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Translation invariant realizability problem on the $d-$dimensional lattice: an explicit construction*

Emanuele Caglioti[†], Maria Infusino[‡], Tobias Kuna[§]

We consider a particular instance of the truncated realizability problem on the $d-$dimensional lattice. Namely, given two functions $\rho_1(\mathbf{i})$ and $\rho_2(\mathbf{i},\mathbf{j})$ non-negative and symmetric on $\mathbb{Z}^d$, we ask whether they are the first two correlation functions of a translation invariant point process. We provide an explicit construction of such a realizing process for any $d \geq 2$ when the radial distribution has a specific form. We also derive from this construction a lower bound for the maximal realizable density and compare it with the already known lower bounds.

1 Introduction

Let d be a positive integer. Given a point process $P = \{P_{\mathbf{i}}\}_{\mathbf{i}\in\mathbb{Z}^d}$ on the $d-$dimensional lattice, $P_{\mathbf{i}} \in \{0,1\}$, whose distribution is described by the probability measure μ, we define the first and second order *correlation function* as follows

$$\begin{cases} \rho_1(\mathbf{i}) := \langle P_{\mathbf{i}} \rangle \\ \rho_2(\mathbf{i},\mathbf{j}) := \langle P_{\mathbf{i}} P_{\mathbf{j}} \rangle - \rho_1(\mathbf{i})\delta(\mathbf{i}-\mathbf{j}) \end{cases},$$

where $\mathbf{i},\mathbf{j} \in \mathbb{Z}^d$, δ is the Dirac delta function and $\langle\cdot\rangle$ denotes the expectation w.r.t. μ.

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The *truncated realizability problem* addresses the inverse question. Namely, given two functions $\rho_1(\mathbf{i})$ and $\rho_2(\mathbf{i},\mathbf{j})$ non-negative and symmetric for all $\mathbf{i},\mathbf{j} \in \mathbb{Z}^d$, does there exist a point process P for which these are the correspondent first and second order correlation functions? Clearly, the truncated realizability problem can be posed for any finite sequence of non-negative and symmetric functions $(\rho_k(\mathbf{i}_1, \mathbf{i}_2, \ldots, \mathbf{i}_k))_{k=1}^n$. When the question is asked for a given infinite sequence $(\rho_k)_{k\in\mathbb{N}}$, then the problem is addressed as full realizability problem (see e.g. [15, 16] for a systematic study of the full realizability problem for point processes and [12, 13] for recent developments).

In the following we will consider the important special case of *translation invariant point processes*, which actually contains all the essential difficulties of the problem. In this case the realizability problem asks if, for given $\rho \in \mathbb{R}^+$ and $g : \mathbb{Z}^d \to \mathbb{R}^+$ symmetric, there exists a translation invariant point process such that its first two correlation functions are given by

$$\begin{cases} \rho_1(\mathbf{i}) = \rho \\ \rho_2(\mathbf{i},\mathbf{j}) = \rho^2 g(\mathbf{i}-\mathbf{j}) \end{cases}. \tag{1}$$

If such a process exists, then it is said to be *realizing* and the pair (ρ, g) is called *realizable* on $\mathbb{Z}^d$. Note that writing the second order correlation in this form is not an additional restriction beyond the assumption of translation invariance. The function g is known in classic fluid theory as *radial distribution*, [6].

The truncated realizability problem is in fact a longstanding problem in the classical theory of fluids (see e.g. [5, 19, 20]), but it has been investigated in many other contexts such as stochastic geometry [17], spatial statistics [3, 21], spatial ecology [18] and neural spike trains [1, 7], just to name a few. In particular, Stillinger, Torquato et al. developed fascinating applications in the study of heterogeneous materials and mesoscopic structures based on the solvability of the truncated realizability problem (see e.g. [4, 22, 23, 24, 25, 26]). A structural investigation of this problem was recently started in [11], where the authors identify the realizability problem as a particular instance of the infinite-dimensional truncated moment problem (see [2, 8, 9, 10, 14] for further recent developments about the truncated realizability problem for point processes). As far as we know, the only earlier reference about the truncated infinite-dimensional moment problem is [28].

In this paper, we will show how to explicitly construct a point process on the $d-$dimensional lattice with $d \geq 2$ such that, for given $\alpha \geq 0$, (1) holds for certain values of ρ and for $g = g^{(\alpha)}$ defined as follows:

$$g^{(\alpha)}(\mathbf{x}) := \begin{cases} 0 & \text{if } \mathbf{x} = 0 \\ \alpha & \text{if } |\mathbf{x}| = 1 \\ 1 & \text{if } |\mathbf{x}| > 1 \end{cases}. \tag{2}$$

Explicit constructions of point processes realizing this lattice problem in the case $d = 1$ were provided in [10, Appendix 1]. Such a problem has been extensively studied for the case $\alpha = 0$ by Stillinger and Torquato in [22] (see also [4, 25]). The function $g^{(0)}$ describes a model with on-site and nearest neighbour exclusion and with no correlation for pairs of sites separated by two or more lattice spacings.

From [10, Section 1], we know that for a fixed α the set of realizable densities ρ is an interval $[0, \bar{\rho}_\alpha(d)]$ with $0 < \bar{\rho}_\alpha(d) \leq 1$. Moreover, in [10] the authors discuss:

(i) certain general methods which, when applied to (2), yield lower bounds for $\bar{\rho}_\alpha(d)$ in any dimension d.

(ii) concrete upper and lower bounds for $\bar{\rho}_\alpha(1)$. In particular, the lower bounds improve those obtained from the general methods (i).

Our $d-$dimensional construction combined with the one-dimensional lower bounds (ii) provides a lower bound for $\bar{\rho}_\alpha(d)$ for any $d \geq 2$ and any $\alpha \geq 0$. We will briefly compare this with the lower bound obtained from the general methods (i). We also follow techniques from [10] to get an upper bound for $\bar{\rho}_\alpha(d)$.

2 An explicit realizing translation invariant point process on $\mathbb{Z}^d$

In the following, we explicitly construct a point process $P = \{P_{\mathbf{i}}\}_{\mathbf{i}\in\mathbb{Z}^d}$ on the $d-$dimensional lattice with $d \geq 2$ such that, for given $\alpha \geq 0$, the following hold for certain values of ρ (depending on α and on d):

$$\langle P_{\mathbf{i}} \rangle = \rho \tag{3}$$

and

$$\langle P_{\mathbf{i}} P_{\mathbf{j}} \rangle = \begin{cases} \rho & \text{if } \mathbf{i} = \mathbf{j} \\ \alpha\rho^2 & \text{if } |\mathbf{i} - \mathbf{j}| = 1 \\ \rho^2 & \text{if } |\mathbf{i} - \mathbf{j}| > 1 \end{cases}, \tag{4}$$

that is, the radial distribution is given by (2).

2.1 Construction in dimension 2

In order to build such a process on $\mathbb{Z}^2$ we start from a realizing one-dimensional process achieving density γ. Namely, given $\alpha \geq 0$, we consider a point process $\{A_i\}_{i\in\mathbb{Z}}$, $A_i \in \{0, 1\}$, defined on the one-dimensional lattice and such that for some $\gamma > 0$ we have

$$\langle A_i \rangle = \gamma,$$

and

$$\langle A_i A_j \rangle = \begin{cases} \gamma & \text{if } i = j \\ \alpha\gamma^2 & \text{if } |i - j| = 1 \\ \gamma^2 & \text{if } |i - j| > 1 \end{cases}.$$

We denote a process of this kind by $BP\gamma$ that stays for *basic process with density* γ. As pointed out in the introduction, there exists a good number of constructions of realizing processes in the one-dimensional case, see e.g. [10, Appendix 1]. The results in the one-dimensional case relevant to our investigation (in particular the range where γ can vary) are recalled in Section 3, which is devoted to the discussion of the maximal realizable density in any dimension.

Let us define two processes $B^{(1)} = \left\{B^{(1)}_{i_1,i_2}\right\}_{(i_1,i_2)\in\mathbb{Z}^2}$ and $B^{(2)} = \left\{B^{(2)}_{i_1,i_2}\right\}_{(i_1,i_2)\in\mathbb{Z}^2}$ on $\mathbb{Z}^2$ as follows. For a fixed $i_1 \in \mathbb{Z}$, the process $\left\{B^{(1)}_{i_1,i_2}\right\}_{i_2\in\mathbb{Z}}$ is a $BP\gamma$ in i_2. For any $i_1, j_1 \in \mathbb{Z}$ with $i_1 \neq j_1$, the processes $\left\{B^{(1)}_{i_1,i_2}\right\}_{i_2\in\mathbb{Z}}$ and $\left\{B^{(1)}_{j_1,j_2}\right\}_{j_2\in\mathbb{Z}}$ are independent. In particular, we have

$$\langle B^{(1)}_{i_1,i_2} B^{(1)}_{j_1,j_2}\rangle = \begin{cases} \gamma^2 & \text{if } i_1 \neq j_1 \\ \gamma & \text{if } i_1 = j_1 \text{ and } i_2 = j_2 \\ \alpha\gamma^2 & \text{if } i_1 = j_1 \text{ and } |i_2 - j_2| = 1 \\ \gamma^2 & \text{if } i_1 = j_1 \text{ and } |i_2 - j_2| > 1 \end{cases} . \tag{5}$$

In other words, the process $B^{(1)}$ can be seen as a sequence of vertical $BP\gamma$'s independent one from each other (see Figure 1 for an example).

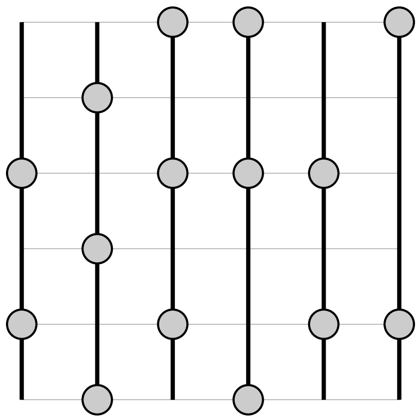

Figure 1: Example of process $B^{(1)}$ (with $\alpha = 0$)

Similarly, the process $B^{(2)}$ is defined as a sequence of horizontal $BP\gamma$'s independent one from each other (see Figure 2 for an example), i.e.

$$\langle B^{(2)}_{i_1,i_2} B^{(2)}_{j_1,j_2}\rangle = \begin{cases} \gamma^2 & \text{if } i_2 \neq j_2 \\ \gamma & \text{if } i_2 = j_2 \text{ and } i_1 = j_1 \\ \alpha\gamma^2 & \text{if } i_2 = j_2 \text{ and } |i_1 - j_1| = 1 \\ \gamma^2 & \text{if } i_2 = j_2 \text{ and } |i_1 - j_1| > 1 \end{cases} . \tag{6}$$

Let us define now the process $P = \{P_{\mathbf{i}}\}_{\mathbf{i}\in\mathbb{Z}^2}$ as

$$P_{i_1,i_2} := B^{(1)}_{i_1,i_2} B^{(2)}_{i_1,i_2},$$

(see Figure 3 for P constructed from the basic processes in Figures 1 and 2). Since the processes $B^{(1)}$ and $B^{(2)}$ are independent, we get

$$\langle P_{i_1,i_2}\rangle = \langle B^{(1)}_{i_1,i_2} B^{(2)}_{i_1,i_2}\rangle = \langle B^{(1)}_{i_1,i_2}\rangle\langle B^{(2)}_{i_1,i_2}\rangle = \gamma\cdot\gamma = \gamma^2.$$

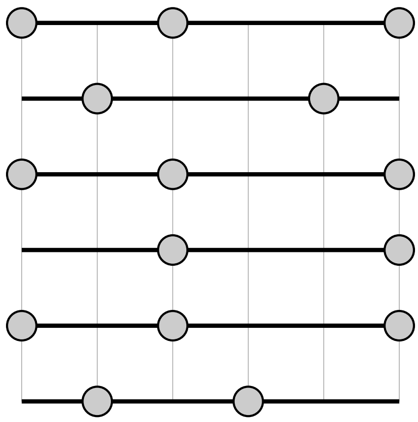

Figure 2: Example of process $B^{(2)}$ (with $\alpha = 0$)

Hence, (3) holds for $\rho = \gamma^2$. From the independence of $B^{(1)}$ and $B^{(2)}$, we also get

$$\langle P_{i_1,i_2} P_{j_1,j_2} \rangle = \langle B^{(1)}_{i_1,i_2} B^{(2)}_{i_1,i_2} B^{(1)}_{j_1,j_2} B^{(2)}_{j_1,j_2} \rangle = \langle B^{(1)}_{i_1,i_2} B^{(1)}_{j_1,j_2} \rangle \langle B^{(2)}_{i_1,i_2} B^{(2)}_{j_1,j_2} \rangle. \tag{7}$$

We can easily check, by using (5) and (6) in (7), that (4) holds for $\rho = \gamma^2$. In fact, we need to consider only the following four cases, because all the others are equivalent to these ones by symmetry.

a) If $i_1 = j_1$ and $i_2 = j_2$ then

$$\langle P_{i_1,i_2} P_{j_1,j_2} \rangle = \gamma \cdot \gamma = \gamma^2.$$

b) If $i_1 = j_1$ and $i_2 \neq j_2$ then

$$\langle P_{i_1,i_2} P_{j_1,j_2} \rangle = \langle B^{(1)}_{i_1,i_2} B^{(1)}_{j_1,j_2} \rangle \gamma^2.$$

Therefore:

- if $i_2 = j_2 + 1$ then $\langle B^{(1)}_{i_1,i_2} B^{(1)}_{j_1,j_2} \rangle = \alpha\gamma^2$ and so $\langle P_{i_1,i_2} P_{j_1,j_2} \rangle = \alpha\gamma^4$
- if $|i_2 - j_2| > 1$ then $\langle B^{(1)}_{i_1,i_2} B^{(1)}_{j_1,j_2} \rangle = \gamma^2$ and so $\langle P_{i_1,i_2} P_{j_1,j_2} \rangle = \gamma^4$.

c) If $i_1 = j_1 + 1$ and $|i_2 - j_2| > 1$ then

$$\langle P_{i_1,i_2} P_{j_1,j_2} \rangle = \langle B^{(1)}_{i_1,i_2} B^{(1)}_{j_1,j_2} \rangle \langle B^{(2)}_{i_1,i_2} B^{(2)}_{j_1,j_2} \rangle = \gamma^4.$$

d) If $|i_1 - j_1| > 1$ and $i_2 \neq j_2$ then

$$\langle P_{i_1,i_2} P_{j_1,j_2} \rangle = \langle B^{(1)}_{i_1,i_2} B^{(1)}_{j_1,j_2} \rangle \langle B^{(2)}_{i_1,i_2} B^{(2)}_{j_1,j_2} \rangle = \gamma^4.$$

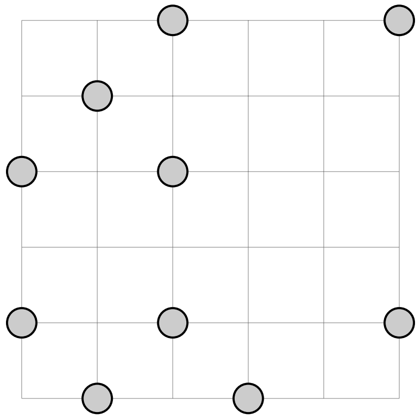

Figure 3: Process P constructed from the processes in Figure 1 and Figure 2

2.2 Construction in higher dimension

The construction presented in the previous subsection easily generalizes to any dimension $d > 2$ by defining $P_{i_1,\dots,i_d} := B^{(1)}_{i_1,\dots,i_d} \cdots B^{(d)}_{i_1,\dots,i_d}$ where, for any fixed $i_2, \dots, i_d \in \mathbb{Z}$, $\{B^{(1)}_{i_1,\dots,i_d}\}_{i_1 \in \mathbb{Z}}$ is a $BP\gamma$ in the variable i_1 with density γ and similarly for the other variables. Therefore, the point process P on $\mathbb{Z}^d$ defined as above satisfies (3) and (4) for $\rho = \gamma^d$.

3 Bounds for the maximal realizable density

In this section, we will discuss the problem of estimating the maximal realizable density $\bar{\rho}_\alpha(d)$. In particular, we will show a general upper bound for any $d \geq 1$ using the technique introduced in [10] for $d = 1$. As for the lower bound, we will recall the results in [10, Appendix 1] for the one-dimensional case and combine them with the explicit construction proposed in Section 2 to produce a lower bound for $\bar{\rho}_\alpha(d)$ for any $d \geq 2$. We will compare this with the lower bound obtained by applying the general methods of [10] to the case when the radial distribution is given by (2).

3.1 Upper bounds for $\bar{\rho}_\alpha(d)$

For $d \geq 1$ and $\alpha \geq 0$, the covariance matrix associated to a given pair $(\rho, g^{(\alpha)})$ realizable on $\mathbb{Z}^d$ must be positive semidefinite. This is equivalent to the non-negativity of the corresponding infinite volume structure function $\hat{S}$ on $\mathbb{R}^d$ (for more details see e.g. [10, Section 2]):

$$\hat{S}(\mathbf{k}) := \rho + \rho^2 \sum_{\mathbf{x} \in \mathbb{Z}^d} e^{i\mathbf{k}\cdot\mathbf{x}}[g^{(\alpha)}(\mathbf{x}) - 1] \geq 0, \ \forall\, \mathbf{k} \in \mathbb{R}^d.$$

This leads to an explicit upper bound for the maximal realizable density $\bar{\rho}_\alpha(d)$. In fact, it is easy to see that for any $\mathbf{k} := (k_1, \dots, k_d) \in \mathbb{R}^d$ we get

$$\begin{aligned}\hat{S}(\mathbf{k}) &= \rho - \rho^2 + \rho^2 \sum_{\mathbf{x}\in\mathbb{Z}^d, |\mathbf{x}|=1} e^{i\mathbf{k}\cdot\mathbf{x}}(\alpha - 1) \\ &= \rho - \rho^2 + \rho^2(\alpha - 1)\sum_{j=1}^{d}(e^{ik_j} + e^{-ik_j}) \\ &= \rho\left[1 - \rho\left(1 - 2(\alpha - 1)\sum_{j=1}^{d}\cos(k_j)\right)\right].\end{aligned}$$

Then, using the non-negativity of $\hat{S}$ on $\mathbb{R}^d$, we get that

$$\rho \leq \frac{1}{f_\alpha(k_1, \dots, k_d)}, \quad \forall\, (k_1, \dots, k_d) \in \mathbb{R}^d,$$

where $f_\alpha(k_1, \dots, k_d) := 1 - 2(\alpha - 1)\sum_{j=1}^{d}\cos(k_j)$. The best upper bound is then obtained for the points of $\mathbb{R}^d$ where f_α attains the maximum. Hence, we have that

$$\bar{\rho}_\alpha(d) \leq \frac{1}{\max\limits_{\mathbf{k}\in\mathbb{R}^d} f_\alpha(\mathbf{k})} =: R_F(\alpha, d).$$

By computing the maximum of f_α over $\mathbb{R}^d$, we get our upper bound

$$R_F(\alpha, d) = \frac{1}{1 + 2d|1 - \alpha|}. \tag{8}$$

As mentioned above, this technique was employed in [10, Appendix 1] to get $R_F(\alpha, 1)$. Furthermore, the authors provided another upper bound $R_Y(\alpha, 1)$ in the one-dimensional case by using the Yamada condition (see [27]). Note that

$$\begin{cases} R_Y(\alpha, 1) = R_F(\alpha, 1), & \text{if } \alpha = \frac{1}{2} \text{ or } \alpha = \frac{k\pm1}{2k}, k \in \mathbb{N} \text{ or } \alpha \geq 1 \\ R_Y(\alpha, 1) < R_F(\alpha, 1) & \text{otherwise.}\end{cases}$$

3.2 Lower bounds for $\bar{\rho}_\alpha(d)$

Applying [10, Theorem 3.2] for $g \equiv g^{(\alpha)}$ when $0 \leq \alpha < 1$ and [10, Theorem 5.1] for $G_2(\mathbf{x}, \mathbf{y}) = g^{(\alpha)}(\mathbf{y} - \mathbf{x})$ for all $\mathbf{x}, \mathbf{y} \in \mathbb{Z}^d$ such that $\mathbf{x} \neq \mathbf{y}$ when $\alpha \geq 1$, we get that

$$\bar{\rho}_\alpha(d) \geq r_A(\alpha, d) := \begin{cases} \frac{1}{e(2d+1-2d\alpha)}, & \text{if } 0 \leq \alpha < 1, \\ \frac{1}{\alpha^{2d}}, & \text{if } \alpha \geq 1. \end{cases} \tag{9}$$

For $d = 1$, this lower bound has been improved in [10, Appendix 1] by explicitly constructing a translation invariant realizing process at some value of ρ and α. Let us summarize in one formula the lower bounds coming from the two main constructions considered in [10, Appendix 1]:

$$\bar{\rho}_\alpha(1) \geq \begin{cases} \frac{1}{(1+\sqrt{1-\alpha})^2}, & \text{if } 0 \leq \alpha < \frac{1}{2}, \\ \frac{1}{1+\sqrt{2-2\alpha}}, & \text{if } \frac{1}{2} \leq \alpha \leq 1, \\ \frac{1}{2\alpha-1}, & \text{if } \alpha \geq 1. \end{cases} \tag{10}$$

In [2] a further explicit construction is provided for the case $\alpha = 0$, which slightly improves this lower bound to $\bar{\rho}_0(1) > 0.265$. In the same work also the upper bound is improved to $\bar{\rho}_0(1) < (326 - \sqrt{3115})/822 \approx 0.3287$. However, it remains an open problem to reduce the gap between lower and upper bounds for $\bar{\rho}_\alpha(1)$ for any $\alpha \geq 0$.

Exactly as in the one-dimensional case, also for $d \geq 2$, one can try to obtain better lower bounds than (9) by using explicit constructions. In the following, we will use the construction we proposed in Section 2 combined with the one-dimensional lower bound (10) to compute a new lower bound for $\bar{\rho}_\alpha(d)$, which we will briefly compare with (9).

If we apply the construction given for $d \geq 2$ in Section 2 starting with a basic process with density $\bar{\rho}_\alpha(1)$, then we get a point process on $\mathbb{Z}^d$ which realizes the pair $\big((\bar{\rho}_\alpha(1))^d, g^{(\alpha)}\big)$ for any $\alpha \geq 0$. This explicit construction guarantees that for any $\alpha \geq 0$,

$$\bar{\rho}_\alpha(d) \geq (\bar{\rho}_\alpha(1))^d.$$

Using the lower bounds (10) in the latter inequality, we directly have the following

$$\bar{\rho}_\alpha(d) \geq r_C(\alpha, d) := \begin{cases} \frac{1}{(1+\sqrt{1-\alpha})^{2d}}, & \text{if } 0 \leq \alpha < \frac{1}{2}, \\ \frac{1}{(1+\sqrt{2-2\alpha})^d}, & \text{if } \frac{1}{2} \leq \alpha \leq 1, \\ \frac{1}{(2\alpha-1)^d}, & \text{if } \alpha \geq 1. \end{cases} \tag{11}$$

Note that:

- if $0 \leq \alpha < \frac{1}{2}$ then $r_C(\alpha, d) \leq r_A(\alpha, d)$
- if $\alpha \geq 1$ then $r_A(\alpha, d) \leq r_C(\alpha, d)$
- if $\frac{1}{2} \leq \alpha \leq 1$ then the relation between the two bounds depends on the dimension d. Actually, for each $d \geq 2$ there exists $\alpha_C(d) \in \left[\frac{1}{2}, 1\right]$ such that $r_A(\alpha, d) \leq r_C(\alpha, d)$ for any $\alpha_C(d) \leq \alpha \leq 1$.

The comparison between the lower bounds $r_C(\alpha, d)$ and $r_A(\alpha, d)$ is illustrated in Figure 4 for $d = 2, \ldots, 6$ and for $0 \leq \alpha < 1$.

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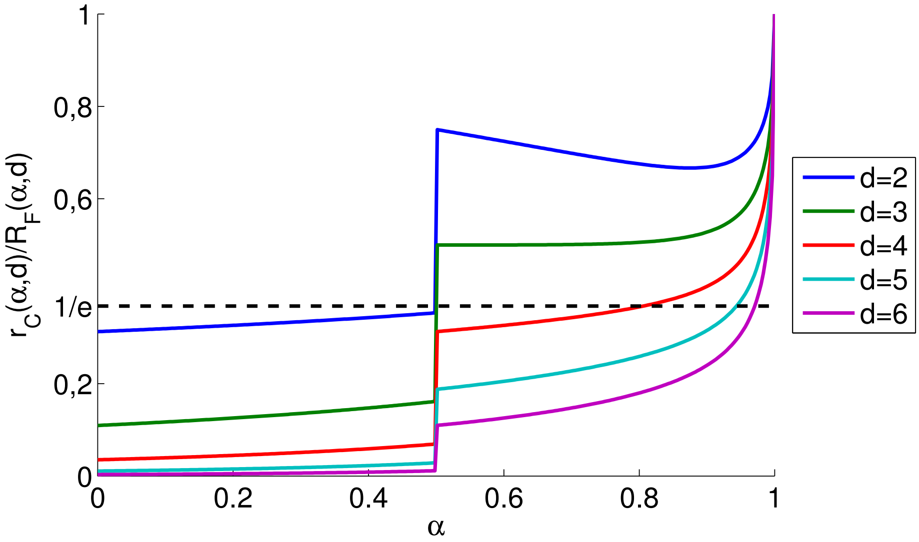

Figure 4: Comparison between the lower bounds $r_C(\alpha, d)$ and $r_A(\alpha, d)$ plotted relatively to the upper bound $R_F(\alpha, d)$ as functions of α with $0 \leq \alpha < 1$. The coloured lines correspond to $\frac{r_C(\alpha,d)}{R_F(\alpha,d)}$ for $d = 2, \ldots, 6$ and the dotted line to $\frac{r_A(\alpha,d)}{R_F(\alpha,d)}$ for any d. For the definitions of $R_F(\alpha, d)$, $r_A(\alpha, d)$, $r_C(\alpha, d)$ see (8), (9), (11), respectively.

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