14)
The set of ECFs $\Theta(T)$ is convex and compact w.r.t. the topology of pointwise convergence on $\mathbb{R}^{\mathcal{F}(T)}$.

The connection of the TCF $\chi^{(X)}$ to the second-order extremal coefficients of a simple max-stable process X is given by

$$\begin{aligned} \chi^{(X)}(s,t) &= 2 - \lim_{\tau \to \infty} \frac{1 - \mathbb{P}\left(X_s \leq \tau, X_t \leq \tau\right)}{1 - \mathbb{P}\left(X_t \leq \tau\right)} \\ &= 2 - \frac{\log \mathbb{P}\left(X_s \leq \tau, X_t \leq \tau\right)}{\log \mathbb{P}\left(X_t \leq \tau\right)} = 2 - \theta^{(X)}(\{s,t\}). \end{aligned} \tag{9}$$

Therefore, it will be convenient to introduce the following map

$$\psi : \mathbb{R}^{\mathcal{F}(T)} \to \mathbb{R}^{T\times T}, \qquad \psi(F)(s,t) := 2 - F(\{s,t\}), \tag{10}$$

such that (9) reads as $\chi^{(X)} = \psi(\theta^{(X)})$. Note that ψ is continuous if we equip both spaces $\mathbb{R}^{\mathcal{F}(T)}$ and $\mathbb{R}^{T\times T}$ with the topology of pointwise convergence. Finally, we restate a continuity result from Strokorb and Schlather (2015) in terms of TCFs (instead of ECFs as in the reference).

Corollary 7 (Strokorb and Schlather (2015), Theorem 25)
Let $X = \{X_t\}_{t\in T}$ be a TM process and $\chi^{(X)}$ its TCF. Then the following statements are equivalent:

(i) $\chi^{(X)}$ *is continuous.*
(ii) $\chi^{(X)}$ *is continuous on the diagonal* $\{(t,t) : t \in T\}$*.*
(iii) X *is stochastically continuous.*

Remark 8 In fact, a TM process $X = \{X_t\}_{t\in T}$ is always stochastically continuous with respect to the semimetric $\eta^X(s,t) = 1 - \chi^{(X)}(s,t)$.

2 TCFs are realized by TM processes

In order to simplify the realization problem for TCFs (termed as Questions (A) to (E) in the introduction) it is desirable to find a subclass of stochastic processes which can realize any given TCF χ. We denote the set of all TCFs and certain subclasses as follows:

$$\begin{aligned}
\mathrm{TCF}(T) &:= \left\{\chi^{(X)} \,:\, \begin{array}{c} X \text{ a stochastic process on } T \text{ with identical} \\ \text{one-dimensional margins and existing } \chi^{(X)} \end{array}\right\},\\
\mathrm{TCF}_\infty(T) &:= \left\{\chi^{(X)} \in \mathrm{TCF}(T) \,:\, X \text{ with essential supremum } \infty\right\},\\
\mathrm{MAX}(T) &:= \left\{\chi^{(X)} \in \mathrm{TCF}(T) \,:\, X \text{ simple max-stable}\right\},\\
\mathrm{TM}(T) &:= \left\{\chi^{(X)} \in \mathrm{TCF}(T) \,:\, X \text{ a TM process}\right\}.
\end{aligned}$$

Remark 9 The class $\mathrm{TCF}_\infty(T)$ represents the TCFs of processes whose margins have no jump at the upper endpoint. To see this, first note that a distribution function $F : \mathbb{R} \to [0,1]$ has no jump at its upper endpoint $u \in (-\infty,\infty]$ if and only if there exists a continuous strictly increasing transformation $f : (-\infty,u) \to \mathbb{R}$ such that $F \circ f^{-1}$ is a distribution function with upper endpoint ∞, and secondly, $\chi^{(X)} = \chi^{(f\circ X)}$ if X is a stochastic process with marginal distribution F and TCF $\chi^{(X)}$.

A priori it is clear that

$$\mathrm{TM}(T) \subset \mathrm{MAX}(T) \subset \mathrm{TCF}_\infty(T) \subset \mathrm{TCF}(T). \tag{11}$$

Further, let us introduce the class of uncentered and normalized covariance functions of binary processes

$$\mathrm{BIN}(T) := \left\{ (s,t) \mapsto \mathbb{P}(Y_s = 1 | Y_t = 1) \ : \ \begin{array}{r} Y \text{ a stochastic process on } T \text{ with} \\ \text{identical one-dimensional margins} \\ \text{with values in } \{0,1\} \text{ and } \mathbb{E}Y_t \neq 0 \end{array} \right\}, \tag{12}$$

which is closely related to the above classes. By definition of $\mathrm{TCF}(T)$ and considering the processes $Y_t = \mathbb{1}_{X_t > \tau}$ indexed by $\tau > 0$, we observe

$$\mathrm{TCF}(T) \subset \text{ sequential closure of } \mathrm{BIN}(T), \tag{13}$$

where the sequential closure is meant w.r.t. pointwise convergence. The following theorem gives an affirmative answer to the question whether $\mathrm{TCF}(T)$ and $\mathrm{MAX}(T)$ coincide *(Question (D) in the Introduction)* and yields also the connection to the other classes. In fact, the class of TM processes can realize already any given TCF.

Theorem 10 *a) For arbitrary sets T the following classes coincide*

$$\mathrm{BIN}(T) = \psi(\Theta_b(T)), \tag{14}$$

$$\begin{aligned} \mathrm{TCF}(T) &= \mathrm{TCF}_\infty(T) = \mathrm{MAX}(T) = \mathrm{TM}(T) = \psi(\Theta(T)) \\ &= \textit{ sequential closure of } \mathrm{BIN}(T) = \textit{ closure of } \mathrm{BIN}(T), \end{aligned} \tag{15}$$

where the map ψ is from (10), $\Theta(T)$ and $\Theta_b(T)$ are from (3) and (4), respectively, and the (sequential) closure is meant w.r.t. pointwise convergence.

b) For infinite sets T the inclusion $\mathrm{BIN}(T) \subsetneq \mathrm{TCF}(T)$ is proper.

c) For finite sets M the equality $\mathrm{BIN}(M) = \mathrm{TCF}(M)$ holds.

Proof a) First, we establish $\mathrm{BIN}(T) = \psi(\Theta_b(T))$:

Let $f \in \mathrm{BIN}(T)$ and let Y be a corresponding process with values in $\{0,1\}$ as in the definition of $\mathrm{BIN}(T)$ (cf. (12)). Let the function $C^{(Y)} : \mathcal{F}(T) \to [0,1]$ be given by $C^{(Y)}(\emptyset) = 0$ and $C^{(Y)}(A) = \mathbb{P}(\exists\, t \in A \text{ such that } Y_t = 1)$ as in Example 3. Then $C(\{t\}) = \mathbb{E}Y_t$ lies in the interval $(0,1]$ and is independent of $t \in T$ due to identical one-dimensional margins. Further, the function f is given by $f(s,t) = \mathbb{P}(Y_s = 1 \mid Y_t = 1) = 2 - C(\{s,t\})/C(\{t\})$. Now, set $\theta(A) := C(A)/C(\{t\})$ for $A \in \mathcal{F}(T)$. Then θ satisfies $\psi(\theta)(s,t) = 2 - \theta(\{s,t\}) = f(s,t)$ and θ is clearly bounded by $1/C(\{t\})$. It follows from Example 3 and Theorem 5 that θ lies in $\Theta(T)$. Hence, $f \in \psi(\Theta_b(T))$.

Conversely, let $\theta \in \Theta_b(T)$ be bounded, say by κ. Clearly, $\kappa \geq \theta(\{t\}) = 1$. Set $C(A) := \theta(A)/\kappa$. Then C satisfies all requirements of Example 3 to determine the f.d.d. of a binary process Y with values in $\{0,1\}$ with $C^{(Y)} = C$. The process Y has identical one-dimensional margins since $\theta(\{t\}) = 1$ for $t \in T$, and $\mathbb{E}Y_t = 1/\kappa > 0$. So Y fulfills the requirements of a process in the definition of $\mathrm{BIN}(T)$. Finally, note that the corresponding function in

BIN(T) is given by $\mathbb{P}(Y_s = 1 \mid Y_t = 1) = 2 - C(\{s,t\})/C(\{t\}) = \psi(\theta)(s,t)$ as desired.

Secondly, the equality $\mathrm{MAX}(T) = \mathrm{TM}(T) = \psi(\Theta(T))$ follows directly from Theorem 5. On the one hand this implies

$$\mathrm{BIN}(T) = \psi(\Theta_b(T)) \subset \psi(\Theta(T)) = \mathrm{TM}(T),$$

and on the other hand, we obtain that TM(T) is compact, as it is the image of the compact set $\Theta(T)$ (Corollary 6) under the continuous map ψ. Now, the assertion (15) follows from

$$\mathrm{TCF}(T) \overset{(13)}{\subset} \text{ sequential closure of } \mathrm{BIN}(T) \subset \text{ closure of } \mathrm{BIN}(T)$$

$$\subset \text{closure of } \mathrm{TM}(T) \subset \mathrm{TM}(T) \overset{(11)}{\subset} \mathrm{MAX}(T) \overset{(11)}{\subset} \mathrm{TCF}_\infty(T) \overset{(11)}{\subset} \mathrm{TCF}(T).$$

b) Let T be an infinite set and let $\chi(s,t) := \delta_{st}$. Indeed χ is an element of MAX(T) realized by the simple max-stable process X on T, where the variables $\{X_t\}_{t\in T}$ are i.i.d. standard Fréchet random variables. Suppose that $\chi \in \mathrm{BIN}(T)$. Then $\mathbb{P}(Y_s = 1, Y_t = 1) = 0$ for all $s, t \in T$ with $s \neq t$. Thus, $\mathbb{P}(\bigcup_{s\in S}\{Y_s = 1\}) = \sum_{s\in S}\mathbb{P}(Y_s = 1) = \infty$ for any countably infinite subset $S \subset T$, a contradiction.

c) If M is finite, elements of $\Theta(M)$ are automatically bounded by $|M|$ and thus, $\Theta(M) = \Theta_b(M)$.

The latter result does not include any regularity considerations beyond the product topology that is somewhat unnatural in infinite-dimensional stochastic contexts. However, in view of Corollary 7, it is possible to identify the role of continuous TCFs in this realization problem and hence address Question (C) as follows.

Corollary 11 *Let $\chi \in \mathrm{TCF}(T)$. Then the following statements are equivalent.*

(i) χ is continuous.
(ii) χ is continuous on the diagonal $\{(t,t) : t \in T\}$.
(iii) There exists a stochastically continuous stochastic process $\{X_t\}_{t\in T}$ with TCF $\chi^{(X)} = \chi$.

Remark 12 In fact, any TM process X with continuous TCF $\chi^{(X)}$ is stochastically continuous. It follows from de Haan's (1984) construction that any simple max-stable process on $\mathbb{R}^d$ (or any other locally compact second countable Hausdorff space) that is continuous in probability, can be realized on a sufficiently regular probability space. Hence, this applies to TM processes with continuous TCFs, since they are simple max-stable and continuous in probability by the preceding corollary.

Remark 13 Lachieze-Rey and Molchanov (2015) discuss regularity conditions on the two-point covering function of a random set, or equivalently, a unit covariance function (cf. Section 6.4) that ensure the existence of a realizing closed set, or equivalently, a realizing $\{0,1\}$-valued process with upper semi-continuous paths. Here, we do not know which regularity conditions on the TCF ensure the existence of a realizing upper semi-continuous process.

3 Basic closure properties and characterization by inequalities

Finally, we collect some immediate and important consequences concerning operations on the set of TCFs and the characterization of the set of TCFs by means of finite-dimensional projections.

Even though not all non-negative correlation functions are TCFs, both classes have some desirable properties in common as we shall see next. Well-known operations on (non-negative) correlation functions include convex combinations, products and pointwise limits. Interestingly, the same operations are still admissible for TCFs (answering Question E).

Corollary 14 *The set of tail correlation functions* $\mathrm{TCF}(T)$ *is convex, closed under pointwise multiplication and compact w.r.t. pointwise convergence.*

Proof These closure properties follow from Theorem 10. Convexity and compactness of $\mathrm{TCF}(T) = \psi(\Theta(T))$ are immediate taking additionally Corollary 6 into account. Moreover, let χ_1 and χ_2 be in $\mathrm{TCF}(T) = \mathrm{TCF}_\infty(T)$ with corresponding processes $X^{(1)}$ and $X^{(2)}$ with upper endpoint $\tau_{\mathrm{up}} = \infty$. We choose them to be independent and set $X^{(3)} := X^{(1)} \wedge X^{(2)}$, which then also has upper endpoint ∞ and satisfies

$$\mathbb{P}(X_s^{(3)} \geq x \,|\, X_t^{(3)} \geq x) = \mathbb{P}(X_s^{(1)} \geq x \,|\, X_t^{(1)} \geq x) \cdot \mathbb{P}(X_s^{(2)} \geq x \,|\, X_t^{(2)} \geq x).$$

Consequently, the TCF χ_3 of $X^{(3)}$ is the product $\chi_3 = \chi_1 \cdot \chi_2$.

Secondly, the set of TCFs can be characterized through finite-dimensional projections.

Corollary 15 *A real-valued function* $\chi : T \times T \to \mathbb{R}$ *is an element of* $\mathrm{TCF}(T)$ *if and only if the restriction* $\chi|_{M\times M}$ *belongs to* $\mathrm{TCF}(M)$ *for all non-empty finite subsets* M *of* T.

Proof If $\chi \in \mathrm{TCF}(T)$, then necessarily $\chi|_{S\times S} \in \mathrm{TCF}(S)$ for any subset $S \in T$. To show the reverse implication, let $\chi|_{M\times M} \in \mathrm{TCF}(M)$ for all $M \in \mathcal{F}(T) \setminus \{\emptyset\}$. Since $\mathrm{TCF}(T) \subset [0,1]^{T\times T}$ is closed, to prove $\chi \in \mathrm{TCF}(T)$ it suffices to show that $U \cap \mathrm{TCF}(T) \neq \emptyset$ for any open neighborhood U of χ in $[0,1]^{T\times T}$. Given U, there is a finite subset of $T \times T$, which we may assume to be of the form $M \times M$, and open sets $A_{(i,j)} \subset [0,1]$, $(i,j) \in M \times M$, such that $\chi \in \bigcap_{(i,j)\in M\times M} \mathrm{pr}_{(i,j)}^{-1}\left(A_{(i,j)}\right) \subset U$ (where $\mathrm{pr}_{(s,t)} : [0,1]^{T\times T} \to [0,1]$ denotes the natural projection). Since $\chi|_{M\times M}$ trivially extends to an element $\tilde{\chi} \in \mathrm{TCF}(T)$ (e.g. copy one of the random variables), we have $\tilde{\chi} \in U \cap \mathrm{TCF}(T) \neq \emptyset$.

In Part II of this exposition, we will see that for a finite set M, the set of TCFs $\mathrm{TCF}(M)$ constitutes a convex polytope in $\mathbb{R}^{|M|\times|M|}$ that can be described by means of a finite system of (affine) inequalities. In this regard Corollary 15 shows that for an arbitrary set T, the class $\mathrm{TCF}(T)$ may also be completely characterized by a system of (affine) inequalities. This is not evident since elements of $\mathrm{TCF}(T)$ are defined a priori through a limiting procedure.

Part II

The realization problem for TCFs on finite sets

In view of Corollary 15 it suffices to study $\mathrm{TCF}(M)$ for finite sets M if one is interested in a complete characterization of the space $\mathrm{TCF}(T)$ for arbitrary T. Therefore, we focus on a non-empty finite set $M = \{1, \dots, n\}$ in this section and set

$$\mathrm{TCF}_n := \mathrm{TCF}(\{1, \dots, n\}).$$

To begin with, we show that TCF_n can be viewed as a convex polytope in Section 4. Its geometry will be studied subsequently. Here, we start off with some basic observations and low-dimensional results in Section 5. Section 6 collects more sophisticated results on TCF_n with deeper insights into the rapidly growing complexity of TCF_n as n grows, including connections between TCF_n and $\mathrm{TCF}_{n'}$ for $n' > n$. Thereby, some obervations from Section 5 will be uncovered as low-dimensional phenomena. At least, it is possible to identify the precise relation of TCF_n to the so-called cut- and correlation-polytopes as well as to the polytope of unit covariances. To complement these general observations, Section 7 reports all results relying on software computations and, in particular, all combinatorial considerations that were necessary in order to push the entire description of the vertices and facets of TCF_n up to $n \leq 6$. Finally, we pursue some open questions on the geometry on TCF_n in Section 8.

4 TCF_n is a convex polytope

Elements of TCF_n are functions on $\{1, \dots, n\} \times \{1, \dots, n\}$, that is to say, they are $n \times n$ matrices. Since TCFs are symmetric and take the value 1 on the diagonal, we may regard TCF_n for $n \geq 2$ as a subset of

$$\mathbb{R}^{E_n} \cong \mathbb{R}^{\binom{n}{2}} = \mathbb{R}^{n(n-1)/2},$$

where E_n is the set of edges of the *complete graph* K_n with vertices $V_n = \{1, \dots, n\}$. It will be convenient to interpret elements of TCF_n as an edge labelling of K_n, which is why we call K_n the *support graph* for TCF_n. Due to Theorem 10 and (12) we know already

$$\mathrm{TCF}_n = \mathrm{BIN}_n := \left\{ \chi \in \mathbb{R}^{E_n} \ : \begin{array}{l} \chi_{ij} = \mathbb{E}(Y_i Y_j)/\mathbb{E}Y_j \text{ where} \\ Y_1, \dots, Y_n \text{ take values in } \{0,1\} \\ \text{and } \mathbb{E}Y_1 = \ldots = \mathbb{E}Y_n > 0 \end{array} \right\}. \tag{16}$$

The following lemma is a reformulation of this fact and will be useful later on.

Lemma 16 *An element $\chi \in \mathbb{R}^{E_n}$ belongs to TCF_n if and only if it can be written as*

$$\chi_{ij} = \mathbb{P}(A_i | A_j), \quad 1 \leq i < j \leq n$$

for some (finite) probability space $(\Omega, \mathcal{A}, \mathbb{P})$ *and measurable subsets* $A_1, \ldots, A_n \in \mathcal{A}$ *which satisfy* $\mathbb{P}(A_1) = \cdots = \mathbb{P}(A_n) > 0$.

Remark 17 In Lemma 16 we may assume that $\mathbb{P}(A_1) = \cdots = \mathbb{P}(A_n) = c$ for any constant $0 < c \leq 1/n$: Otherwise enlarge Ω, such that $A := \bigcup_{i=1}^n A_i \neq \Omega$. On A define the measure $\mathbb{Q} := c/\mathbb{P}(A_1) \cdot \mathbb{P}|_A$. Then $\mathbb{Q}(A) \leq 1$ and, thus, $\mathbb{Q}$ extends to a probability measure on Ω with $\mathbb{Q}(A_i) = c$ and $\mathbb{Q}(A_i|A_j) = \chi_{ij}$.

Likewise, we set

$$\Theta_n := \Theta(\{1, \ldots, n\})$$

and, since $\theta_\emptyset = 0$ and $\theta_i = 1$ for $i = 1, \ldots, n$, we may regard Θ_n for $n \geq 2$ as a subset of

$$\mathbb{R}^{\mathcal{F}_n^{(2)}} \cong \mathbb{R}^{2^n - n - 1},$$

where $\mathcal{F}_n^{(2)}$ is the set of subsets of V_n with at least two elements. Remember from (10) that

$$\mathrm{TCF}_n = \psi_n(\Theta_n) \qquad \text{where} \qquad \psi_n : \mathbb{R}^{\mathcal{F}_n^{(2)}} \to \mathbb{R}^{E_n}, \quad \psi_n(\theta)_{ij} = 2 - \theta_{ij}, \quad (17)$$

and note that $\psi_n = 2 - \mathrm{pr}_{E_n}$ is essentially a projection onto the $\binom{n}{2}$ coordinates of $\mathbb{R}^{E_n}$. Before we proceed, we need to revise some notation for convex polytopes.

Notation and facts concerning convex polytopes (cf. Ziegler (1995)). A subset $P \subset \mathbb{R}^p$ is a *convex polytope* if P is bounded and can be represented as $P = \{x \in \mathbb{R}^p : Cx \leq c\}$ for a $q \times p$ matrix C and a q-vector c for some $q \in \mathbb{N}$ (where $\leq$ is meant componentwise). The rows of C and c represent hyperplanes in $\mathbb{R}^d$ and the inequality $\leq$ determines the corresponding halfspace to which P belongs. The system $Cx \leq c$ will be called an *$\mathcal{H}$-representation* (or *halfspace representation*) of P.

An $\mathcal{H}$-representation will be called a *facet representation* if it is minimal in the sense that none of the rows in C and c can be deleted in order to define P, i.e. $P \neq \{x \in \mathbb{R}^p : C_{-i}x \leq c_{-i}\}$ for all $i = 1, \ldots, q$, where C_{-i} and c_{-i} are the modified versions of C and c with the i-th row removed. In fact, an $\mathcal{H}$-representation $Cx \leq c$ is a facet representation if every row of C and c yields in fact a *facet inducing* inequality of P, where an inequality $C_i x \leq c_i$ is facet inducing if $\dim(P \cap \{x \in \mathbb{R}^p : C_i x = c_i\}) = \dim(P) - 1$. The latter is equivalent to the existence of $\dim(P)$ affinely independent points $x^1, \ldots, x^{\dim(P)} \in P$ solving the equation $C_i x = c_i$. By a slight abuse of notation, we will usually refer to the inequality $C_i x \leq c_i$ as a *facet* of P if it induces a facet (instead of calling the set $P \cap \{x \in \mathbb{R}^p : C_i x = c_i\}$ a facet).

Equivalently, a subset $P \subset \mathbb{R}^p$ is a convex polytope if P equals the convex hull of a finite subset $S \subset \mathbb{R}^p$. Then S will be called a *$\mathcal{V}$-representation* of P. A minimal $\mathcal{V}$-representation, with respect to set inclusion, will be called a *vertex representation*. In fact, the vertex representation is unique and given by the set $\mathrm{Ex}(P)$ of extremal points, or *vertices*, of P, i.e. the points of P that cannot be decomposed non-trivially as a convex combination of two other points of P. Note that in general a $\mathcal{V}$-representation of P may consist of more points than the vertex set $\mathrm{Ex}(P)$.

Moreover, if $P \subset \mathbb{R}^p$ is a convex polytope and $\pi : \mathbb{R}^p \to \mathbb{R}^{p'}$ is an affine map $x \mapsto Ax+b$, then the image $\pi(P)$ is again a convex polytope and secondly, any intersection of P with an affine subspace of $\mathbb{R}^p$ is a convex polytope.

Corollary 18 *For all $n \in \mathbb{N}$ the sets Θ_n and TCF_n are convex polytopes.*

Proof For Θ_n this property is evident from Theorem 5 and (8). But then the affine map ψ_n maps Θ_n to the convex polytope $\mathrm{TCF}_n = \psi_n(\Theta_n)$.

Now, that we know that TCF_n is a convex polytope, we seek to understand its geometric structure. At best, we would like to determine its vertex and facet representation (and we will indeed do so in Section 7 up to $n \leq 6$). To repeat the terminology adopted from convex geometry in this context, note that an $\mathcal{H}$-representation of TCF_n (and in particular, a facet representation) allows one to check whether a given matrix is indeed a TCF, since any $\mathcal{H}$-representation of TCF_n constitutes a set of necessary and sufficient conditions for being a TCF. In a facet representation no condition is obsolete. Complementary, a $\mathcal{V}$-representation (and in particular, a vertex representation) of TCF_n is more useful if one wants to generate valid TCFs. Any TCF can be obtained as a convex combination of the elements of a $\mathcal{V}$-representation. In a vertex representation no point is obsolete.

5 Basic observations and low-dimensional results for TCF_n

This section comprises two first general observations. First, every polytope TCF_n satisfies a certain system of inequalities (to be called *hypermetric inequalities*) and, second, we identify its $\{0,1\}$-valued vertices as so-called *clique partition points*. With regard to the explicit vertex and facet structure of TCF_n in low dimensions, both findings might lead to tempting conjectures on the geometry of TCF_n eventually refuted by the more sophisticated methods applied in Section 6.

Hypermetric inequalities Remember that we identified the set of all TCFs on $V_n = \{1, \ldots, n\}$ with a subset of $\mathbb{R}^{E_n} = \mathbb{R}^{\binom{n}{2}}$ while it originally was interpreted as a set of symmetric $n \times n$ matrices with 1's on the diagonal. In the sequel we will identify points $x = (x_{ij})_{1 \leq i < j \leq n} \in \mathbb{R}^{E_n}$ with $n \times n$ matrices $(x_{ij})_{1 \leq i,j \leq n}$ via $x_{ji} = x_{ij}$ and $x_{ii} := 1$.

Let $b = (b_1, \dots, b_n) \in \mathbb{Z}^n$. The point $(x_{ij})_{1\le i<j\le n} \in \mathbb{R}^{E_n}$ satisfies the *hypermetric inequality defined by* b if

$$\sum_{1\le i,j\le n} b_i b_j x_{ij} \ge \sum_{i=1}^{n} b_i$$

$$\text{or, equivalently,} \qquad \sum_{1\le i<j\le n} (-b_i b_j) x_{ij} \le \frac{1}{2}\sum_{i=1}^{n} b_i(b_i - 1). \tag{18}$$

Remark 19 In Deza and Laurent (1997) the inequalities $\sum_{1\le i<j\le n} b_i b_j x_{ij} \le 0$ with $\sum_{1\le i\le n} b_i = 1$ are termed hypermetric. All these inequalities are valid for the cut polytope $\mathrm{CUT}_n^{\square}$ to be introduced here in Section 6.4 (Deza and Laurent, 1997, Lemma 28.1.3). For TCF_n the variant (18) is an appropriate "counterpart".

Lemma 20 *All hypermetric inequalities (in the sense of* (18)*) are valid for elements of* TCF_n.

Proof Let $Y_1, \dots, Y_n$ be a $\{0,1\}$-valued stochastic model for $\chi \in \mathrm{TCF}_n$. Set $a := \mathbb{E}(Y_1) > 0$. Then for $b \in \mathbb{Z}^n$

$$\sum_{1\le i,j\le n} b_i b_j \chi_{ij} = \sum_{1\le i,j\le n} b_i b_j \frac{\mathbb{E}(Y_i Y_j)}{a} = \frac{1}{a}\mathbb{E}\left[\sum_{i=1}^{n} b_i Y_i\right]^2 \ge \frac{1}{a}\mathbb{E}\left[\sum_{i=1}^{n} b_i Y_i\right] = \sum_{i=1}^{n} b_i,$$

as for any integer k we have $k^2 \ge k$.

Clique partition polytopes A subset $\{C_1, \dots, C_k\}$ of the powerset of $V_n = \{1, \dots, n\}$ is a *partition* of V_n if $k \ge 1$, $C_r \cap C_s = \emptyset$ for $r \ne s$ and $\bigcup_{r=1}^{k} C_r = V_n$. A partition of V_n defines a *clique partition point* $\gamma(\{C_1, \dots, C_k\}) \in \{0,1\}^{E_n}$ by

$$\gamma(\{C_1, \dots, C_k\})_{ij} = \sum_{r=1}^{k} \mathbb{1}_{\{i,j\}\subset C_r}, \quad 1 \le i < j \le n.$$

The *clique partition polytope* is defined as the convex hull of the clique partition points (Grötschel and Wakabayashi, 1990) in $\mathbb{R}^{E_n}$

$$\mathrm{CPP}_n := \mathrm{conv}\left(\{\gamma(\{C_1, \dots, C_k\}) : \{C_1, \dots, C_k\} \text{ partition of } V_n\}\right).$$

Being $\{0,1\}$-valued, the clique partition points are automatically the extremal points of their convex hull:

$$\mathrm{Ex}\left(\mathrm{CPP}_n\right) = \left(\{\gamma(\{C_1, \dots, C_k\}) : \{C_1, \dots, C_k\} \text{ partition of } V_n\}\right).$$

It turns out that all $\{0,1\}$-valued vertices of TCF_n are precisely the clique partition points.

Proposition 21 $\mathrm{TCF}_n \cap \{0,1\}^{E_n} = \mathrm{Ex}(\mathrm{CPP}_n)$ *for all* $n \in \mathbb{N}$. *In particular* $\mathrm{CPP}_n \subset \mathrm{TCF}_n$.

Proof Since $\mathrm{TCF}_n \cap \{0,1\}^{E_n} \subset \mathrm{Ex}(\mathrm{TCF}_n)$ it suffices to show the first statement. For $n = 2$ we have $\mathrm{TCF}_2 = [0,1]$ and $\{0,1\} = \mathrm{Ex}(\mathrm{CPP}_2)$. For $n \geq 3$ the points in TCF_n have to satisfy the triangle-inequalities (all permutations of $\chi_{1,2} + \chi_{2,3} - \chi_{1,3} \leq 1$, see (2) and also (18) with $b = (1,-1,1,0,\ldots,0)$). For points $\chi \in \mathrm{TCF}_n \cap \{0,1\}^{E_n}$, viewed via the support graph K_n, this implies for any triple of nodes i,j,k, where the edges $\{i,j\}$ and $\{j,k\}$ have value 1, that also the edge $\{i,k\}$ has value 1. Thus, a simple inductive argument shows: for any pair of nodes i,j, which are connected by a path of edges with value 1, the edge from i to j has also value 1. This shows that the points in $\mathrm{TCF}_n \cap \{0,1\}^{E_n}$ are clique partition points. In order to see that any clique partition point $\gamma(\{C_1,\ldots,C_k\})$ belongs to $\mathrm{TCF}_n \cap \{0,1\}^{E_n}$ choose $\Omega = \{1,\ldots,k\}$ with uniform distribution $\mathbb{P}$ and $A_i = \{r_i\}$, $1 \leq i \leq n$, with r_i uniquely determined by $i \in C_{r_i}$ and apply Lemma 16.

For $n \leq 4$ the clique partition polytope and TCF_n even coincide.

Proposition 22 $\mathrm{TCF}_n = \mathrm{CPP}_n$ *for* $n \leq 4$.

Proof For $n \leq 4$ we computed explicitly that $\mathrm{Ex}(\mathrm{TCF}_n) = \mathrm{Ex}(\mathrm{CPP}_n)$ from the characterization (17) (Strokorb, 2013, Tables 3.1 and 3.3) and confirmed this result using the software `polymake`. This implies $\mathrm{TCF}_n = \mathrm{CPP}_n$ for $n \leq 4$.

Low-dimensional phenomena Even though for $n \leq 4$ the polytope TCF_n and the clique partition polytope CPP_n coincide, the property $\mathrm{TCF}_n = \mathrm{CPP}_n$ will turn out to be a low-dimensional phenomenon. Starting from $n = 5$ the vertices of TCF_n are not $\{0,1\}$-valued anymore (see Corollary 28 in Section 6), in particular $\mathrm{CPP}_n \subsetneq \mathrm{TCF}_n$ for $n \geq 5$. Still, up to $n \leq 5$ all facet inducing inequalities of TCF_n turn out to be hypermetric and one might be tempted to believe that certain hypermetric inequalities provide an $\mathcal{H}$-representation for TCF_n also in higher dimensions. Again, this property constitutes only another low-dimensional phenomenon. Starting from $n = 6$ not all facets of TCF_n are hypermetric anymore (see Proposition 32 in Section 6).

6 Sophisticated results on the geometry of TCF_n

A fundamental observations in this section concerns the lifting of vertices and facets to higher dimensions (Section 6.1). It means that vertices (and facets) of TCF_n will also appear as vertices (and facets) of $\mathrm{TCF}_{n'}$ for $n' > n$ if the coordinates (or coefficients) are filled up with zeros at appropriate places. Note that both statemenents are not evident, but a deep structural result only revealed by some delicate combinatorial arguments. Subsequently, we prove that every rational number in the interval $[0,1]$ will appear as coordinate value in the vertex set of TCF_n starting from a sufficiently large n (Proposition 27 in Section 6.2) and that TCF_n possesses non-hypermetric facets starting from $n \geq 6$ (Proposition 32 in Section 6.3). Taken together, these results give insights into the rapidly growing complexity of TCF_n as n grows and confound the aim of a full description of vertices and facets of TCF_n for arbitrary n. Finally, Section 6.4 provides an alternative ("dual") description of the polytope TCF_n (which we recognized already as the *projection* of the polytope Θ_n) as an *intersection* with the so-called correlation polytope or, equivalently, with the so-called cut-polytope.

6.1 **Lifting of vertices and facets to higher dimensions**

First, we deal with connections between TCF_n and TCF_{n+1}. A particularly important feature is the lifting property. That is every vertex of TCF_n will appear again in the list of vertices of TCF_{n+1} with some zeros added.

Lemma 23 (Projections and liftings of points and vertices)
For $\chi \in \mathrm{TCF}_{n+1}$ let $\chi|_{K_n}$ denote the restriction of χ to the subgraph $K_n \subset K_{n+1}$ (delete all $\chi_{i,n+1}$, $1 \le i \le n$). Conversely, let $\chi^0 \in \mathbb{R}^{E_{n+1}}$ denote the extension of a point $\chi \in \mathrm{TCF}_n$ by

$$\chi^0_{i,n+1} = 0, \quad 1 \le i \le n.$$

a) The assignment $\chi \mapsto \chi|_{K_n}$ maps TCF_{n+1} onto TCF_n.
b) The assignment $\chi \mapsto \chi^0$ embeds TCF_n into TCF_{n+1} and $\mathrm{Ex}(\mathrm{TCF}_n)$ into $\mathrm{Ex}(\mathrm{TCF}_{n+1})$.
c) If $\chi \in \mathrm{Ex}(\mathrm{TCF}_{n+1})$ and $\chi_{i,n+1} = 0$ for all $1 \le i \le n$, then $\chi|_{K_n} \in \mathrm{Ex}(\mathrm{TCF}_n)$.

Proof a) Let $Y_1, \dots, Y_{n+1}$ be a binary process that models χ. Simply deleting Y_{n+1} gives a model for $\chi|_{K_n} \in \mathrm{TCF}_n$. Surjectivity follows from b).
b) Let $Y_1, \dots, Y_n$ be a binary process that models χ. Let $a = \mathbb{E}(Y_1)$. Add a disjoint point ω_0 to the underlying probability space Ω and replace the probability measure $\mathbb{P}$ by $\frac{1}{1+a} \cdot \mathbb{P}|_\Omega + \frac{a}{1+a} \cdot \delta_{\omega_0}$. Extend $Y_1, \dots, Y_n$ by 0 on ω_0, let $Y_{n+1} = \mathbf{1}_{\{\omega_0\}}$. Now, $Y_1, \dots, Y_{n+1}$ is a model for χ^0, since $Y_i Y_{n+1} = 0$, $1 \le i \le n$. If $\chi^0 \notin \mathrm{Ex}(\mathrm{TCF}_{n+1})$, there is a representation $\chi^0 = \lambda y + (1-\lambda) z$, with $y, z \in \mathrm{TCF}_{n+1}$, $0 < \lambda < 1, y \ne z$. Since χ^0 is zero on the new edges, the points y, z also have to be zero on the new edges, so $y|_{K_n} \ne z|_{K_n}$ and $y|_{K_n}, z|_{K_n} \in \mathrm{TCF}_n$ by a). Thus, $\chi = \chi^0|_{K_n} \notin \mathrm{Ex}(\mathrm{TCF}_n)$.
c) If $\chi|_{K_n} \notin \mathrm{Ex}(\mathrm{TCF}_n)$, then $\chi|_{K_n} = \lambda y + (1-\lambda) z$, with $y, z \in \mathrm{TCF}_n$, $0 < \lambda < 1, y \ne z$. By b) we know $y^0, z^0 \in \mathrm{TCF}_{n+1}$. Since $\chi_{i,n+1} = 0$ for all $1 \le i \le n$, we have $\chi = (\chi|_{K_n})^0 = \lambda y^0 + (1-\lambda) z^0 \notin \mathrm{Ex}(\mathrm{TCF}_{n+1})$.

We call χ^0 a *lifting* of χ. The following lemma generalizes the lifting of vertices and will be applied to deduce Proposition 27.

Lemma 24 (Lifting of vertices arising from partitions)
Let $C_1, \dots, C_k \subset V_n$ be disjoint subsets of the vertex set $V_n = \{1, \dots, n\}$ each containing at least two elements of V_n. For $1 \le r \le k$ let $\chi^r \in \mathrm{Ex}(\mathrm{TCF}(C_r))$. Similarly to the interpretation of TCFs on $V_n = \{1, \dots, n\}$ as elements of

$\mathbb{R}^{E_n}$, *we interpret* χ^r *as an element of* $\mathbb{R}^{E(C_r)}$, *where* $E(C_r)$ *is the set of edges of the complete graph with vertex set* $C_r \subset V_n$. *Define* $\chi \in \mathbb{R}^{E_n}$ *by*

$$\chi_{ij} = \begin{cases} \chi^r_{ij} & \text{if } \{i,j\} \subset C_r \text{ for some } 1 \le r \le k, \\ 0 & \text{else.} \end{cases}$$

Then $\chi \in \mathrm{Ex}(\mathrm{TCF}_n)$.

Proof Because of the lifting property (Lemma 23), it suffices to consider the case $V_n = \bigcup_{r=1}^k C_r$, where $C_r = \{i_1^{(r)}, \ldots, i_{|C_r|}^{(r)}\}$. First, we show that $\chi \in \mathrm{TCF}_n$. To this end, choose (finite) set models

$$(\Omega_r, \mathbb{P}_r), \quad A^r_{i_1^{(r)}}, \ldots, A^r_{i^{(r)}_{|C_r|}} \subset \Omega_r, \quad 1 \le r \le k$$

for χ^r as in Lemma 16 such that $\chi^{(r)}_{ij} = \mathbb{P}(A^r_i \mid A^r_j)$. By Remark 17 these models can be chosen such that $\mathbb{P}_r(A^r_i)$ does not depend on r. Then a stochastic model for χ is obtained through the normalized disjoint union of these models, i.e. where $\Omega = \bigcup_{r=1}^k \Omega_r$, $\mathbb{P} = \frac{1}{k}\sum_{r=1}^k \mathbb{P}_r(\cdot \cap \Omega_r)$ and $A_i = A^r_i$ if $i \in C_r$. (Note that for each $i \in V_n$ there exists a unique r with $i \in C_r$, since the sets C_r are disjoint and cover V_n.)

Now, we show that $\chi \in \mathrm{Ex}(\mathrm{TCF}_n)$. Suppose not. Then $\chi = \lambda y + (1-\lambda)z$ with $1 < \lambda < 0$ and $y, z \in \mathrm{TCF}_n$ with $y \neq z$. Necessarily $y_{ij} = 0$ and $z_{ij} = 0$ whenever $\chi_{ij} = 0$. Thus, $y|_{K^r_n} \neq z|_{K^r_n}$ for some $1 \le r \le k$ when K^r_n denotes the complete subgraph of K_n defined by C_r. Since $y|_{K^r_n}, z|_{K^r_n} \in \mathrm{TCF}(C_r)$ by Lemma 23, we obtain $\chi^r = \chi|_{K^r_n} = \lambda y|_{K^r_n} + (1-\lambda) z|_{K^r_n}$ contradicting $\chi^r \in \mathrm{Ex}(\mathrm{TCF}(C_r))$.

In order to deduce the lifting property also for inequalities and facets, we adapt ideas from (Deza and Laurent, 1997, Lemma 26.5.2). We show that, starting from $n = 3$, no facet inducing inequality will ever become obsolete as n grows. For instance, the triangle inequality (2) cannot be deduced from a set of other valid inequalities for TCF_n. One needs $n \ge 3$, since the inequality $\chi_{12} \le 1$, although facet-inducing for $n = 2$, is no longer facet-inducing for $n \ge 3$, see Table 3 and Proposition 25 b).

Proposition 25 (Lifting of valid inequalities and facets)
Suppose that

$$a_0 + a_{1,2}\chi_{1,2} + \ldots + a_{n-1,n}\chi_{n-1,n} \ge 0 \tag{19}$$

is a valid inequality for TCF_n. *The lifting of this inequality to* $\mathbb{R}^{E_{n+1}}$ *is the corresponding inequality which is extended by*

$$a_{i,n+1} = 0, \quad 1 \le i \le n.$$

a) Every lifting of a valid inequality of TCF_n *defines a valid inequality of* TCF_{n+1}.
b) For $n \ge 3$, *the lifting of a facet of* TCF_n *defines a facet of* TCF_{n+1}.

Proof a) The lifting of a valid inequality for TCF_n is always valid for TCF_{n+1}, even for $n = 2$, since the lifted equation applied to $\chi \in \mathrm{TCF}_{n+1}$ returns the same value as the orginal equation applied to $\chi|_{K_n}$, which is a point of TCF_n, see Lemma 23.

b) Now suppose that (19) is a facet for TCF_n. By the above, its lifting is a valid inequality for TCF_{n+1}. We show that it defines a facet if $n \geq 3$. First, note that there has to be a coefficient $a_{i,j} \neq 0$. Since $n \geq 3$, there is some index $k \notin \{i, j\}$. To simplify notation, we assume $k = 1 < i < j \leq n$.
Further, let $m := \binom{n}{2}$ and let $a = (a_0, a_{1,2}, a_{1,3}, \ldots, a_{n-1,n}) \in \mathbb{R}^{m+1}$ denote the vector of coefficients that appear in the inequality (19). Since (19) induces a facet of TCF_n, there exist m affinely independent points $\chi^k \in \mathrm{TCF}_n \subset \mathbb{R}^m$, $1 \leq k \leq m$ that solve the inequality (19) as an equation. Affine independence of the m points χ^k means that the m points $(1, \chi^k) \in \mathbb{R}^{m+1}$ are linearly independent in $\mathbb{R}^{m+1}$. By assumption, they solve $\langle (1, \chi^k), a\rangle = 0$, $1 \leq k \leq m$. Let $W \subset \mathbb{R}^{m+1}$ denote the vector space spanned by $(1, \chi^k), 1 \leq k \leq m$. Then $\dim(W) = m$ and $W \perp a$.
Since $a_{i,j} \neq 0$ for some $1 < i < j$, a non-zero entry occurs after the n^{th} entry of a. Thus, a suitable unit vector shows $U_n := \{0\}^n \oplus \mathbb{R}^{m+1-n} \not\subset \{a\}^{\perp}$. Since $W \perp a$, the inclusion $W \cap U_n \subset U_n$ is necessarily strict, which entails $\dim(W \cap U_n) \leq m - n$. Let $\mathrm{pr} : W \to \mathbb{R}^n$ denote the projection onto the first n coordinates. By elementary linear algebra and since $\mathrm{Ker}(\mathrm{pr}) = W \cap U_n$ by definition, $\dim(\mathrm{Im}(\mathrm{pr})) = \dim W - \dim(\mathrm{Ker}(\mathrm{pr})) \geq m - (m-n) = n$. Thus, $\mathrm{pr}(W) = \mathbb{R}^n$ and the set $\{\mathrm{pr}((1, \chi^k))\}_{1 \leq k \leq m} = \{(1, \chi^k_{1,2}, \ldots, \chi^k_{1,n})\}_{1 \leq k \leq m}$ contains n linearly independent vectors, which we may assume to be indexed by $1 \leq k \leq n$ (reordering the χ^k if necessary).
Finally, we construct $\binom{n+1}{2}$ affinely independent solutions in TCF_{n+1} for the lifted equation

$$a_0 + a_{1,2}\chi_{1,2} + \ldots + a_{n,n+1}\chi_{n,n+1} = 0, \quad \text{with} \quad a_{i,n+1} = 0, \quad 1 \leq i \leq n.$$

To simplify notation, assume that the new coordinates $\chi_{1,n+1}, \ldots, \chi_{n,n+1}$ are added to the right of the previous coordinates $\chi_{1,2}, \ldots, \chi_{n-1,n}$. We show that the $m + n = \binom{n+1}{2}$ points (recall $m := \binom{n}{2}$)

(a) $(\chi^k, 0, \ldots, 0) \in \mathbb{R}^{m+n}$, $\quad 1 \leq k \leq m$, (with n 0's added),
(b) $(\chi^k, \mathrm{pr}((1, \chi^k))) \in \mathbb{R}^{m+n}$, $\quad 1 \leq k \leq n$,

solve the lifted equation, belong to TCF_{n+1} and are affinely independent.
The first statement follows from the choice of the χ^k. The points in (a) belong to TCF_{n+1} by Lemma 23. For (b), let $Y_1, \ldots, Y_n$ be a stochastic model for χ^k. Extend this model to $n + 1$ variables $Y_1, \ldots, Y_n, Y_{n+1}$ by $Y_{n+1} := Y_1$. Since $\mathrm{pr}((1, \chi^k)) = (1, \chi^k_{1,2}, \ldots, \chi^k_{1,n})$, this yields $(\chi^k, \mathrm{pr}((1, \chi^k))) \in \mathrm{TCF}_{n+1}$.
Linear independence of the $m + n$ points

$$\{(1, \chi^k, 0, \ldots, 0)\}_{1 \leq k \leq m} \cup \{(1, \chi^k, \mathrm{pr}((1, \chi^k)))\}_{1 \leq k \leq n}$$

follows from the independence of $\mathrm{pr}((1,\chi^k))$, $1 \leq k \leq n$ and the choice of the χ^k.

Remark 26 By a slight abuse of notation, we will also call any vertex in the permutation orbit of χ^0 a lifting of the vertex χ and any facet in the permutation orbit of a lifted facet a lifting of the respective facet.

6.2 **Unboundedness of denominators**

The following proposition shows that every rational number in the interval $[0,1]$ will appear as coordinate value in the vertex set of TCF_n starting from a sufficiently large n. The result is even sharper in that it detects a single vertex, whose coordinate values comprise a given finite subset of $[0,1]$-valued rational numbers.

Proposition 27 (Unboundedness of denominators)
For each finite subset $Q \subset \mathbb{Q} \cap [0,1]$ of rational numbers in the interval $[0,1]$ there exists an $n \in \mathbb{N}$ and a point $\chi \in \mathrm{Ex}(\mathrm{TCF}_n)$ whose coordinate-values $(\chi_{ij})_{1 \leq i<j \leq n}$ include the set Q.
(By the lifting property, this holds for all $n' \geq n$, too.)

Proof By Lemma 24 it suffices to consider singletons $Q = \{q\}, q \in \mathbb{Q} \cap [0,1]$. The proof only uses the following properties of $\chi \in \mathrm{TCF}_n$:

- "Positivity" $\chi_{ij} \geq 0$ and
- the permutations of the valid inequalities

$$\sum_{i=1}^{r} \chi_{i,r+1} - \sum_{1 \leq i<j \leq r} \chi_{i,j} \leq 1, \quad r \geq 2$$

  which are hypermetric with b-vector $b = (1,\ldots,1,-1,0,\ldots,0)$ (with $r \geq 2$ times the entry 1), in particular permutations of the "triangle inequality" $\chi_{1,3} + \chi_{2,3} - \chi_{1,2} \leq 1$. The validity of these inequalities has been shown in Lemma 20.

The cases $q = 0$ and $q = 1$ are trivial.

(I) We show that for rationals $q = \frac{1}{m}$ and $q = \frac{m-1}{m}$ it suffices to choose $n = 2m+1$. Let $\Omega = \{\omega_1, \omega_{2,1}, \ldots, \omega_{2,m}, \omega_{3,1}, \ldots, \omega_{3,m}\}$ be a set with $2m+1$ elements and define a positive function g on Ω by

$$g(\omega_1) = \frac{1}{m}; \quad g(\omega_{2,i}) = \frac{m-1}{m} \quad \text{and} \quad g(\omega_{3,i}) = \frac{1}{m}, \quad 1 \leq i \leq m.$$

Normalizing g by $c := \frac{m^2+1}{m}$ yields a probability measure $\mathbb{P}$ on Ω by $\mathbb{P}(\{\omega\}) = g(\omega)/c$. Now, we define $2m+1$ subsets of Ω as follows:

$$A_{1,i} = \{\omega_1, \omega_{2,i}\}, \quad A_{2,i} = \{\omega_{2,i}, \omega_{3,i}\}, \quad 1 \leq i \leq m, \quad A_{3,1} = \{\omega_{3,1}, \ldots, \omega_{3,m}\}.$$

Since all of these $2m+1$ sets have the same probability $1/c$, they define a point $\chi \in \mathrm{TCF}_{2m+1}$ as in Lemma 16.

When viewed as an edge labelling χ can be described as follows: Let $\{v_{1,1},\dots,v_{1,m},v_{2,1},\dots,v_{2,m},v_{3,1}\}$ denote the nodes of the support graph of χ. A pair of nodes v_{i_1,i_2}, v_{j_1,j_2} is connected by an edge with label $\chi_{(i_1,i_2),(j_1,j_2)} = \mathbb{P}(A_{i_1,i_2} \mid A_{j_1,j_2})$. Draw the nodes $\{v_{1,1},\dots,v_{1,m}\}$ at the bottom level, they form a complete subgraph, all edges labelled by $\frac{1}{m}$. Above them draw the nodes $v_{2,1},\dots,v_{2,m}$, where $v_{2,i}$ is connected to $v_{1,i}$ with an edge labelled $\frac{m-1}{m}$. Finally, the top node $v_{3,1}$ is connected to each $v_{2,1},\dots,v_{2,m}$ with an edge labelled $\frac{1}{m}$.

We show now that $\chi \in \mathrm{Ex}(\mathrm{TCF}_{2m+1})$. To this end, consider a representation $\chi = \lambda y + (1-\lambda)z$, $0<\lambda<1$, $y,z \in \mathrm{TCF}_{2m+1}$. Whenever χ satisfies a valid inequality as an equality, the same has to be true for y and z. Consider y. All χ-edges with label 0 have label 0 for y, too. Denote the unknown label $y_{(1,1),(2,1)}$ of the y-edge from $v_{1,1}$ to $v_{2,1}$ by $1-a \in [0,1]$. Note that χ satisfies a triangle inequality as an equality at $v_{2,1}, v_{1,1}, v_{1,2}$, since $\frac{m-1}{m} + \frac{1}{m} - 0 = 1$. This enforces $y_{(1,1),(1,2)} = a$. Now the triangle $v_{1,1}, v_{1,2}, v_{2,2}$ enforces $y_{(1,2),(2,2)} = 1-a$. Repeating this argument gives $y_{(1,i),(2,i)} = 1-a$ for all $1 \le i \le m$. From this, again just using triangles, it follows $y_{(1,i),(1,j)} = a$ for all $1 \le i < j \le m$ and $y_{(2,i),(3,1)} = a$ for all $1 \le i \le m$. Finally, observe that χ satisfies the hypermetric inequality given by $b = (0,\dots,0,1,1,\dots,1,-1)$, with m 1's, as an equality $\sum_{i=1}^m \chi_{(3,1),(2,i)} - \sum_{1\le i<j\le m} \chi_{(2,i),(2,j)} = m \cdot \frac{1}{m} - 0 = 1$. Applied to y, this forces $m \cdot a = 1$, thus $a = 1/m$. This shows $y = \chi$. The same argument applies to z. Hence $y = \chi = z$ and $\chi \in \mathrm{Ex}(\mathrm{TCF}_{2m+1})$.

(II) Now let $q = \frac{k}{m}$ for some $1 \le k \le m-1$. We modify the above construction to obtain a $\chi \in \mathrm{Ex}(\mathrm{TCF}_{2m+3})$ with some coordinate value equal to q. Extend Ω by two points to $\Omega' := \Omega \cup \{\omega_{3,m+1}, \omega_{3,m+2}\}$. Extend g by

$$g(\omega_{3,m+1}) = \frac{k}{m} \quad \text{and} \quad g(\omega_{3,m+2}) = \frac{m-k}{m}.$$

Normalizing g defines now $\mathbb{P}'$. Use the same definitions for the sets $A_{i,j}$ as above and add the two sets

$$A_{3,2} = \{\omega_{3,1},\dots,\omega_{3,m-k},\omega_{3,m+1}\} \quad \text{and} \quad A_{3,3} = \{\omega_{3,m+1},\omega_{3,m+2}\}.$$

All sets have the same probability (the inverse of the normalizing constant) and thus, they define a point $\chi \in \mathrm{TCF}_{2m+3}$. Its support graph has two more nodes $v_{3,2}, v_{3,3}$, corresponding to $A_{3,2}$ and $A_{3,3}$. The new edges are

$$\chi_{(2,i),(3,2)} = \frac{1}{m}, \quad 1 \le i \le m-k, \quad \chi_{(3,1),(3,2)} = \frac{m-k}{m}, \quad \chi_{(3,2),(3,3)} = \frac{k}{m}.$$

Repeating the arguments from the first part shows $y = \chi$ on the "old" edges. Now, using the new triangles at $v_{3,2}, v_{2,i}, v_{1,i}$ for $1 \le i \le m-k$, we get

$$y_{(2,i),(3,2)} = \frac{1}{m}, \quad 1 \le i \le m-k.$$

Note that a permutation of the hypermetric inequality $b = (1, \dots, 1, -1, 0, \dots, 0)$ with $m-k+1$ leading 1's is fulfilled by χ as an equality, if the -1 corresponds to $v_{3,2}$ and the 1's correspond to $v_{2,1}, \dots, v_{2,m-k}, v_{3,3}$. Applied to y, this yields $(m-k) \cdot \frac{1}{m} + y_{(3,2),(3,3)} = 1$, thus $y_{(3,2),(3,3)} = \frac{k}{m}$. Finally, the triangle at $v_{3,1}, v_{3,2}, v_{3,3}$ implies $y_{(3,1),(3,2)} = \frac{m-k}{m}$. Thus, $y = \chi$ and the same argument applies to z. Hence, $\chi \in \mathrm{Ex}(\mathrm{TCF}_{2m+3})$.

For $n \leq 4$ we have seen that $\mathrm{CPP}_n = \mathrm{TCF}_n$ (Proposition 22). This is complemented by the following result.

Corollary 28
For $n \geq 5$ we have $\mathrm{Ex}(\mathrm{TCF}_n) \not\subset \{0,1\}^{E_n}$ and, in particular, $\mathrm{CPP}_n \subsetneq \mathrm{TCF}_n$.

Proof By the lifting of extremal points (Lemma 23) it suffices to prove this for $n = 5$. For $q = \frac{1}{2}$ the construction (I) in the proof of Proposition 27 yields an example with $n = 5$.

Remark 29 For $q = \frac{1}{2}$ the above construction (I) is optimal: it gives the smallest possible n for the occurence of q as the coordinate value of a vertex of TCF_n. To realize $q = \frac{1}{3}$ the construction (I) uses $n = 7$, but a coordinate value $\frac{1}{3}$ already occurs for $n = 6$, as the computation of $\mathrm{Ex}(\mathrm{TCF}_6)$ in Section 7 shows.

6.3 Non-hypermetric facets of TCF_n for $n \geq 6$

We give a proof for the existence of non-hypermetric facets. First, we provide two simple necessary conditions for hypermetricity. Of course, multiplying a given (affine) inequality by some constant $q \neq 0$ does not change the halfspace it describes. Thus, one is often interested, if a given inequality is hypermetric up to a suitable multiplication.

Lemma 30 *Suppose that an inequality $\sum_{1 \leq i < j \leq n} c_{ij} x_{ij} \leq c_0$ (with rational coefficients) is equivalent to a hypermetric inequality, i.e., it becomes a hypermetric inequality defined by some $b \in \mathbb{Z}^n$ after multiplication with a suitable constant $q \in \mathbb{Q} \setminus \{0\}$. Then we have:*

a) The edges $\{i,j\} \subset E_n$ with $c_{ij} \neq 0$ form a complete subgraph of the support graph K_n.
b) The vectors $v_1 := (c_{1,3}, \dots, c_{1,n})$ and $v_2 := (c_{2,3}, \dots, c_{2,n})$ are linearly dependent.

Proof a) By assumption $c_{ij} = -q^{-1} \cdot b_i b_j$ for some $q \in \mathbb{Q} \setminus \{0\}$. Thus, the non-zero c_{ij} correspond to the edges of the complete subgraph with nodes $\{1 \leq i \leq n \,|\, b_i \neq 0\}$.
b) Again, $c_{ij} = -q^{-1} \cdot b_i b_j$. If $b_2 = 0$, then $v_2 = 0$, thus, v_1, v_2 are dependent. If $b_2 \neq 0$, then $v_1 = (b_1/b_2) \cdot v_2$.

Remark 31 Note that criterion a) of Lemma 30 also implies: if there is at least one 0-coefficient, there have to be at least n 0-coefficients, and if the first $n-1$ coefficients $c_{1,2}, \dots, c_{1,n}$ are positive, all have to be positive.

The following proposition shows the existence of non-hypermetric facets of TCF_n starting from $n \geq 6$. It was inspired by the 2nd inequality of Generator 7 in Table 5.

Proposition 32 (Non-hypermetric facets of TCF_n for $n \geq 6$)
For $n \geq 6$ there are non-hypermetric facets of TCF_n.
An example, for arbitrary $n \geq 6$, is given by the facet inducing inequality

$$\sum_{i=1}^{5} x_{i,6} - \sum_{i=1}^{4} x_{i,i+1} - x_{1,5} \leq 2.$$

Proof By the lifting of facets (Proposition 25), it suffices to consider the case $n = 6$. We start with a simple observation for 0-1-vectors of even length: For $y \in \{0,1\}^{2k}, k \in \mathbb{N}$, the inequality

$$\sum_{i=1}^{2k-1} y_i \cdot (y_{2k} - y_{\pi(i)}) \leq (k-1) \cdot y_{2k} \tag{20}$$

holds, where π is the cyclic permutation of $1, \dots, 2k-1$, i.e., $\pi(i) = i+1$, $i < 2k-1$ and $\pi(2k-1) = 1$. The observation is trivial if $y_{2k} = 0$. To handle the case $y_{2k} = 1$ observe that $y_i(1 - y_{\pi(i)}) = 1$ if and only if $y_i = 1$ and $y_{\pi(i)} = 0$. There can be at most $k-1$ occurrences of the word "10" in the string $y_1, \dots, y_{2k-1}, y_1$. Applying (20) to arbitrary binary random variables $Y_1, \dots, Y_{2k}$ and taking expectations yields

$$\sum_{i=1}^{2k-1} \mathbb{E}(Y_i Y_{2k}) - \sum_{i=1}^{2k-1} \mathbb{E}(Y_i Y_{\pi(i)}) \leq (k-1)\mathbb{E}(Y_{2k}).$$

If, additionally, $a := \mathbb{E}(Y_1) = \dots = \mathbb{E}(Y_{2k}) > 0$, dividing by a gives the following valid inequality for TCF_{2k}, where $x_{i,j} := \frac{1}{a}\mathbb{E}(Y_i Y_j)$,

$$\sum_{i=1}^{2k-1} x_{i,2k} - \sum_{i=1}^{2k-1} x_{i,\pi(i)} \leq (k-1) \tag{21}$$

(which has a very simple supporting graph when we identify $x_{2k-1,1}$ with $x_{1,2k-1}$). Assume now $k \geq 3$. Since the coefficients of $x_{1,2}$ and $x_{2,3}$ are -1 and the coefficient of $x_{1,3}$ is 0, the non-zero coefficients do not define a complete subgraph of the support graph. Thus, Lemma 30 a) shows that the above inequality is not hypermetric for $k \geq 3$.

Finally, we show that for $k = 3$, the inequality (21) defines a facet for $\mathrm{TCF}_6 \subset \mathbb{R}^{E_6}$: To this end, we define $|E_6| = 15$ points $x^r, y^r, z^r \in \{0,1\}^{E_6}$, $1 \le r \le 5$ by

$$
\begin{aligned}
&(a) \quad x^r_{i,j} = 1 \quad :\Leftrightarrow \quad \{i,j\} \subset A_r := \{r, \pi^2(r), 6\},\\
&(b) \quad y^r_{i,j} = 1 \quad :\Leftrightarrow \quad \{i,j\} \subset B_r := \{r, \pi(r), \pi^3(r), 6\},\\
&(c) \quad z^r_{i,j} = 1 \quad :\Leftrightarrow \quad (\{i,j\} \subset B_r \quad \text{or} \quad \{i,j\} = \{\pi^2(r), \pi^4(r)\}).
\end{aligned}
$$

Note that these points are clique partion points and thus belong to the set TCF_6 by Proposition 21. Using the support graph of (21) for $k = 3$, it can be easily seen that they solve (21) for $k = 3$ as an equality. Moreover, these 15 points are affinely independent, since they are even linearly independent as the determinant of the corresponding 15×15 0-1-matrix is $-2 \neq 0$.

6.4 Embedding TCF_n into the Correlation and Cut polytopes

We saw already in the proof of Corollary 18 that the polytope TCF_n can be viewed essentially as a *projection* of the convex polytope Θ_n onto several coordinates as in (17). In this section we will see that the polytope TCF_n can be embedded into the so-called *correlation polytope* (or, equivalently, the so-called *cut polytope*, see Proposition 37 below). Thereby, we obtain a "dual" description of TCF_n as the *intersection* of a polytope with an affine subspace.

To this end, we need to review some notation and results from Deza and Laurent (1997). Remember that E_n denotes the set of edges of the complete graph K_n with vertices $V_n = \{1, \dots, n\}$. For $R \subset V_n$ we define a *correlation vector* $\pi(R) \in \{0,1\}^{V_n \cup E_n}$ by

$$\pi(R)_i = \mathbb{1}_{i \in R}, \quad 1 \le i \le n \qquad \text{and} \qquad \pi(R)_{ij} = \mathbb{1}_{i\in R}\mathbb{1}_{j \in R}, \quad 1 \le i < j \le n.$$

The *correlation polytope* is then defined as the convex hull of these 2^n correlation vectors in $\mathbb{R}^{V_n \cup E_n}$

$$\mathrm{COR}^{\square}_n := \mathrm{conv}\left(\{\pi(R) \,:\, R \subset V_n\}\right).$$

Lemma 33 (Deza and Laurent (1997) Prop. 5.3.4)
A point $p \in \mathbb{R}^{V_n \cup E_n}$ belongs to $\mathrm{COR}^{\square}_n$ if and only if it can be written as $p_i = \mathbb{P}(A_i)$, $1 \le i \le n$ and $p_{ij} = \mathbb{P}(A_i \cap A_j)$, $1 \le i < j \le n$ for some probability space $(\Omega, \mathcal{A}, \mathbb{P})$ and measurable subsets $A_1, \dots, A_n \in \mathcal{A}$.

Secondly, let $S \subset V_{n+1}$. A *cut vector* $\delta(S) \in \{0,1\}^{E_{n+1}}$ is defined through

$$\delta(S)_{ij} = \mathbb{1}_{|S \cap \{i,j\}|=1}, \qquad 1 \le i < j \le n+1.$$

Since $\delta(S) = \delta(S^c)$, there are, in fact, $2^{n+1}/2 = 2^n$ different points $\delta(S)$. The *cut polytope* is defined as the convex hull of these cut vectors in $\mathbb{R}^{E_{n+1}}$

$$\mathrm{CUT}^{\square}_{n+1} := \mathrm{conv}\left(\{\delta(S) \,:\, S \subset V_{n+1}\}\right).$$

Being $\{0,1\}$-valued, the correlation vectors and the cut vectors are automatically the extremal points of their convex hulls

$$\operatorname{Ex}\left(\mathrm{COR}_n^\square\right) = \{\pi(R) : R \subset V_n\} \quad \text{and} \quad \operatorname{Ex}\left(\mathrm{CUT}_{n+1}^\square\right) = \{\delta(S) : S \subset V_{n+1}\}.$$

It is a well-known result that $\mathrm{COR}_n^\square \subset \mathbb{R}^{V_n \cup E_n}$ and $\mathrm{CUT}_{n+1}^\square \subset \mathbb{R}^{E_{n+1}}$ can be transformed into each other by a linear bijection.

Proposition 34 (Deza and Laurent (1997), Section 5.2)) *The covariance mapping $\zeta_n : \mathbb{R}^{V_n \cup E_n} \to \mathbb{R}^{E_{n+1}}$, which maps $p \in \mathbb{R}^{V_n \cup E_n}$ to $\zeta_n(p) = x \in \mathbb{R}^{E_{n+1}}$ via*

$$x_{i,n+1} = p_i, \quad 1 \le i \le n \qquad \text{and} \qquad x_{ij} = p_i + p_j - 2p_{ij}, \quad 1 \le i < j \le n,$$

induces a linear bijection

$$\zeta_n : \mathrm{COR}_n^\square \to \mathrm{CUT}_{n+1}^\square.$$

Remark 35 In (Deza and Laurent, 1997) the inverse $\xi_n := \zeta_n^{-1}$ is termed covariance mapping. For us, it was more instructive to work with ζ_n instead of ξ_n.

A probabilistic description of $\mathrm{CUT}_{n+1}^\square$ is as follows. Here the symmetric difference between sets A and B will be denoted by $A \triangle B = (A \setminus B) \cup (B \setminus A)$.

Lemma 36 *A point $x \in \mathbb{R}^{E_{n+1}}$ belongs to the cut polytope $\mathrm{CUT}_{n+1}^\square$ if and only if one of the following two equivalent statements holds true:*

(i) $x_{i,n+1} = \mathbb{P}(A_i)$, $1 \le i \le n$ *and* $x_{ij} = \mathbb{P}(A_i \triangle A_j)$, $1 \le i < j \le n$ *for some probability space* $(\Omega, \mathcal{A}, \mathbb{P})$ *and measurable subsets* $A_1, \dots, A_n \in \mathcal{A}$.
(ii) $x_{ij} = \mathbb{P}(B_i \triangle B_j)$, $1 \le i < j \le n+1$ *for some probability space* $(\Omega, \mathcal{A}, \mathbb{P})$ *and measurable subsets* $B_1, \dots, B_{n+1} \in \mathcal{A}$.

Proof The equivalence to (i) is an immediate consequence of Lemma 33 and Proposition 34. The equivalence of (i) and (ii) can be seen as follows: (i) $\Rightarrow$ (ii): Set $B_i = A_i$, $1 \le i \le n$ and $B_{n+1} = \emptyset$. (ii) $\Rightarrow$ (i): Set $A_i = B_i \triangle B_{n+1}$, $1 \le i \le n$ and use that $(C \triangle D) \triangle (E \triangle D) = C \triangle E$ for any triplet of sets C, D, E.

Finally, this enables us to interpret TCF_n as an intersection of $\mathrm{COR}_n^\square$ (resp. $\mathrm{CUT}_{n+1}^\square$) with an affine subspace of $\mathbb{R}^{V_n \cup E_n}$ (resp. $\mathbb{R}^{E_{n+1}}$) in the following sense.

Proposition 37 (Embedding TCF_n into the correlation polytope) *The injective affine map $\iota_n : \mathbb{R}^{E_n} \to \mathbb{R}^{V_n \cup E_n}$ which maps $\chi \in \mathbb{R}^{E_n}$ to $\iota_n(\chi) = p \in \mathbb{R}^{V_n \cup E_n}$ via*

$$p_i = \frac{1}{n}, \quad 1 \le i \le n \qquad \text{and} \qquad p_{ij} = \frac{\chi_{ij}}{n}, \quad 1 \le i < j \le n,$$

induces a bijection

$$\iota_n : \mathrm{TCF}_n \to \mathrm{COR}_n^\square \cap \left\{ p \in \mathbb{R}^{V_n \cup E_n} : p_i = \frac{1}{n}, i = 1, \dots, n \right\}.$$

Proof The map ι_n is injective by definition. First, we show that $\iota_n(\mathrm{TCF}_n) \subset \mathrm{COR}_n^\square$. Because of Lemma 16 and Remark 17, a point $\chi \in \mathrm{TCF}_n$ has a stochastic model $A_1, \ldots, A_n$ with $\mathbb{P}(A_1) = \cdots = \mathbb{P}(A_n) = 1/n$ and $\chi_{ij} = \mathbb{P}(A_i \cap A_j)/\mathbb{P}(A_j)$. Lemma 33, applied to $A_1, \ldots, A_n$ and $\mathbb{P}$, shows that ι_n maps TCF_n to $\mathrm{COR}_n^\square$. Now, suppose that $p \in \mathrm{COR}_n^\square \cap \bigcap_{i=1}^n \{p_i = 1/n\}$. By Lemma 33 there is a stochastic model with sets $A_1, \ldots, A_n$, $\mathbb{P}(A_1) = \ldots = \mathbb{P}(A_n) = 1/n$, $\mathbb{P}(A_i \cap A_j) = p_{ij}$. Thus, $\chi = (n \cdot p_{ij})_{1 \le i < j \le n}$ is a preimage of p in TCF_n.

Note that we just established the following equivalences

$$\chi \in \mathrm{TCF}_n \quad \Leftrightarrow \quad \iota_n(\chi) \in \mathrm{COR}_n^\square \quad \Leftrightarrow \quad \zeta_n \circ \iota_n(\chi) \in \mathrm{CUT}_{n+1}^\square.$$

In particular, one can pull back facets from $\mathrm{CUT}_{n+1}^\square$ to $\mathrm{COR}_n^\square$ with the covariance mapping ζ_n, and further, we obtain an $\mathcal{H}$-representation for TCF_n using $\zeta_n \circ \iota_n$. Thus, any $\mathcal{H}$-representation of $\mathrm{COR}_n^\square$ or $\mathrm{CUT}_{n+1}^\square$ yields an $\mathcal{H}$-representation of TCF_n as follows.

Proposition 38 (Pulling back $\mathcal{H}$-representations)

a) (Deza and Laurent (1997) Prop. 26.1.1, p. 402)
The covariance mapping $\xi_n := \zeta_n^{-1}$ maps a valid inequality for $\mathrm{CUT}_{n+1}^\square$ (resp. facet of $\mathrm{CUT}_{n+1}^\square$)

$$\sum_{1 \le i < j \le n+1} c_{ij} x_{ij} \le c_0 \tag{22}$$

to the following valid inequality $\mathrm{COR}_n^\square$ (resp. facet of $\mathrm{COR}_n^\square$)

$$\sum_{1 \le i \le n} b_i p_i + \sum_{1 \le i < j \le n} (-2c_{ij}) p_{ij} \le c_0 \quad \text{with} \quad b_i = \sum_{1 \le s < i} c_{si} + \sum_{i < s \le n+1} c_{is}. \tag{23}$$

b) The above valid inequality (resp. facet) of $\mathrm{CUT}_{n+1}^\square$ induces the following valid inequality for TCF_n via $\zeta_n \circ \iota_n$

$$\sum_{1 \le i < j \le n} (-2c_{ij}) \chi_{ij} \le n \cdot c_0 - 2 \sum_{1 \le i < j \le n} c_{ij} - \sum_{i=1}^{n} c_{i,n+1}. \tag{24}$$

If applied to all elements of an $\mathcal{H}$-representation of $\mathrm{CUT}_{n+1}^\square$ (e.g. all facets of $\mathrm{CUT}_{n+1}^\square$), this gives an $\mathcal{H}$-representation for TCF_n.

Proof b) It suffices to replace x_{ij} in Inequality (22) by

$$(\zeta_n \circ \iota_n(\chi))_{ij} = \begin{cases} \frac{1}{n} & j = n+1, \\ \frac{2}{n} - \frac{2}{n}\chi_{ij} & 1 \le i < j \le n. \end{cases}$$

and to reorder the resulting terms.

Dual views on TCF_n Summarizing, we obtain two complementary views on the polytope TCF_n which may be illustrated as follows.

$$\begin{tikzcd} \Theta_n \arrow[d, "\psi_n"'] & & \\ \mathrm{TCF}_n \arrow[r, hook, "\iota_n"'] & \mathrm{COR}_n^{\square} \arrow[r, "\zeta_n"'] & \mathrm{CUT}_{n+1}^{\square} \end{tikzcd} \qquad \begin{tikzcd} \mathbb{R}^{\mathcal{F}_n^{(2)}} \arrow[d, "\psi_n"'] & & \\ \mathbb{R}^{E_n} \arrow[r, hook, "\iota_n"'] & \mathbb{R}^{V_n \cup E_n} \arrow[r, "\zeta_n"'] & \mathbb{R}^{E_{n+1}} \end{tikzcd}$$

Here ψ_n is given by the "projection" map (17), the map ι_n is the embedding from Proposition 37 and ζ_n the covariance mapping from Proposition 34. While any $\mathcal{V}$-representation of Θ_n easily yields a $\mathcal{V}$-representation of TCF_n essentially by a projection, any $\mathcal{H}$-representation of $\mathrm{CUT}_{n+1}^{\square}$ easily yields an $\mathcal{H}$-representation of TCF_n essentially by an intersection. Unfortunately, Θ_n is a priori given by its facets (an $\mathcal{H}$-represenation), while $\mathrm{CUT}_{n+1}^{\square}$ is a priori given by its vertices (a $\mathcal{V}$-representation) and not the other way around, such that both views come along with certain drawbacks. At least the facets of $\mathrm{CUT}_{n+1}^{\square}$ are classified to some extent.

The facets of $\mathrm{CUT}_{n+1}^{\square}$ **and their generators** (Deza and Laurent, 1997, Part V) Let us consider the following two kinds of actions on $\mathbb{R}^{E_{n+1}}$. On the one hand the symmetric group S_{n+1} acts on $\mathbb{R}^{E_{n+1}}$ by node permutations: $(\sigma(x))_{ij} := x_{\sigma(i)\sigma(j)}$ for $\sigma \in S_{n+1}$. These actions are simply called *permutations*. On the other hand each of the 2^n cut vectors $\delta(S)$ acts on $\mathbb{R}^{E_{n+1}}$ by

$$(\delta(S)(x))_{ij} = \begin{cases} 1 - x_{ij} & \text{if } \delta(S)_{ij} = 1, \\ x_{ij} & \text{otherwise,} \end{cases}$$

for any $S \subset V_{n+1} = \{1, \ldots, n+1\}$, i.e. coordinates x_{ij} corresponding to the edges of the cut beween S and S^c are replaced by $1 - x_{ij}$. These actions are called *switchings*. Note that $\delta(S) \circ \delta(R) = \delta(S \triangle R)$ and that $\delta(S) \circ \sigma = \sigma \circ \delta(\sigma(S))$. In fact, both kinds of actions can be restricted to the cut polytope $\mathrm{CUT}_{n+1}^{\square}$. For any $\sigma \in S_{n+1}$ and any $S \subset V_{n+1}$

$$\sigma(x) \in \mathrm{CUT}_{n+1}^{\square} \quad \Leftrightarrow \quad x \in \mathrm{CUT}_{n+1}^{\square} \quad \Leftrightarrow \quad \delta(S)(x) \in \mathrm{CUT}_{n+1}^{\square}.$$

These permutations and switchings on the polytope $\mathrm{CUT}_{n+1}^{\square}$ induce, of course, corresponding actions on its facets. First, it is not surprising that (22) is a facet inducing inequality of $\mathrm{CUT}_{n+1}^{\square}$ if and only if

$$\sum_{1 \le i < j \le n+1} c_{\sigma(i)\sigma(j)} x_{ij} \le c_0$$

is facet inducing for $\mathrm{CUT}_{n+1}^{\square}$. Second, any facet inducing inequality (22) can be *switched* by a cut vector $\delta(S)$ to another facet inducing inequality of $\mathrm{CUT}_{n+1}^{\square}$ which is given by

$$\sum_{1 \le i < j \le n+1} (1 - 2\delta(S)_{ij}) c_{ij} x_{ij} \le c_0 - \sum_{1 \le i < j \le n+1} \delta(S)_{ij} c_{ij}.$$

Let $O^{SP}(g, c_0)$ denote the full orbit of a facet $g(x) \leq c_0$ under all possible finite applications of switchings and permutations to $g(x) \leq c_0$. The set of all facets of $\mathrm{CUT}^{\square}_{n+1}$ splits into finitely many such orbits, say O^{SP}_i, $i \in I$. Choosing one facet $g^{(i)}(x) \leq c_0^{(i)}$ from each orbit O^{SP}_i yields a set of representatives $g^{(i)}(x) \leq c_0^{(i)}$, $i \in I$, of the facets of $\mathrm{CUT}^{\square}_{n+1}$, up to switchings and permutations. In this way *generators* for the facets of $\mathrm{CUT}^{\square}_{n+1}$ are given in the literature. It is a feature of the cut polytope that it always has a set of *homogeneous generators*, i.e. with $c_0^{(i)} = 0$, $i \in I$ (Deza and Laurent, 1997, Section 26.3.2).

The facets of $\mathrm{CUT}^{\square}_{n+1}$ and corresponding generators are known for $n \leq 7$ (Deza and Laurent, 1997, p. 504). In Table 6 (Appendix A) we list the 11 generators of the 116 764 facets of $\mathrm{CUT}^{\square}_{7}$ that will be used to derive the facets of TCF_6.

Relations to unit covariances In their works on McMillan's (1955) realization problem concerning covariances of binary processes Quintanilla (2008), Lachieze-Rey (2013); Lachièze-Rey (2015) and Shepp (1963, 1967) considered $\{-1, 1\}$-valued random vectors $(U_1, \ldots, U_n)$ (instead of $\{0, 1\}$-valued vectors) and studied the set of *unit covariances*

$$\mathcal{U}_n := \left\{ u \in \mathbb{R}^{E_n} \;:\; \begin{array}{l} u_{ij} = \mathbb{E}(U_i U_j) \text{ where} \\ U_1, \ldots, U_n \text{ take values in } \{-1, 1\} \end{array} \right\}.$$

As a consequence of Lemma 36 (ii) (set $B_i = \{U_i = 1\}$ therein) the cut polytope $\mathrm{CUT}^{\square}_{n}$ and the set of unit covariances $\mathcal{U}_n$ are affine equivalent via the bijective mapping $g_n : \mathbb{R}^{E_n} \to \mathbb{R}^{E_n}$, $g_n(x) = \frac{1}{2}(1 - x)$ through

$$\mathrm{CUT}^{\square}_{n} = g_n(\mathcal{U}_n). \tag{25}$$

Let us further denote for $c \in [0, 1]$ as in Shepp (1963)

$$\mathcal{U}_n(c) := \left\{ u \in \mathbb{R}^{E_n} \;:\; \begin{array}{l} u_{ij} = \mathbb{E}(U_i U_j) \text{ where} \\ U_1, \ldots, U_n \text{ take values in } \{-1, 1\} \\ \text{and } \mathbb{P}(U_1 = 1) = \cdots = \mathbb{P}(U_n = 1) = c \end{array} \right\}.$$

It is immediate that $\mathcal{U}_n(c) = \mathcal{U}_n(1 - c)$ and repeating an argument from Shepp (1963), p. 10, it is not difficult to see that $\mathcal{U}_n(c)$, $0 \leq c \leq 1/2$ are increasing towards $\mathcal{U}_n(1/2) = \mathcal{U}_n$. The latter equality follows from the fact that the unit covariance of a $\{-1, 1\}$-valued random vector remains unchanged after multiplication with an independent $\{-1, 1\}$-valued zero mean variable. The affine equivalence (25) can be refined to

$$\mathrm{CUT}^{\square}_{n}(c) = g_n(\mathcal{U}_n(c)), \quad c \in [0, 1] \tag{26}$$

if we set

$$\mathrm{CUT}^{\square}_{n}(c) := \mathrm{pr}_n(\mathrm{CUT}^{\square}_{n+1} \cap \{x \in \mathbb{R}^{E_{n+1}} \;:\; x_{i,n+1} = c,\ 1 \leq i \leq n\})$$

and $\mathrm{pr}_n : \mathbb{R}^{E_{n+1}} \to \mathbb{R}^{E_n}$ is the projection onto the edges not containing the vertex $n+1$. A probabilistic description of the polytopes $\mathrm{CUT}_n^{\square}(c)$, $c \in [0,1]$ follows from the equivalence (i) in Lemma 36 (set $A_i = \{U_i = 1\}$) and thereby proves the refinement (26) as follows.

Lemma 39 *A point $x \in \mathbb{R}^{E_n}$ belongs to $\mathrm{CUT}_n^{\square}(c)$ if and only if can be written as $x_{ij} = \mathbb{P}(A_i \triangle A_j)$, $1 \le i < j \le n$ for some probability space $(\Omega, \mathcal{A}, \mathbb{P})$ and measurable subsets $A_1, \ldots, A_n \in \mathcal{A}$ satisfying $\mathbb{P}(A_i) = c$, $1 \le i \le n$.*

A direct connection of unit covariances to TCF_n can be obtained from Lemma 16 and Remark 17 (set $U_i = 2 \cdot \mathbf{1}_{A_i} - 1$ therein) as

$$f_n(\mathrm{TCF}_n) = \mathcal{U}_n(1/n),$$

where $f_n : \mathbb{R}^{E_n} \to \mathbb{R}^{E_n}$ is the bijective affine mapping $f_n(x) = \frac{4}{n}x - \frac{4}{n} + 1$. It can be easily checked that the following diagram commutes if ζ_n and ι_n are the respective affine mappings from Propositions 34 and 37.

$$\begin{tikzcd}
\mathrm{TCF}_n \arrow[r, hook, "\zeta_n \circ \iota_n"] \arrow[d, "f_n"'] & \mathrm{CUT}_{n+1}^{\square} \arrow[d, "\mathrm{pr}_n"] \\
\mathcal{U}_n(1/n) \arrow[r, "g_n"'] & \mathrm{CUT}_n^{\square}(1/n)
\end{tikzcd}
\qquad
\begin{tikzcd}
\mathbb{R}^{E_n} \arrow[r, hook, "\zeta_n \circ \iota_n"] \arrow[d, "f_n"'] & \mathbb{R}^{E_{n+1}} \arrow[d, "\mathrm{pr}_n"] \\
\mathbb{R}^{E_n} \arrow[r, "g_n"'] & \mathbb{R}^{E_n}
\end{tikzcd}$$

We remark the simple form of the mapping $(g_n \circ f_n)(x) = \frac{2}{n}(1-x)$. The following lemma shows that the polytopes $\mathrm{CUT}_n^{\square}(c)$, $0 < c \le 1/n$ and $\mathcal{U}_n(c)$, $0 < c \le 1/n$ are also affine isomorphic.

Lemma 40 *For $\lambda \in [0,1]$ we have*

$$\begin{aligned}
\mathrm{CUT}_n^{\square}(\lambda/n) &= \lambda \cdot \mathrm{CUT}_n^{\square}(1/n) \\
\mathcal{U}_n(\lambda/n) &= \lambda \cdot \mathcal{U}_n(1/n) + (1-\lambda).
\end{aligned}$$

Proof The second relation follows from the first by applying the map g_n. We prove the first statement using Lemma 39 for both inclusions ("$\subset$" and "$\supset$"), where we may assume that $A := \bigcup_{i=1}^n A_i \ne \Omega$ (otherwise add a point to Ω). An element $x \in \mathrm{CUT}_n^{\square}(\lambda/n)$ admits the representation $x_{ij} = \mathbb{P}(A_i \triangle A_j)$ for sets $A_1, \ldots, A_n$ with $\mathbb{P}(A_i) = \lambda/n$. It follows that $\mathbb{P}(A) \le \lambda$ and we can extend $\mathbb{P}' := (1/\lambda) \cdot \mathbb{P}|_A$ to a probability measure on Ω which gives $x_{ij} = \lambda \mathbb{P}'(A_i \triangle A_j)$ with $(\mathbb{P}'(A_i \triangle A_j))_{1 \le i < j \le n} \in \mathrm{CUT}_n^{\square}(1/n)$. Conversely, $x \in \mathrm{CUT}_n^{\square}(1/n)$ admits the representation $x_{ij} = \mathbb{P}(A_i \triangle A_j)$ for sets $A_1, \ldots, A_n$ with $\mathbb{P}(A_i) = 1/n$ and we can extend the measure $\mathbb{P}' := \lambda \cdot \mathbb{P}|_A$ to Ω which gives $\lambda \cdot x_{ij} = \mathbb{P}'(A_i \triangle A_j)$ with $(\mathbb{P}'(A_i \triangle A_j))_{1 \le i < j \le n} \in \mathrm{CUT}_n^{\square}(\lambda/n)$.

Together with $(g_n \circ f_n)^{-1}(y) = 1 - \frac{n}{2}y$ this identifies the polytope TCF_n as

$$\mathrm{TCF}_n = 1 - \frac{1}{2c}\mathrm{CUT}_n^{\square}(c) = 1 - \frac{1}{4c}\left(1 - \mathcal{U}_n(c)\right), \qquad \text{for any } c \in (0, 1/n]. \quad (27)$$

Hence, any better understanding on one of the polytopes in (27) will automatically transfer to all the other ones.

7 Computational results

We computed the vertices and facets of TCF_n for $n \leq 6$ using the software `R` (R Core Team, 2013) and `polymake` (Gawrilow and Joswig, 2000). Their explicit representatives are documented in the tables of Appendix A. In order to obtain the vertices and facets of TCF_6, we had to use both views on TCF_6 described at the end of Section 6.4: a $\mathcal{V}$-representation of TCF_6 was obtained via the polytope Θ_6, the reduction to the vertex representation $\mathrm{Ex}(\mathrm{TCF}_6)$ took extra efforts. An $\mathcal{H}$-representation for TCF_6 was obtained via the embedding into $\mathrm{CUT}_7^\square$ (using the known facet-representation), from which we extracted a facet-representation of TCF_6 using the previously computed vertices $\mathrm{Ex}(\mathrm{TCF}_6)$. Below we give a detailed description of our methods.

The vertices and facets of TCF_n for $2 \leq n \leq 5$
For $n \leq 4$ the vertices and facets of TCF_n were computed already in Strokorb (2013) p. 62. In particular, all vertices are $\{0,1\}$-valued, hence clique partition points (cf. Proposition 22).

The vertices and facets of TCF_5 have been obtained directly using `R` and `polymake` via the two different approaches presented in Section 6.4 (leading to the same result): via the polytope Θ_5 and the embedding into the correlation polytope $\mathrm{COR}_5^\square$ (defined by its vertices). Here, for $n = 5$, the software `R` was simply used to generate the input for `polymake`. From these computations we see that TCF_5 has 214 vertices in 11 permutation orbits as listed in Table 2 (Appendix A). While 52 vertices in 7 permutation orbits are $\{0,1\}$-valued (the expected clique partition points), for the first time also $\{0,1/2\}$-valued vertices turn up (162 in 4 permutation orbits).

Representatives for the permutation orbits of the facets of TCF_n for each $2 \leq n \leq 5$ are listed in Table 3 in the Appendix A. Since all facets turned out to be hypermetric, we describe them by their defining vectors $b \in \mathbb{Z}^n$. In particular, we obtain the following result.

Proposition 41 *For $n \leq 5$ all facets of TCF_n are hypermetric.*

Let us now turn to the case $n = 6$, which needed additional arguments to reduce the computational burden.

The vertices of TCF_6
According to our computational results, the polytope TCF_6 possesses 28895 vertices in 88 permutation orbits, whose representatives are listed in Table 4 in the Appendix A. For the first time, also $\{0,1/3,2/3\}$-valued vertices occur, more precisely,

- 203 vertices in 11 orbits are $\{0,1\}$-valued,
- 4662 vertices in 16 orbits are $\{0,1/2\}$-valued,
- 2430 vertices in 11 orbits are $\{0,1/2,1\}$-valued,
- 21600 vertices in 50 orbits are $\{0,1/3,2/3\}$-valued.

It was not feasible to use the simple embedding of TCF_6 into $\mathrm{CUT}_6^{\square}$ from Section 6.4 and `polymake` to compute the vertices by common standard hardware in reasonable time. Instead, we used the projection of the Θ_6 polytope in (17) to obtain a $\mathcal{V}$-representation for TCF_6, from which - with some additional efforts - we extracted the vertex representation.

1st step: *Computing a $\mathcal{V}$-representation of* TCF_6.

With `R` we generated the input for `polymake` (63 inequalities with 58 coefficients each) to define the polytope Θ_6 in $\mathbb{R}^{57}$. Then `polymake` computed the 200 214 extremal points of Θ_6 in less then 20 minutes by standard hardware. We projected the extremal points of Θ_6 onto the 15 coordinates for TCF_6, applied the coordinatewise $2-x$-transformation, and removed duplicates. This gave us 168 894 points in $[0,1]^{15}$ with convex hull TCF_6 (a $\mathcal{V}$-representation of TCF_6). Their coordinate values were all fractions $\frac{a}{b}, 0 \leq a \leq b \leq 9$.

2nd step: *Reduction to a vertex representation of* TCF_6.

It was not feasible to extract the subset of extremal points directly by `polymake`. Using `R` we determined the 521 permutation orbits of these 168 894 convex hull points and chose 521 representatives. These representatives included the 11 well-known representatives for $\mathrm{Ex}(\mathrm{TCF}_6) \cap \{0,1\}^{15}$ (i.e., the clique partition points of the complete graph K_6, see Proposition 21), and the 4 liftings of the 4 representatives for $\mathrm{Ex}(\mathrm{TCF}_5) \cap \{0,1/2\}^{10}$ described above (see Table 2 in the Appendix A). This gave us a list of 15 representatives known to be extremal and 506 undecided ones.

The extremal ones among them were identified as follows.

a) First, we took the union of the full permutation orbits of the 15 known representatives, a set of 1175 points, and added the undecided 506 candidates. The resulting list of 1681 points was handed over to `polymake`, which computed the 1259 extremal points of their convex hull (among them the previously mentioned set of 1175 points). Any candidate from the 506-list not appearing among these 1259 extremal points is a strict convex combination of points from TCF_6, thus not extremal. This left us with the 15 representatives known to extremal plus only $84 = 1259 - 1175$ undecided representatives from the previous list of 506.

b) For each of the remaining 84 undecided representatives we computed with `polymake`, if there is a hyperplane positively separating this selected representative from the union of all orbits of the 15 representatives known to extremal and the 83 other undecided representatives (in each case roughly 30000 points). If so, the selected representative is extremal, otherwise not. For a proof of this statement see the following Lemma 42. In this way we found 73 extremal representatives among the 84 undecided ones, which led to the 15+73= 88 representatives for $\mathrm{Ex}(\mathrm{TCF}_6)$ in Table 4 (Appendix A).

In order to justify the last step, the following lemma is needed.

Lemma 42 *Let $A \subset \mathbb{R}^n$ and $B \subset \mathbb{R}^n$ be two disjoint finite sets with the property that either $B \subset \mathrm{Ex}(A \cup B)$ or $B \cap \mathrm{Ex}(A \cup B) = \emptyset$ (property $(*)$ in* *the proof). Let x be a point from B. Then $x \in \mathrm{Ex}(A \cup \{x\})$ if and only if $x \in \mathrm{Ex}(A \cup B)$.*

(Our application in mind is $A \subset \mathbb{R}^{\binom{n}{2}}$, a union of S_n-orbits, $B \subset \mathbb{R}^{\binom{n}{2}}$ another S_n-orbit. Then the above condition $(*)$ holds, since S_n acts via invertible linear maps.)

Proof Note that the following identities hold trivially for a finite set $A \subset \mathbb{R}^n$: $\mathrm{Ex}(A) \subset A$ $(*1)$ and $\mathrm{conv}(A) = \mathrm{conv}(\mathrm{Ex}(A))$ $(*2)$. Hence, the assertion is a consequence of the following.
"$\Leftarrow$": $x \notin \mathrm{Ex}(A \cup \{x\}) \overset{(*1)}{\Rightarrow} \mathrm{Ex}(A \cup \{x\}) \subset A \overset{(*2)}{\Rightarrow} x \in \mathrm{conv}(A)$, thus x is a convex combination of points from A (which are different from x, since $x \in B$, $A \cap B = \emptyset$), thus $x \notin \mathrm{Ex}(A \cup B)$.
"$\Rightarrow$": $x \notin \mathrm{Ex}(A \cup B) \overset{(*)}{\Rightarrow} B \cap \mathrm{Ex}(A \cup B) = \emptyset \overset{(*1)}{\Rightarrow} \mathrm{Ex}(A \cup B) \subset A \overset{(*2)}{\Rightarrow} \mathrm{conv}(A \cup B) \subset \mathrm{conv}(A) \Rightarrow x \in \mathrm{conv}(A)$, as above now $x \notin \mathrm{Ex}(A \cup \{x\})$ follows.

The facets of TCF_6

It turned out that TCF_6 has 18720 facets which split into 67 permutation orbits. For an annotated complete list see Table 5 in the Appendix A. The 67 representatives for TCF_6 are grouped into 11 classes, according to their "ancestral cut polytope generator" (see below). The first 6 generators led to 6 classes with 17 representatives for TCF_6, which are all hypermetric. A list of the corresponding 17 b-vectors is given in Table 7 (Appendix A). The remaining 5 generators induced 50 representatives and all of them are non-hypermetric (this is easily checked using Lemma 30 and Remark 31 for all but the 7th inequality derived from generator 9, for this one the vectors $c_{2,4}, c_{2,5}, c_{2,6}$ and $c_{3,4}, c_{3,5}, c_{3,6}$ are independent and the same reasoning as for criterion (b) of Lemma 30 works). Thus, the number of hypermetric orbits is 17 out of 67 ($\approx 25.4\%$), with 858 hypermetric facets out of 18720 (just $\approx 4.6\%$).

We obtained this list of representatives for the facets of TCF_6 in using known results about the cut polytope $\mathrm{CUT}_7^{\square}$ (Section 6.4), the previously computed vertex set $\mathrm{Ex}(\mathrm{TCF}_6)$ and the software `R`:

1st step: Choose one of the 11 homogeneous generators $g_i \leq 0$, $i \in \{1, \dots, 11\}$ for the facets of the cut polytope $\mathrm{CUT}_7^{\square}$ (see Table 6 (Appendix A) and Section 6.4). Compute the list of all facets of $\mathrm{CUT}_7^{\square}$ generated by g_i w.r.t. switchings and permutations (cf. Section 6.4). This results in an $a_i \times 22$ matrix with $a_i \leq 40320$ for all i (see also Deza and Laurent (1997) Figure 30.6.1).

2nd step: Apply the simple map from Proposition 38 to all rows of the matrix from step 1. This yields a set of valid inequalities for TCF_6 (an $a_i \times 16$ matrix), which is permutation invariant by construction. Choose representatives of the permutation orbits (the largest count was 93 representatives).

3rd step: Use the 28 895 precomputed vertices in $\mathrm{Ex}(\mathrm{TCF}_6)$ to decide for each representative from step 2, if it defines a facet of TCF_6. For that, first determine which vertices from $\mathrm{Ex}(\mathrm{TCF}_6)$ solve the inequality as an equality.

Then check if the rank of the matrix of solutions with an added 1-column in front is at least 15. We used the vertex set $6 \cdot \mathrm{Ex}(\mathrm{TCF}_6)$ to make all computations integer valued, so the rank-checking procedure should be computationally reliable in this case. This gives a list of representatives for certain permutation orbits of TCF_6-facets "stemming from the cut polytope generator g_i".

4th step: If done for all 11 generators, the union of the 11 lists obtained in step 3 gives a complete list of representatives of the facets of TCF_6. This holds true, since the set of all valid inequalities obtained in the second step for all $1 \le i \le 11$ defines TCF_6 by Proposition 38, thus we know that the facets of TCF_6 are a subset. Finally, we checked that representatives from different lists have different permutation orbits. Thus, the 11 lists partition a minimal set of facet representatives for TCF_6 according to the unique "ancestral cut polytope generator".

Remark 43 It is feasible to generate all 116 764 facets of $\mathrm{CUT}_7^{\square}$ in step 1, and go through steps 2 and 3 (testing 391 representatives from step 2), to just obtain the 67 facet representatives, but then relating them to the different cut polytope generators needs extra bookkeeping.

Remark 44 One can exploit the interaction of the permutation group actions on $\mathrm{CUT}_{n+1}^{\square}$ and TCF_n to avoid the large row counts in step 1 and 2. Starting from a list $h_j \le c_j, j \in J$ of facet representatives for the cut polytope $\mathrm{CUT}_{n+1}^{\square}$ w.r.t. *permutations* ($|J| = 108$ in the case $n = 6$) there is a way to immediately compute a list of at most $(n+1) \cdot |J|$ valid inequalities for TCF_n that contains a complete collection of facet representatives for TCF_n as a sublist (details omitted). This might get interesting if one wants to investigate TCF_n for $n \ge 7$ using knowledge about $\mathrm{CUT}_{n+1}^{\square}$.

8 Some open questions on the geometry of TCF_n

Finally, we pursue some questions which arose while studying the convex polytope TCF_n that remained open to us. To this end, let $\mathrm{PSD}_n \subset \mathbb{R}^{E_n}$ be the space of symmetric and positive semi-definite $n \times n$ matrices in the sense of (1). As mentioned in the introduction, it is well-known that all elements of TCF_n are positive semi-definite, that is

$$\mathrm{TCF}_n \subset \mathrm{PSD}_n.$$

It is natural to ask whether certain subsets of inequalities from facets of TCF_n imply already positive semi-definiteness. A simple candidate for such a question could be all facets at the exposed vertices $v_0 = (0, 0, \ldots, 0)$ and $v_1 = (1, 1, \ldots, 1)$ of TCF_n. Let us denote the polytope which is defined by these facets by $\mathrm{TCF}_n(v_0, v_1)$. The following problem can be seen in a similar vein to Matheron's conjecture (Matheron, 1993).

(F) For which values of n does $\mathrm{TCF}_n(v_0, v_1) \subset \mathrm{PSD}_n$ *hold?*

Therefore, let us take a closer look at the facets of TCF_n at the exposed vertices v_0 and v_1. The facets at $v_0 = (0, 0, \dots, 0)$ are just the positivity inequalities $\chi_{ij} \geq 0$, which are hypermetric with $b = \mathbb{1}_{\{i,j\}}$. To investigate the facets of TCF_n at $v_1 = (1, 1, \dots, 1)$, the following simple lemma is helpful.

Lemma 45 *A hypermetric inequality given by $b \in \mathbb{Z}^n$ is satisfied as an equality by v_1 if and only if $\sum_{i=1}^n b_i \in \{0, 1\}$.*

Proof $\sum_{1 \leq i,j \leq n} b_i b_j \cdot 1 = \sum_{i=1}^n b_i$ if and only if $(\sum_{i=1}^n b_i)^2 = \sum_{i=1}^n b_i$.

A hypermetric inequality is *pure hypermetric* if its corresponding b-vector satisfies $b \in \{-1, 0, 1\}^n$. Using this lemma and inspecting Tables 3, 5 and 7 we derive the following proposition.

Proposition 46 (Facets of TCF_n at v_1)
a) For $n = 2$ the (exceptional) facet at v_1 is pure hypermetric with $\sum_{i=1}^n b_i = 0$.
b) For $3 \leq n \leq 5$ the facets at v_1 are pure hypermetric with $\sum_{i=1}^n b_i = 1$.
c) For $n = 6$ the facets at v_1 are hypermetric with $\sum_{i=1}^n b_i = 1$. Some are not pure.

Thus, the pure hypermetricity of the hypermetric facets at v_1 is another low-dimensional phenomenon: For $n = 6$ there exist non-pure hypermetric facets at v_1. By the lifting property for $n \geq 3$ (Proposition 25), the same holds true for $n \geq 7$. However, we may ask (cf. also Lemma 45):

(G) Are there non-hypermetric facets at v_1 for $n \geq 7$?
Are there hypermetric facets at v_1 with $\sum_{i=1}^n b_i = 0$ for $n \geq 7$?

Let $\mathrm{TCF}_n^{\mathrm{hyp}}(v_0, v_1)$, resp. $\mathrm{TCF}_n^{\mathrm{pure}}(v_0, v_1)$, be given by the hypermetric, resp. pure hypermetric, facets at v_0 and v_1.

Remark 47 By definition $\mathrm{TCF}_n(v_0, v_1) \subset \mathrm{TCF}_n^{\mathrm{hyp}}(v_0, v_1) \subset \mathrm{TCF}_n^{\mathrm{pure}}(v_0, v_1)$. All these sets are polytopes, since positivity (= the facets of TCF_n at v_0) and triangle inequalities (which are certainly among the pure hypermetric facets of TCF_n at v_1 for $n \geq 3$) suffice already to imply $\mathrm{TCF}_n^{\mathrm{pure}}(v_0, v_1) \subset [0, 1]^{E_n}$ (which also holds true for $n = 2$), i.e., all of these sets are bounded and thus indeed polytopes. These polytopes are called *spindles*, since each facet contains one of the two vertices v_0, v_1.

The following proposition collects some partial answers to Question (F).

Proposition 48 (Partial answers to Question (F))
a) For $2 \leq n \leq 5$ we have $\mathrm{TCF}_n(v_0, v_1) = \mathrm{TCF}_n^{\mathrm{hyp}}(v_0, v_1) = \mathrm{TCF}_n^{\mathrm{pure}}(v_0, v_1) \subset \mathrm{PSD}_n$.
b) For $n = 6$ we have $\mathrm{TCF}_6(v_0, v_1) = \mathrm{TCF}_6^{\mathrm{hyp}}(v_0, v_1) \neq \mathrm{TCF}_6^{\mathrm{pure}}(v_0, v_1)$.
c) For $n \geq 6$ we have $\mathrm{TCF}_n^{\mathrm{hyp}}(v_0, v_1) \not\subset \mathrm{PSD}_n$. In particular $\mathrm{TCF}_6(v_0, v_1) \not\subset \mathrm{PSD}_6$.

Proof a) The equalities follow from Table 3. The inclusion $\mathrm{TCF}_n^{\mathrm{pure}}(v_0, v_1) \subset \mathrm{PSD}_n$ has been solved by hand in Strokorb (2013) Proposition 3.6.5. for the cases $n \leq 4$. The idea for $n = 4$ was to compute the extremal points of the polytope defined by positivity and triangle inequalities and to check p.s.d. for them. This suffices since PSD_n is convex. For $n = 5$ we used `polymake` to compute the extremal points of the polytope defined by positivity, triangle and pentagonal inequalities (see Table 3), and `R` to check p.s.d.

b) This follows from Proposition 46.

c) For $n \geq 6$ consider the point $x \in \mathbb{R}^{E_n}$ with $x_{in} = 0.5$, $1 \leq i \leq n-1$; $x_{ij} = 0$ otherwise. Let X denote the associated matrix. For $b = (b_1, \ldots, b_n) \in \mathbb{Z}^n$ and $s := \sum_{i=1}^n b_i$ we have

$$bXb^t = \sum_{i=1}^{n} b_i^2 + b_n \sum_{i=1}^{n-1} b_i = \sum_{i=1}^{n-1} b_i^2 + b_n \cdot s.$$

This shows $bXb^t \geq s$ for $s \in \{0, 1\}$, for $s = 1$ use $\sum_{i=1}^{n-1} b_i^2 + b_n \geq \sum_{i=1}^{n-1} b_i + b_n = 1$. Thus, all hypermetric inequalities with $\sum_{i=1}^{n} b_i \in \{0, 1\}$ are satisfied, in particular those at v_1 (c.f. Lemma 45), and x is non-negative. On the other hand, x is not positive semi-definite: For $a = (1, \ldots, 1, -2)$ the above formula shows $aXa^t = (n-1) - 2(n-3) = 5 - n \leq -1$.

Thus, we expect "if and only if $n \leq 5$" to be the answer to Question F.

Our final question is motivated by the following observation. Let HYP_n denoted the set of points $x = (x_{ij})_{1 \leq i < j \leq n} \in \mathbb{R}^{E_n}$ that satisfy all hypermetric inequalities (cf. Section 5).

Lemma 49 *For all $n \geq 2$ the inclusions $\mathrm{TCF}_n \subset \mathrm{HYP}_n \subset \mathrm{PSD}_n$ hold.*

Proof The first inclusion is a reformulation of Lemma 20. Now let $x \in \mathrm{HYP}_n$. By assumption we have $\sum_{1 \leq i,j \leq n} b_i b_j x_{ij} \geq \sum_{i=1}^n b_i$ for all $b = (b_1, \ldots, b_n) \in \mathbb{Z}^n$. This holds for b and $-b$. Thus, $\sum_{1 \leq i,j \leq n} b_i b_j x_{i,j} \geq 0$ for all $b \in \mathbb{Z}^n$. Division by integers extends this to $\mathbb{Q}^n$, and continuity to $\mathbb{R}^n$.

Remark 50 By Proposition 41 the sets TCF_n and HYP_n even coincide for $n \leq 5$. This is no longer true for $n \geq 6$. A point $x \in \mathrm{HYP}_6 \setminus \mathrm{TCF}_6$ is given by $x_{i,6} = 1/2, 1 \leq i \leq 5$, $x_{1,2} = x_{2,3} = x_{3,4} = x_{4,5} = x_{1,5} = 1/2$, and $x_{i,j} = 0$ otherwise. Indeed, since $(\sum_{i=1}^5 x_{i,6}) - x_{1,3} - x_{3,5} - x_{2,5} - x_{2,4} - x_{1,4} = 2.5 > 2$, the point x does not satisfy a permutation of the TCF_6-facet from Proposition 32. We omit the computations showing $x \in \mathrm{HYP}_6$. By lifting, this extends to examples $x^0 \in \mathrm{HYP}_n \setminus \mathrm{TCF}_n$ for all $n \geq 6$.

(H) *Do the inequalities of all hypermetric facets of TCF_n define a polytope, say $\mathrm{TCF}_n^{\mathrm{hyp}}$, already contained in PSD_n?*

This holds true for $n \leq 5$ by Proposition 48, and remains open for $n \geq 6$. Note that $\mathrm{TCF}_n^{\mathrm{hyp}}$ is a polytope by $\mathrm{TCF}_n^{hyp} \subset \mathrm{TCF}_n^{hyp}(v_0, v_1)$ and Remark 47.

Discussion

In this article, we deal with the realization problem for the tail correlation function (TCF), which is an omnipresent bivariate tail dependence measure in the extremes literature. We make this specific by formulating Questions (A)-(E) in the introduction. Here, we discuss our contribution to these questions. In doing so we address Questions (A)-(E) partially in reversed order according to their growing complexity.

Questions (E) and (D) can be answered fully and affirmatively by Corollary 14 and Theorem 10, respectively. That is, convex combinations, products and pointwise limits are admissible operations on the set of TCFs and Theorem 10 shows that the class of TM processes, a subclass of max-stable processes, is rich enough to realize any given TCF. Concerning the regularity of the corresponding TM process, we identify continuity of its TCF as a necessary and sufficient condition for its stochastic continuity (Corollary 11), which contributes to Question (C). Theorem 10 also opens up links to binary ($\{0,1\}$-valued) processes and thereby provides a substantial reduction of Questions (A) and (B). Corollary 15 reduces them even further to the study of TCFs on finite base spaces. Together with Corollary 18, we reveal that membership in the set of TCFs (even on infinite spaces) can be completely characterized by a system of affine inequalities, which – if known – would provide a complete answer to Question (A).

To identify and classify these affine inequalities, a better understanding of the geometry of the polytope TCF_n of $n \times n$ tail correlation functions (matrices) for arbitrary n is needed. Its facet inducing inequalities constitute such a list (actually, an $\mathcal{H}$-representation would suffice already). Lemma 20 contributes to Question (A) in that it provides a rich class of necessary conditions (all hypermetric inequalities) for membership in TCF_n, whereas Proposition 21 identifies any clique partition point to be an admissible TCF. In Section 6.4, we discuss that the polytope TCF_n can be viewed either as an affine *projection* of the polytope Θ_n (whose facets are well-understood) or as an affine *intersection* with the *correlation polytope* (whose vertices are well-understood). Both views immediately suggest algorithms that can be easily implemented in order to obtain the vertices and facets of TCF_n that in theory would work "for arbitrary n". This would solve Question (A) computationally. Due to the complexity of the problem, software computations lead to a full description of facets and vertices of TCF_n only up to $n = 6$ (Section 7).

Indeed, several of our results reveal the rapidly growing complexity of Question (A) as n grows. Starting from $n = 3$, no facet inducing inequality of TCF_n will ever become obsolete (Proposition 25). For instance, the triangle inequality (2) cannot be deduced from any other set of valid inequalities for TCF_n. By contrast, *all* facet inducing inequalities that define the polytope of ECFs Θ_n become obsolete for $\Theta_{n'}$ for higher $n' > n$, and still Θ_n has 2^n facets in dimension n. Starting from $n \geq 6$ there exist (actually plenty of) non-hypermetric facets of TCF_n (Proposition 32). Moreover, we derived the facets of TCF_6 from the facets of the cut polytope $\mathrm{CUT}_7^{\square}$ which had 11 generators for 116 764 facets. The next step would take into account the polytope $\mathrm{CUT}_8^{\square}$, which has already more than 217 million facets which can be subdivided into 147 orbits under permutations and switchings (Deza and Laurent, 1997, p. 505). It is even possible to choose n sufficiently large, such that a given finite set of rational numbers from the interval $[0,1]$ turns up as coordinate values of a single vertex of TCF_n (Proposition 27). Altogether, these results confound the aim of a full answer to Question (A).

Finally, if Question (A) is already so difficult to answer, what more can be eventually said about Question (B)? That is, given a TCF χ, say on a finite space, how to construct a specific stochastic model that realizes χ? Again, from our dual views on TCF_n as affine "projection of" or "intersection with" other polytopes, it is easy to formulate naive ad-hoc algorithms providing an entire convex polytope of solutions to such a problem, cf. Strokorb (2013), p. 65. Perhaps more interestingly, in case of $T = \mathbb{R}^d$, Strokorb et al (2015) characterize subclasses of radially symmetric and monotonously decreasing TCFs with some sharp bounds on membership in the class of TCFs on $\mathbb{R}^d$ (cf. Table 2 therein) and recover realizing max-stable models. Surprisingly often, it is possible to obtain explicitly several such realizing models sharing an identical TCF, but with rather different spectral profiles. In this sense, the reader should not overrate the finding of a specific model meeting a given TCF even though the TM models helped us here to approach the realization problem.

To conclude with, independently of our research (Fiebig et al, 2014) and motivated from an insurance context, Embrechts et al (2015) dealt with almost the same questions (in particular Questions A and B) for random vectors with an emphasis on the construction of realizing copulas as we learned on the EVA 2015 in AnnArbor. Our approach offers (at least theoretically) an algorithm that can solve Questions A and B for random vectors completely (even though the feasibilty of such an algorithm breaks down very quickly as the dimension grows and we have doubts on its practical use in higher dimensions). This answers one of the questions raised in the discussion of Embrechts et al (2015).

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A Tables

Vertex and facet counts										
	TCF_n					Θ_n				
n	2	3	4	5	6	2	3	4	5	6
# vertices	2	5	15	214	28 895	2	6	42	1292	200 214
# facets	2	6	22	110	18 720	2	7	15	31	63
# permutation orbits of vertices	2	3	5	11	88	2	4	10	45	583
# permutation orbits of facets	2	2	3	7	67	2	3	4	5	6
	$\mathrm{COR}^{\square}_n$					$\mathrm{CUT}^{\square}_{n+1}$				
n	2	3	4	5	6	2	3	4	5	6
# vertices	4	8	16	32	64	4	8	16	32	64
# facets	4	16	56	368	116 764	4	16	56	368	116 764
# permutation orbits of vertices	3	4	5	6	7	2	3	3	4	4
# permutation orbits of facets	3	5	10	29	428	2	2	5	11	108
# perm./switch. orbits of vertices						1	1	1	1	1
# permu./switch. orbits of facets						1	1	2	3	11

Table 1 Vertex and facet counts for the polytope of tail correlation functions $\mathrm{TCF}_n \subset \mathbb{R}^{\binom{n}{2}}$, the polytope of extremal coefficient functions $\Theta_n \subset \mathbb{R}^{2^n-n-1}$, the correlation polytope $\mathrm{COR}^{\square}_n \subset \mathbb{R}^{n+\binom{n}{2}}$ and the cut polytope $\mathrm{CUT}^{\square}_n \subset \mathbb{R}^{\binom{n+1}{2}}$. For Θ_n the number of facets (2^n-1) and orbits of facets (n) follow from Lemma 2. Since $\mathrm{COR}^{\square}_n$ and $\mathrm{CUT}^{\square}_{n+1}$ are linearly equivalent, they have the same number of vertices (2^n by definition) and facets (see Deza and Laurent (1997) p. 503-505 for the respective numbers as well as for the permutation/switching orbits of $\mathrm{CUT}^{\square}_{n+1}$). All other numbers rely on computations using the software `R` and `polymake`. The counts for TCF_n and Θ_n in case $n \leq 4$ have been obtained previously "by hand" in Strokorb (2013) p. 62-63.

Vertices of TCF_5											
7 $\{0,1\}$-valued representatives											
0	0	0	0	0	0	0	0	0	0	1	five 1-cliques
0	0	0	0	0	0	0	0	0	1	10	one 2-clique
0	0	0	0	0	0	0	1	1	1	10	one 3-clique
0	0	0	0	0	0	1	1	0	0	15	two 2-cliques
0	0	0	0	1	1	1	1	1	1	5	one 4-clique
0	0	0	1	1	1	0	1	0	0	10	one 2-clique and one 3-clique
1	1	1	1	1	1	1	1	1	1	1	one 5-clique
4 $\{0,1/2\}$-valued representatives											
0	0	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	30	
0	0	1/2	1/2	1/2	0	1/2	1/2	1/2	1/2	60	
0	0	0	1/2	1/2	1/2	0	1/2	1/2	1/2	60	
1/2	0	0	1/2	1/2	0	0	1/2	0	1/2	12	

Table 2 The 11 representatives $(\chi_{1,2},\dots,\chi_{4,5})$ for the 214 elements of $\mathrm{Ex}(\mathrm{TCF}_5)$. Columns (1)-(10) list the coordinates $\chi_{1,2},\dots,\chi_{4,5}$, Column (11) gives the orbit length under permutations and the last column is a comment on the generating clique partition (see Section 5).

Facets of TCF_n **for** $2 \le n \le 5$					
$n=2$	$b=(1,1)$	*positivity inequality* $x_{1,2} \ge 0$	$(\times\ 1)$	2 facets	v_0
	$b=(1,-1)$	$x_{1,2} \le 1$ (this facet disappears for $n \ge 3$)	$(\times\ 1)$		v_1
$n=3$	$b=(1,1,0)$	lifting of *positivity ineq.*	$(\times\ 3)$	6 facets	v_0
	$b=(1,1,-1)$	*triangle inequality*	$(\times\ 3)$		v_1
$n=4$	$b=(1,1,0,0)$	lifting of *positivity ineq.*	$(\times\ 6)$	22 facets	v_0
	$b=(1,1,-1,0)$	lifting of *triangle ineq.*	$(\times 12)$		v_1
	$b=(1,1,1,-1)$	*tetrahedron inequality*	$(\times\ 4)$		
$n=5$	$b=(1,1,0,0,0)$	lifting of *positivity ineq.*	$(\times 10)$	110 facets	v_0
	$b=(1,1,-1,0,0)$	lifting of *triangle ineq.*	$(\times 30)$		v_1
	$b=(1,1,1,-1,0)$	lifting of *tetrahedron ineq.*	$(\times 20)$		
	$b=(1,1,1,1,-1)$	*pyramid inequality*	$(\times\ 5)$		
	$b=(1,1,1,1,-2)$	*2-weighted variant of pyramid ineq.*	$(\times\ 5)$		
	$b=(1,1,1,-1,-1)$	*pentagonal inequality*	$(\times 10)$		v_1
	$b=(2,1,1,-1,-1)$	*2-weighted variant of pentagonal ineq.*	$(\times 30)$		

Table 3 Permutation orbit representatives for the facets of TCF_n for $2 \le n \le 5$. Since all facets are hypermetric, they can be described by their corresponding b-vector (see Section 5). The number in brackets is the orbit length. The last column indicates whether the respective facet contains one of the exposed vertices $v_0 = (0,0,\dots,0)$ or $v_1 = (1,1,\dots,1)$.

Vertices of TCF_6															
7 $\{0,1\}$-vd. repr'tives (liftings from TCF_5)															
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	15
0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	20
0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	45
0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	15
0	0	0	0	0	0	0	1	1	1	0	1	0	0	0	60
0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	6
4 new $\{0,1\}$-vd. repr'tives (not liftings)															
0	0	0	0	1	0	0	1	0	1	0	0	0	0	0	15
0	0	0	0	1	1	1	1	0	1	1	0	1	0	0	15
0	0	0	1	1	1	1	0	0	1	0	0	0	0	1	10
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
4 $\{0,½\}$-vd. repr'tives (liftings from TCF_5)															
0	0	0	0	0	0	0	0	1/2	1/2	1/2	0	1/2	1/2	1/2	360
0	0	0	0	0	0	0	1/2	1/2	1/2	0	1/2	1/2	0	0	72
0	0	0	0	0	0	0	1/2	1/2	1/2	0	1/2	1/2	1/2	1/2	360
0	0	0	0	0	0	0	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	180
12 new $\{0,½\}$-vd. repr'tives (not liftings)															
0	0	0	0	1/2	0	1/2	1/2	0	1/2	1/2	1/2	1/2	0	0	360
0	0	0	0	1/2	0	1/2	1/2	0	1/2	1/2	1/2	1/2	0	1/2	720
0	0	0	0	1/2	0	1/2	1/2	0	1/2	1/2	1/2	1/2	1/2	1/2	360
0	0	0	1/2	1/2	0	1/2	0	1/2	1/2	1/2	0	0	0	1/2	360
0	0	0	1/2	1/2	0	1/2	0	1/2	1/2	1/2	0	1/2	1/2	1/2	120
0	0	0	1/2	1/2	1/2	1/2	0	0	1/2	0	0	1/2	1/2	1/2	180
0	0	0	1/2	1/2	1/2	1/2	0	0	1/2	1/2	1/2	1/2	1/2	1/2	90
0	0	0	1/2	1/2	1/2	1/2	0	1/2	1/2	0	1/2	1/2	1/2	1/2	360
0	0	0	1/2	1/2	1/2	1/2	0	1/2	1/2	1/2	0	1/2	1/2	0	360
0	0	0	1/2	1/2	1/2	1/2	0	1/2	1/2	1/2	0	1/2	1/2	1/2	360
0	0	0	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	60
0	0	1/2	1/2	1/2	1/2	0	1/2	1/2	1/2	0	1/2	1/2	1/2	1/2	360
11 new $\{0,½,1\}$-vd. repr'tives (not liftings)															
0	0	0	0	1/2	1	1/2	1/2	0	1/2	1/2	0	1/2	1/2	1/2	180
0	0	0	0	1/2	1	1/2	1/2	1/2	1/2	1/2	1/2	1/2	0	1/2	360
0	0	0	1	1/2	1/2	1/2	0	0	1/2	0	1/2	0	1/2	1/2	180
0	0	0	1/2	1/2	1	1/2	0	1/2	1/2	0	1/2	1/2	0	0	180
0	0	0	1/2	1/2	1	1/2	0	1/2	1/2	0	1/2	1/2	1/2	1/2	360
0	0	0	1/2	1/2	1	1/2	1/2	1/2	1/2	1/2	1/2	0	0	1/2	180
0	0	0	1/2	1/2	1	1/2	1/2	1/2	1/2	1/2	1/2	0	1/2	1/2	360
0	0	0	1/2	1/2	1	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	180
0	0	1	1/2	1/2	1/2	0	1/2	1/2	0	1/2	1/2	1/2	1/2	1/2	90
0	0	1/2	1/2	1/2	1/2	0	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1	180
0	0	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1	1/2	1/2	180
50 new $\{0,⅓,⅔\}$-vd. repr'tives (not liftings)															
0	0	0	0	1/3	1/3	1/3	1/3	0	2/3	2/3	2/3	2/3	2/3	2/3	120
0	0	0	0	1/3	1/3	1/3	1/3	2/3	2/3	2/3	0	2/3	1/3	1/3	360
0	0	0	0	1/3	2/3	2/3	2/3	1/3	2/3	2/3	1/3	2/3	2/3	2/3	180
0	0	0	0	2/3	1/3	1/3	1/3	1/3	2/3	2/3	0	2/3	0	1/3	360
0	0	0	0	2/3	2/3	2/3	2/3	0	2/3	2/3	1/3	2/3	1/3	1/3	120
0	0	0	1/3	1/3	1/3	1/3	0	2/3	2/3	2/3	1/3	2/3	1/3	1/3	360
0	0	0	1/3	1/3	1/3	1/3	2/3	2/3	2/3	0	1/3	1/3	1/3	2/3	720
0	0	0	1/3	1/3	2/3	2/3	0	2/3	2/3	1/3	2/3	1/3	2/3	1/3	360
0	0	0	1/3	1/3	2/3	2/3	1/3	1/3	2/3	1/3	2/3	2/3	2/3	2/3	720
0	0	0	1/3	1/3	2/3	2/3	1/3	2/3	2/3	1/3	2/3	2/3	1/3	1/3	360
0	0	0	1/3	2/3	1/3	1/3	0	1/3	2/3	2/3	0	2/3	0	0	360
0	0	0	1/3	2/3	1/3	1/3	2/3	1/3	2/3	0	0	1/3	0	1/3	360
0	0	0	1/3	2/3	1/3	1/3	2/3	1/3	2/3	1/3	0	1/3	1/3	1/3	720
0	0	0	1/3	2/3	2/3	2/3	0	0	2/3	1/3	0	1/3	1/3	1/3	720
0	0	0	1/3	2/3	2/3	2/3	1/3	0	2/3	1/3	1/3	2/3	1/3	1/3	720
0	0	0	1/3	2/3	2/3	2/3	1/3	1/3	2/3	1/3	1/3	2/3	0	0	360
0	0	0	1/3	2/3	2/3	2/3	1/3	1/3	2/3	2/3	1/3	2/3	1/3	1/3	360
0	0	0	2/3	2/3	2/3	2/3	0	1/3	2/3	1/3	1/3	1/3	1/3	2/3	360
0	0	1/3	1/3	1/3	1/3	0	1/3	1/3	2/3	2/3	2/3	2/3	2/3	2/3	180
0	0	1/3	1/3	1/3	1/3	0	2/3	2/3	2/3	1/3	1/3	1/3	1/3	2/3	360
0	0	1/3	1/3	1/3	2/3	0	1/3	2/3	1/3	1/3	2/3	2/3	1/3	1/3	720
0	0	1/3	1/3	1/3	2/3	1/3	1/3	1/3	1/3	2/3	2/3	2/3	2/3	2/3	360
0	0	1/3	1/3	1/3	2/3	1/3	1/3	2/3	1/3	1/3	2/3	2/3	0	0	180
0	0	1/3	1/3	1/3	2/3	1/3	1/3	2/3	1/3	1/3	2/3	2/3	0	1/3	360
0	0	1/3	1/3	1/3	2/3	1/3	1/3	2/3	1/3	2/3	1/3	2/3	2/3	1/3	360
0	0	1/3	1/3	1/3	2/3	1/3	1/3	2/3	1/3	2/3	2/3	2/3	1/3	2/3	720
0	0	1/3	1/3	1/3	2/3	1/3	1/3	2/3	2/3	2/3	2/3	2/3	2/3	2/3	360
0	0	1/3	1/3	1/3	2/3	1/3	2/3	2/3	1/3	2/3	2/3	0	1/3	2/3	360
0	0	1/3	1/3	1/3	2/3	1/3	2/3	2/3	2/3	1/3	2/3	1/3	2/3	2/3	360
0	0	1/3	1/3	1/3	2/3	2/3	2/3	2/3	2/3	2/3	2/3	2/3	2/3	2/3	60
0	0	1/3	1/3	2/3	1/3	0	2/3	1/3	2/3	0	1/3	0	1/3	1/3	360
0	0	1/3	1/3	2/3	1/3	1/3	1/3	1/3	2/3	2/3	1/3	2/3	1/3	1/3	360
0	0	1/3	1/3	2/3	2/3	1/3	1/3	0	1/3	1/3	1/3	2/3	1/3	2/3	720
0	0	1/3	1/3	2/3	2/3	1/3	1/3	0	1/3	1/3	1/3	2/3	2/3	2/3	360
0	0	1/3	1/3	2/3	2/3	1/3	1/3	1/3	1/3	2/3	0	2/3	1/3	0	720
0	0	1/3	1/3	2/3	2/3	1/3	1/3	1/3	1/3	2/3	1/3	2/3	0	1/3	720
0	0	1/3	1/3	2/3	2/3	1/3	2/3	0	1/3	2/3	1/3	0	1/3	1/3	720
0	0	1/3	1/3	2/3	2/3	1/3	2/3	0	1/3	2/3	1/3	1/3	2/3	1/3	720
0	0	1/3	1/3	2/3	2/3	1/3	2/3	1/3	1/3	2/3	1/3	1/3	0	1/3	360
0	0	1/3	1/3	2/3	2/3	1/3	2/3	1/3	2/3	2/3	1/3	2/3	1/3	1/3	720
0	0	1/3	1/3	2/3	2/3	2/3	2/3	0	2/3	2/3	1/3	2/3	1/3	1/3	360
0	0	1/3	2/3	2/3	2/3	1/3	1/3	1/3	2/3	0	1/3	0	1/3	2/3	360
0	0	1/3	2/3	2/3	2/3	2/3	1/3	1/3	2/3	1/3	1/3	1/3	1/3	2/3	180
0	0	2/3	2/3	2/3	1/3	1/3	1/3	1/3	1/3	1/3	1/3	2/3	2/3	2/3	60
0	1/3	1/3	1/3	1/3	1/3	1/3	1/3	2/3	2/3	2/3	1/3	2/3	2/3	2/3	360
0	1/3	1/3	1/3	1/3	1/3	1/3	2/3	2/3	2/3	1/3	2/3	2/3	2/3	2/3	720
0	1/3	1/3	1/3	1/3	1/3	2/3	2/3	2/3	1/3	2/3	2/3	2/3	2/3	2/3	360
0	1/3	1/3	1/3	2/3	1/3	1/3	2/3	1/3	2/3	0	2/3	1/3	2/3	1/3	720
0	1/3	1/3	1/3	2/3	1/3	2/3	2/3	1/3	0	1/3	2/3	2/3	1/3	1/3	360
0	1/3	1/3	1/3	2/3	1/3	2/3	2/3	1/3	2/3	2/3	1/3	2/3	1/3	1/3	360

Table 4 The 88 {...}-valued representatives (vd. repr'tives) $(\chi_{1,2},\ldots,\chi_{5,6})$ for the 28895 elements of $\mathrm{Ex}(TCF_6)$ (see Section 7). Columns (1)-(15) list the coordinates $\chi_{1,2},\ldots,\chi_{5,6}$. The last column gives the orbit length under permutations.

Facets of TCF_6																	
Generator 1																	
Positivity																	
-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7657	15
Triangle inequality																	
-1	1	0	0	0	1	0	0	0	0	0	0	0	0	0	1	3521	60
Generator 2																	
Tetrahedron inequality																	
-1	-1	1	0	0	-1	1	0	0	1	0	0	0	0	0	1	1554	60
Pentagonal inequality																	
-1	-1	1	1	0	-1	1	1	0	1	1	0	-1	0	0	2	1043	60
Generator 3																	
Pyramid inequality																	
-1	-1	-1	1	0	-1	-1	1	0	-1	1	0	1	0	0	1	110	30
2-weighted pentagonal inequality																	
-2	-2	2	2	0	-1	1	1	0	1	1	0	-1	0	0	3	135	180
2-weighted pyramid inequality																	
-1	-1	-1	2	0	-1	-1	2	0	-1	2	0	2	0	0	3	102	30
“new inequalities” from here on																	
-2	-2	2	2	2	-1	1	1	1	1	1	1	-1	-1	-1	4	129	60
-1	-1	-1	1	2	-1	-1	1	2	-1	1	2	1	2	-2	4	129	30
Generator 4																	
-1	-1	-1	1	1	-1	-1	1	1	-1	1	1	1	1	-1	2	554	15
Generator 5																	
-2	-2	-2	2	2	-1	-1	1	1	-1	1	1	1	1	-1	3	20	60
-1	-1	-1	-1	2	-1	-1	-1	2	-1	-1	2	-1	2	2	3	20	6
-4	-2	2	2	2	-2	2	2	2	1	1	1	-1	-1	-1	5	61	60
-2	-2	-2	2	4	-1	-1	1	2	-1	1	2	1	2	-2	5	53	120
Generator 6																	
-1	-1	-1	-1	1	-1	-1	-1	1	-1	-1	1	-1	1	1	1	15	6
-3	-3	3	3	3	-1	1	1	1	1	1	1	-1	-1	-1	6	15	60
-1	-1	-1	-1	3	-1	-1	-1	3	-1	-1	3	-1	3	3	6	15	6
Generator 7: Clique-Web-Generator; all following inequalities are not hypermetric																	
-1	-1	-1	1	1	-1	-1	1	1	0	0	1	1	0	-1	2	95	180
-1	-1	0	0	1	0	-1	0	1	0	-1	1	-1	1	1	2	95	72
-1	-1	-1	1	1	-1	-1	1	1	0	0	1	1	1	0	3	15	360
-1	-1	-1	1	1	-1	0	0	1	0	1	0	1	1	0	3	15	360
-1	-1	-1	1	1	-1	0	0	1	0	1	1	1	1	-1	3	15	720
-1	-1	0	0	1	-1	1	1	1	1	1	1	-1	-1	0	3	15	360
-1	-1	0	0	1	0	-1	0	1	0	1	1	1	1	-1	3	15	360
-1	-1	0	1	1	-1	1	0	1	1	1	1	0	-1	-1	3	15	360
Generator 8: Clique-Web-Generator																	
-2	-2	-2	1	2	-1	-1	1	1	-1	1	1	1	1	0	3	18	120
-2	-2	-1	2	2	-1	-1	1	1	-1	1	1	0	1	-1	3	18	360
-1	-1	-1	-1	2	-1	-1	-1	2	-1	-1	2	0	1	2	3	18	120
-3	-2	-1	2	2	-1	-2	2	2	0	1	1	1	1	-1	4	83	180
-2	-2	-2	1	3	-1	-1	1	2	-1	1	2	1	2	-2	4	86	120
-3	-2	1	2	2	-2	2	1	2	1	1	1	0	-1	-1	5	15	360
-3	-2	1	2	2	-2	2	2	2	1	1	1	-1	-1	-1	5	15	360
-3	-2	1	2	2	-1	2	2	2	0	1	1	-1	-1	-1	5	15	360
-2	-2	-2	2	3	-1	-1	1	2	-1	1	2	1	2	-1	5	15	120
-2	-2	-1	2	3	-1	-1	1	2	-1	1	2	0	2	-1	5	15	360
-2	-2	-1	2	3	-1	-1	1	2	-1	1	2	1	2	-2	5	15	360
-2	-2	-1	2	3	-1	-1	1	2	0	1	1	1	2	-2	5	15	720
-2	-2	1	2	3	-1	1	1	2	1	1	2	-1	-2	-2	5	15	360
Generator 9: Clique-Web-Generator																	
-2	-2	-2	-2	3	-1	-1	-1	2	-1	-1	2	-1	2	2	3	15	30
-3	-3	-3	3	5	-1	-1	1	2	-1	1	2	1	2	-2	6	15	120
-2	-2	-2	-2	5	-1	-1	-1	3	-1	-1	3	-1	3	3	6	15	30
-5	-5	3	3	3	-3	2	2	2	2	2	2	-1	-1	-1	7	73	60
-5	-3	3	3	5	-2	2	2	3	1	1	2	-1	-2	-2	8	15	360
-3	-3	-3	5	5	-1	-1	2	2	-1	2	2	2	2	-3	8	15	60
-3	-2	-2	2	5	-2	-2	2	5	-1	1	3	1	3	-3	8	15	180
Generator 10: Parachute-Generator																	
-1	-1	0	0	1	0	-1	0	1	1	-1	0	1	1	-1	2	93	360
-1	-1	0	0	1	-1	0	1	0	1	0	1	1	-1	1	3	15	720
-1	-1	0	0	1	-1	0	1	1	1	1	0	-1	1	0	3	15	720
-1	-1	0	0	1	0	-1	0	1	1	-1	1	1	0	1	3	15	720
-1	-1	0	0	1	0	-1	1	0	1	-1	1	1	0	1	3	15	720
-1	-1	0	0	1	0	-1	1	1	1	0	1	1	0	-1	3	15	720
Generator 11: Grishukhin-Generator																	
-1	-1	-1	0	1	-1	-1	0	1	-1	1	0	1	0	1	2	19	90
-1	-1	-1	0	1	-1	-1	0	1	0	-1	1	1	0	1	2	19	360
-2	-2	-1	1	2	-1	0	1	1	0	1	1	-1	1	0	3	87	360
-2	-2	1	2	2	-1	0	1	1	0	1	1	-1	-1	-1	3	88	180
-2	-2	-1	2	2	-1	0	1	1	0	1	1	1	1	-1	4	15	180
-2	-2	1	1	2	-1	0	1	1	0	1	1	1	-1	0	4	15	360
-2	-2	1	1	2	-1	0	1	1	1	0	1	1	-1	0	4	15	720
-2	-2	1	2	2	-1	0	1	1	1	1	1	-1	0	-1	4	15	720
-2	-1	-1	2	2	-1	0	1	1	1	0	0	1	1	-1	4	15	360
-2	-1	-1	2	2	-1	0	1	1	1	0	1	1	0	-1	4	15	720
-2	-1	1	1	1	-1	2	2	2	0	0	1	-1	-1	-1	4	15	360
-2	-1	1	2	2	0	1	1	1	-1	0	1	-1	0	-1	4	15	720
-2	0	1	1	1	1	2	2	2	-1	-1	0	-1	-1	-1	4	15	360
-1	-1	-1	0	2	-1	-1	0	2	-1	1	2	1	2	-1	4	15	180
-1	-1	-1	0	2	-1	-1	0	2	0	-1	2	1	1	1	4	15	360
-1	-1	-1	0	2	-1	0	1	2	0	1	2	-1	1	-1	4	15	360

Table 5 The 67 representatives for the 18720 facets of TCF_6 as computed from the 11 generators of the facets of $CUT_7^{\square}$ and the 28895 vertices of TCF_6 (see Section 7 and Tables 6 and 4). When we use the format $\sum_{1 \leq i < j \leq 6} c_{ij} x_{ij} \leq c_0$ for the facet inducing inequalities of TCF_6, columns (1)-(16) list the coefficients $c_{1,2}, c_{1,3}, \ldots, c_{5,6}$ followed by the constant c_0, column (17) is the total number of vertices from TCF_6 solving it as an equation and finally, column (18) is the orbit length under permutations. By “new inequalities” we mean that the following inequalities cannot be obtained as liftings from TCF_5 (see Section 6.1).

Generators for the cut polytope $\mathrm{CUT}_7^{\square}$	
Name in Deza and Laurent (1997)	Coefficients $c_{1,2},\ldots,c_{6,7}$
1. $Q_7(1,1,-1,0,0,0,0)$	1 -1 0 0 0 0 -1 0 0 0 0 0 0 0 0 0 0 0 0 0 0
2. $Q_7(1,1,1,-1,-1,0,0)$	1 1 -1 -1 0 0 1 -1 -1 0 0 -1 -1 0 0 1 0 0 0 0 0
3. $Q_7(2,1,1,-1,-1,-1,0)$	2 2 -2 -2 -2 0 1 -1 -1 -1 0 -1 -1 -1 0 1 1 0 1 0 0
4. $Q_7(1,1,1,-1,-1,-1,-1)$	1 1 1 -1 -1 -1 1 1 -1 -1 -1 1 -1 -1 -1 -1 -1 -1 1 1 1
5. $Q_7(2,2,1,-1,-1,-1,-1)$	4 2 -2 -2 -2 -2 2 -2 -2 -2 -2 -1 -1 -1 -1 1 1 1 1 1 1
6. $Q_7(3,1,1,-1,-1,-1,-1)$	3 3 -3 -3 -3 -3 1 -1 -1 -1 -1 -1 -1 -1 -1 1 1 1 1 1 1
7. $\mathrm{CW}_7^1(1,1,1,1,1,-1,-1)$	0 1 1 0 -1 -1 0 1 1 -1 -1 0 1 -1 -1 0 -1 -1 -1 -1 1
8. $\mathrm{CW}_7^1(2,2,1,1,-1,-1,-1)$	3 2 1 -2 -2 -2 1 2 -2 -2 -2 0 -1 -1 -1 -1 -1 -1 1 1 1
9. $\mathrm{CW}_7^1(3,2,2,-1,-1,-1,-1)$	5 5 -3 -3 -3 -3 3 -2 -2 -2 -2 -2 -2 -2 -2 1 1 1 1 1 1
10. Par_7	-1 -1 0 -1 -1 0 1 0 1 0 -1 1 0 0 -1 -1 -1 -1 1 0 1
11. Gr_7	1 1 1 -2 -1 0 1 1 -2 0 -1 1 -2 -1 0 -2 0 -1 1 1 -1

Table 6 The 11 homogeneous generators for the 116 764 facets of $\mathrm{CUT}_7^{\square}$ under all switchings and permutations as in Deza and Laurent (1997) p. 504 and their 21 coefficients $c_{1,2},\ldots,c_{6,7}$ of $\sum_{1\le i<j\le 7} c_{ij}x_{ij} \le 0$. Generators 1-6 are hypermetric "in the cut sense", i.e., the given b-vectors determine the c_{ij} via $c_{ij} = b_i \cdot b_j$. Generators 7-9 are called clique-web inequalities (the vectors have a different meaning here). Generator 10 is a parachute inequality and generator 11 a Grishukhin inequality.

Hypermetric facets of TCF_6 **and their corresponding** b**-vector**			
Generator 1	$b=(1,1,0,0,0,0)$	lifting of *positivity inequality*	v_0
	$b=(1,1,-1,0,0,0)$	lifting of *triangle inequality*	v_1
Generator 2	$b=(1,1,1,-1,0,0)$	lifting of *tetrahedron inequality*	
	$b=(1,1,1,-1,-1,0)$	lifting of *pentagonal inequality*	v_1
Generator 3	$b=(1,1,1,1,-1,0)$	lifting of *pyramid inequality*	
	$b=(2,1,1,-1,-1,0)$	lifting of *2-weighted pentagonal inequality*	
	$b=(1,1,1,1,-2,0)$	lifting of *2-weighted pyramid inequality*	
	$b=(2,1,1,-1,-1,-1)$		v_1
	$b=(1,1,1,1,-1,-2)$		v_1
Generator 4	$b=(1,1,1,1,-1,-1)$		
Generator 5	$b=(2,1,1,1,-1,-1)$		
	$b=(1,1,1,1,1,-2)$		
	$b=(2,2,1,-1,-1,-1)$		
	$b=(2,1,1,1,-1,-2)$		
Generator 6	$b=(1,1,1,1,1,-1)$		
	$b=(3,1,1,-1,-1,-1)$		
	$b=(1,1,1,1,1,-3)$		

Table 7 The 17 representatives for the 858 hypermetric facets of TCF_6 and their corresponding b-vectors (see Section 5). The list is in the same order as in Table 5. The last column indicates whether the respective facet contains one of the exposed vertices $v_0 = (0,0,\ldots,0)$ or $v_1 = (1,1,\ldots,1)$.