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

Emanuele Caglioti<sup>†</sup>      Maria Infusino<sup>‡</sup>      Tobias Kuna<sup>§</sup>

## Abstract

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.

**Keywords:** truncated moment problem; realizability; point processes; translation invariant; infinite dimensional moment problem.

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

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  $(\rho_k(\mathbf{i}_1, \mathbf{i}_2, \dots, \mathbf{i}_k))_{k=1}^n$ . When the question is asked for a given infinite sequence  $(\rho_k)_{k \in \mathbb{N}}$ , then the problem is addressed as

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full realizability problem (see e.g. [15, 16] for a systematic study of the full realizability problem for point processes and [7, 8] 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  $g : \mathbb{Z}^d \rightarrow \mathbb{R}^+$  symmetric, there exists a translation invariant point process such that its first two correlation functions are given by

$$\begin{cases} \rho_1(\mathbf{i}) = \rho \\ \rho_2(\mathbf{i}, \mathbf{j}) = \rho^2 g(\mathbf{i} - \mathbf{j}) \end{cases} \quad (1.1)$$

If such a process exists, then it is said to be *realizing* and the pair  $(\rho, g)$  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, 23], spatial ecology [18] and neural spike trains [1, 9], 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, 21, 22, 24, 25, 26]). A structural investigation of this problem was recently started in [13], where the authors identify the realizability problem as a particular instance of the infinite-dimensional truncated moment problem (see [2, 10, 11, 12, 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  $\alpha \geq 0$ , (1.1) holds for certain values of  $\rho$  and for  $g = g^{(\alpha)}$  defined as follows:

$$g^{(\alpha)}(\mathbf{x}) := \begin{cases} 0 & \text{if } \mathbf{x} = 0 \\ \alpha & \text{if } |\mathbf{x}| = 1 \\ 1 & \text{if } |\mathbf{x}| > 1 \end{cases} \quad (1.2)$$

Explicit constructions of point processes realizing this lattice problem in the case  $d = 1$  were provided in [12, Appendix 1]. Such a problem has been extensively studied for the case  $\alpha = 0$  by Stillinger and Torquato in [21] (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 [12, Section 1], we know that for a fixed  $\alpha$  the set of realizable densities  $\rho$  is an interval  $[0, \bar{\rho}_\alpha(d)]$  with  $0 < \bar{\rho}_\alpha(d) \leq 1$ . Moreover, in [12] the authors discuss:

- (i) certain general methods which, when applied to (1.2), 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 [12] 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  $P = \{P_i\}_{i \in \mathbb{Z}^d}$  on the  $d$ -dimensional lattice with  $d \geq 2$  such that, for given  $\alpha \geq 0$ , the following hold for certain values of  $\rho$  (depending on  $\alpha$  and on  $d$ ):

$$\langle P_i \rangle = \rho \quad (2.1)$$

and

$$\langle P_i P_j \rangle = \begin{cases} \rho & \text{if } i = j \\ \alpha \rho^2 & \text{if } |i - j| = 1 \\ \rho^2 & \text{if } |i - j| > 1 \end{cases}, \quad (2.2)$$

that is, the radial distribution is given by (1.2).

### 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  $\gamma$ . 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*  $\gamma$ . As pointed out in the introduction, there exists a good number of constructions of realizing processes in the one-dimensional case, see e.g. [12, Appendix 1]. The results in the one-dimensional case relevant to our investigation (in particular the range where  $\gamma$  can vary) are recalled in Section 3, which is devoted to the discussion of the maximal realizable density in any dimension.

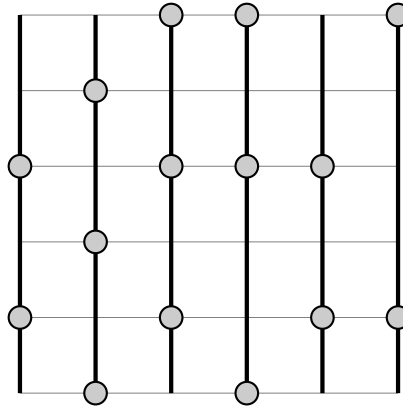
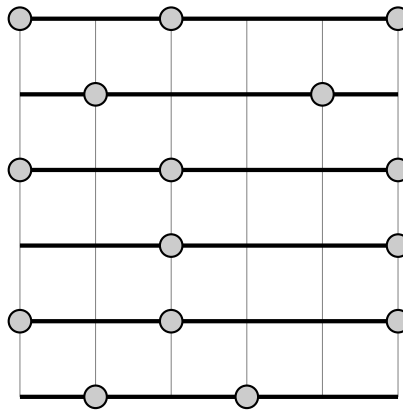
Let us define two processes  $B^{(1)} = \{B_{i_1, i_2}^{(1)}\}_{(i_1, i_2) \in \mathbb{Z}^2}$  and  $B^{(2)} = \{B_{i_1, i_2}^{(2)}\}_{(i_1, i_2) \in \mathbb{Z}^2}$  on  $\mathbb{Z}^2$  as follows. For a fixed  $i_1 \in \mathbb{Z}$ , the process  $\{B_{i_1, i_2}^{(1)}\}_{i_2 \in \mathbb{Z}}$  is a  $BP\gamma$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

$$\langle B_{i_1, i_2}^{(1)} B_{j_1, j_2}^{(1)} \rangle = \begin{cases} \gamma^2 & \text{if } i_1 \neq j_1 \\ \gamma & \text{if } i_1 = j_1 \text{ and } i_2 = j_2 \\ \alpha \gamma^2 & \text{if } i_1 = j_1 \text{ and } |i_2 - j_2| = 1 \\ \gamma^2 & \text{if } i_1 = j_1 \text{ and } |i_2 - j_2| > 1 \end{cases}. \quad (2.3)$$

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).

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.

$$\langle B_{i_1, i_2}^{(2)} B_{j_1, j_2}^{(2)} \rangle = \begin{cases} \gamma^2 & \text{if } i_2 \neq j_2 \\ \gamma & \text{if } i_2 = j_2 \text{ and } i_1 = j_1 \\ \alpha \gamma^2 & \text{if } i_2 = j_2 \text{ and } |i_1 - j_1| = 1 \\ \gamma^2 & \text{if } i_2 = j_2 \text{ and } |i_1 - j_1| > 1 \end{cases}. \quad (2.4)$$


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

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

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

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

(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

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

Hence, (2.1) holds for  $\rho = \gamma^2$ . From the independence of  $B^{(1)}$  and  $B^{(2)}$ , we also get

$$\langle P_{i_1, i_2} P_{j_1, j_2} \rangle = \langle B_{i_1, i_2}^{(1)} B_{i_1, i_2}^{(2)} B_{j_1, j_2}^{(1)} B_{j_1, j_2}^{(2)} \rangle = \langle B_{i_1, i_2}^{(1)} B_{j_1, j_2}^{(1)} \rangle \langle B_{i_1, i_2}^{(2)} B_{j_1, j_2}^{(2)} \rangle. \quad (2.5)$$

We can easily check, by using (2.3) and (2.4) in (2.5), that (2.2) 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

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

Therefore:

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

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

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

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

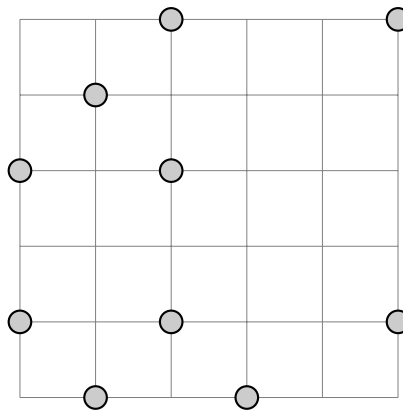


Figure 3: Process  $P$  constructed from the processes in Figure 1 and Figure 2

## 2.2 Construction in higher dimension

The construction presented in the previous subsection easily generalizes to any dimension  $d > 2$  by defining  $P_{i_1, \dots, i_d} := B_{i_1, \dots, i_d}^{(1)} \cdots B_{i_1, \dots, i_d}^{(d)}$  where, for any fixed  $i_2, \dots, i_d \in \mathbb{Z}$ ,  $\{B_{i_1, \dots, i_d}^{(1)}\}_{i_1 \in \mathbb{Z}}$  is a  $BP\gamma$  in the variable  $i_1$  with density  $\gamma$  and similarly for the other variables. Therefore, the point process  $P$  on  $\mathbb{Z}^d$  defined as above satisfies (2.1) and (2.2) 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 [12] for  $d = 1$ . As for the lower bound, we will recall the results in [12, 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 [12] to the case when the radial distribution is given by (1.2).

### 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. [12, Section 2]):

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

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  $f_\alpha$  attains the maximum. Hence, we have that

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

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

$$R_F(\alpha, d) = \frac{1}{1 + 2d|1 - \alpha|}. \quad (3.1)$$

As mentioned above, this technique was employed in [12, 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

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

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

Applying [12, Theorem 3.2] for  $g \equiv g^{(\alpha)}$  when  $0 \leq \alpha < 1$  and [12, 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

$$\bar{\rho}_\alpha(d) \geq r_A(\alpha, d) := \begin{cases} \frac{1}{e(2d+1-2d\alpha)}, & \text{if } 0 \leq \alpha < 1, \\ \frac{1}{\alpha^{2d}}, & \text{if } \alpha \geq 1. \end{cases} \quad (3.2)$$

For  $d = 1$ , this lower bound has been improved in [12, Appendix 1] by explicitly constructing a translation invariant realizing process at some value of  $\rho$  and  $\alpha$ . Let us summarize in one formula the lower bounds coming from the two main constructions considered in [12, Appendix 1]:

$$\bar{\rho}_\alpha(1) \geq \begin{cases} \frac{1}{(1+\sqrt{1-\alpha})^2}, & \text{if } 0 \leq \alpha < \frac{1}{2}, \\ \frac{1}{1+\sqrt{2-2\alpha}}, & \text{if } \frac{1}{2} \leq \alpha \leq 1, \\ \frac{1}{2\alpha-1}, & \text{if } \alpha \geq 1. \end{cases} \quad (3.3)$$

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 (3.2) by using explicit constructions. In the following, we will use the construction we proposed in Section 2 combined with the one-dimensional lower bound (3.3) to compute a new lower bound for  $\bar{\rho}_\alpha(d)$ , which we will briefly compare with (3.2).

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  $((\bar{\rho}_\alpha(1))^d, g^{(\alpha)})$  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 (3.3) in the latter inequality, we directly have the following

$$\bar{\rho}_\alpha(d) \geq r_C(\alpha, d) := \begin{cases} \frac{1}{(1+\sqrt{1-\alpha})^{2d}}, & \text{if } 0 \leq \alpha < \frac{1}{2}, \\ \frac{1}{(1+\sqrt{2-2\alpha})^d}, & \text{if } \frac{1}{2} \leq \alpha \leq 1, \\ \frac{1}{(2\alpha-1)^d}, & \text{if } \alpha \geq 1. \end{cases} \quad (3.4)$$

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  $\alpha_C(d) \in [\frac{1}{2}, 1]$  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  $d = 2, \dots, 6$  and for  $0 \leq \alpha < 1$ .

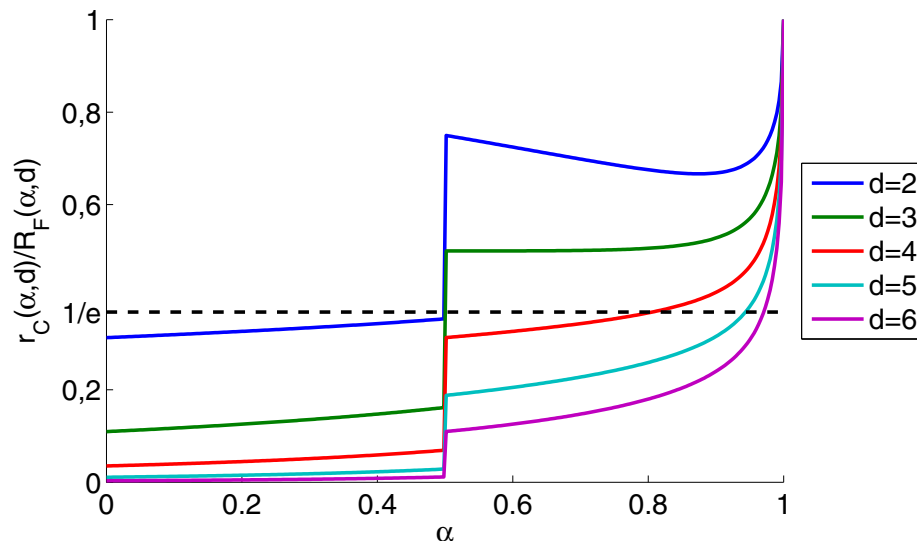


Figure 4: Comparison between the lower bounds  $r_C(\alpha, d)$  and  $r_A(\alpha, d)$  plotted relatively to the upper bound  $R_F(\alpha, d)$  as functions of  $\alpha$  with  $0 \leq \alpha < 1$ . The coloured lines correspond to  $\frac{r_C(\alpha, d)}{R_F(\alpha, d)}$  for  $d = 2, \dots, 6$  and 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 (3.1), (3.2), (3.4), respectively.

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