Ruling Out Certain 5-Spectra with One Repeated Eigenvalue for the Symmetric NIEP *

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Abstract

Here, prior work, that ruled out certain spectra with two repeated eigenvalues for the 5-by-5 S-NIEP, is extended. Previously unresolved spectra with just one repeated eigenvalue are shown not to occur. The repeat could be either positive or negative, but the two situations are different. In both situations, the prior result with two repeats is a special case.

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1 Introduction

In [3], we considered spectra with 5 real eigenvalues, a repeated positive eigenvalue and a repeated negative eigenvalue, that were previously unresolved for the symmetric nonnegative inverse eigenvalue problem (S-NIEP). A method was developed that showed that a large portion (not all) of these spectra could not be realized. As the nonrealizable spectra form an open set in $\mathbb{R}^5$, it must happen that these nonrealizable spectra imply that many nearby spectra (with fewer repeated eigenvalues) are also nonrealizable. Unfortunately, it is difficult to explicitly exploit this analytical fact. Here, we refine our method and, with additional complication, apply it to real 5-spectra with just one repeated eigenvalue. Again, many spectra are excluded, including our prior results as a special case. Interestingly, the two cases (a repeated positive eigenvalue, and a repeated negative eigenvalue) are analytically different. In all cases, we consider only spectra with 3 positive eigenvalues (including the Perron root) and 2 negative eigenvalues, as all other $+/-$ balances have been resolved. We also restrict attention (primarily) to spectra within this case that are not otherwise resolved. As before, the starting point for a proposed 5-spectrum is to consider, via the interlacing inequalities,

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the possible spectra of the five 4-by-4 principal submatrices. In the prior work [3], spectra of the form

$$1, a, a-(a+d), -(a+d)$$

were considered, with $a, d > 0$ and $a+d, 2d < 1 < a+2d$ (unresolved cases were among these). A sufficient condition for nonrealizability was found ([3, Theorem 1]) to be

$$2(a+d)^3 > 1 + a^3 + (a+2d-1)^3.$$

Note the typo in the statement of the theorem, where $\geq$ appears instead of $>$.

Section 2 contains a discussion of the current state of knowledge about the 5-by-5 S-NIEP with 2 repeated eigenvalues, relative to our work in [3].

Computationally obtained graphical depictions of our results, usually in comparison to prior results (primarily of [8]), are given in figures 1-11. These are the primary basis for comments in the text about comparison to prior results. Proofs about comparisons appear in appendices.

2 5-Spectra with Repeated Positive and Negative Eigenvalues

In [3], we considered spectra with 5 real eigenvalues, a repeated positive eigenvalue and a repeated negative eigenvalue and we proved:

Theorem 1. ([3, Theorem 1]) *Let $0 < a, d$ satisfy $a+d, 2d < 1 < a+2d$. If $2(a+d)^3 > 1 + a^3 + (a+2d-1)^3$, then $1, a, a, -(a+d), -(a+d)$ are not the eigenvalues of a 5-by-5 symmetric nonnegative matrix.*

After this result was published, another result appeared about symmetric realization of spectra with 5 eigenvalues.

Theorem 2. ([6, Theorem 4]) *Let $\sigma = \{\lambda_1, \ldots, \lambda_5\}$ be a list of monotonically decreasing real numbers such that $\sum_{i=1}^{5} \lambda_i \geq \frac{\lambda_1}{2}$. Necessary and sufficient conditions for σ to be the spectrum of a nonnegative symmetric matrix are:*

1. $\lambda_1 = \max_{\lambda \in \sigma} |\lambda|$,
2. $\lambda_2 + \lambda_5 \leq \sum_{i=1}^{5} \lambda_i$,
3. $\lambda_3 \leq \sum_{i=1}^{5} \lambda_i$.

And about to appear from the same authors is another paper on the same subject [7]. This one primarily deals with realizable spectra and also points out some comments made here but with a different parametrization.

A spectrum $1, a, a, -(a+d), -(a+d)$ under the hypothesis of Theorem 1, clearly satisfies conditions 1 and 2 but not 3 from Theorem 2. Note that in this case $\sum_{i=1}^{5} \lambda_i \geq \frac{\lambda_1}{2}$ leads us to $d \leq \frac{1}{4}$. In a, d-space, fig. 1 describes these results. The grey triangle, without the border, is the domain of Theorem 1. The dashed slightly curved line 1 is the exclusionary curve given by Theorem 1. No spectrum corresponding to points above it is symmetrically realizable. The dotted curve 2 is an exclusionary boundary deduced from a cubic Johnson-Loewy-London necessary condition [2, 4].

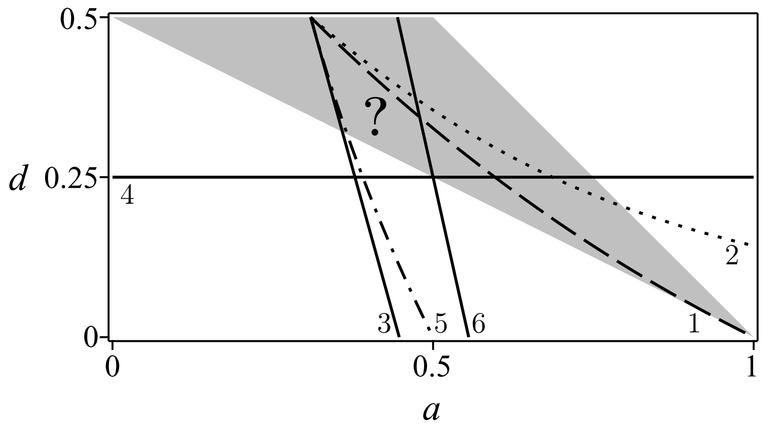

fig. 1: Curve 1 $\equiv 2(a+d)^3 - a^3 - (a+2d-1)^3 = 1$, curve 2 $\equiv 50(a+d)^3 + (1-2d)^2 - 50a^3 = 25$, line 3 $\equiv 10a - (\sqrt{5}-5)d = 2\sqrt{5}$, line 4 $\equiv d = 1/4$, curve 5 $\equiv 4a(a+d) = 1$, line 6 $\equiv 9a + 2d = 5$.

Line 3 corresponds to constant diagonal S-NIEP realizable spectra, deduced from the result of [8]. Any spectrum corresponding to points on the left or on it is symmetrically realizable with constant diagonal. Line 4 is $d = \frac{1}{4}$ and no spectrum corresponding to points under or on it is symmetrically realizable because of Theorem 2. In [5] a family of matrices was exhibited that, when translated to our parameters, realizes spectra on the dashdotted curve 5. Since spectra southwest of realizable ones are also realizable, by increasing the Perron root and re-scaling, points to the left of this curve are also realizable and this observation was claimed in [7], as well. In [7, Theorem 5.1] it was also shown that spectra to the right of line 6 on the grey region are not realizable. This reduces the unknown region described in [3], but still leaves a region of unresolved spectra, the one with a question mark in fig. 1.

3 5-Spectra with a Repeated Positive Eigenvalue

Throughout this section, we consider 5-spectra of the form

$$1, a, a, -(a+d_1), -(a+d_2)$$

with $a + d_2 < 1$ because of the Perron condition, $1 > a, d_2 > d_1 > 0$, and $1 < a + d_1 + d_2$, as otherwise existence has been characterized [1]. Of course, $1 > d_1 + d_2$, as the trace must be positive; the inequality may be taken to be strict, as trace 0 spectra have been characterized for $n = 5$ in the S-NIEP [8].

If these are the eigenvalues of a 5-by-5 symmetric nonnegative matrix $A = (a_{ij})$, then we suppose that each 4-by-4 principal submatrix A_i of A, resulting from deleting row and column i, has eigenvalues

$$p_i, a, q_i, -(a+c_i), \quad i = 1, \dots, 5,$$

in which p_i, $1 \geq p_i \geq a$, is the Perron root, $a \geq q_i \geq -(a+d_1)$ and $d_1 \leq c_i \leq d_2$ all by interlacing. By Perron-Frobenius $p_i \geq a + c_i \geq a + d_1 > a$, so that $1 \geq p_i > a$.

Now, we have $4\text{Tr }(A) = \sum_{i=1}^{5} \text{Tr }(A_i)$, and, because of nonnegativity

$$4\text{Tr }(A^3) = \sum_{i=1}^{5} \text{Tr }((A^3)_i) \geq \sum_{i=1}^{5} \text{Tr }(A_i^3).$$

From the latter, we obtain

$$4(1 + 2a^3 - (a + d_1)^3 - (a + d_2)^3) \geq \sum_{i=1}^{5} p_i^3 + 5a^3 + \sum_{i=1}^{5} q_i^3 - \sum_{i=1}^{5} (a + c_i)^3$$

which gives, algebraically

$$\sum_{i=1}^{5} p_i^3 + \sum_{i=1}^{5} q_i^3 \leq 4 + 3a^3 - 4(a + d_1)^3 - 4(a + d_2)^3 + \sum_{i=1}^{5} (a + c_i)^3. \tag{1}$$

Via optimization, we also give a lower bound for $\sum_{i=1}^{5} p_i^3 + \sum_{i=1}^{5} q_i^3$, so that we can compare it to (1) and reach a contradiction, in certain cases.

As in the prior analysis, we will see that $q_i < 0$. Since $p_i \geq a + c_i$ by Perron-Frobenius, we put

$$p_i = a + c_i + t_i, \text{ with } t_i \in [0, 1 - a - c_i],\ i = 1, \ldots, 5.$$

Now

$$\text{Tr }(A_i) = p_i + q_i - c_i = a + t_i + q_i \geq 0.$$

Also $0 \leq a_{ii} = \text{Tr }(A) - \text{Tr }(A_i) = 1 - d_1 - d_2 - (a + t_i + q_i)$, from which we obtain

$$-(a + t_i) \leq q_i \leq -(a + t_i) + 1 - d_1 - d_2 = 1 - a - d_1 - d_2 - t_i < -t_i,$$

so that $q_i < 0$ and

$$q_i = -(a + t_i) + s_i, \text{ with } s_i \in [0, 1 - d_1 - d_2].$$

From $4\text{Tr }(A) = \sum_{i=1}^{5} \text{Tr }(A_i)$, we obtain

$$4(1 - d_1 - d_2) = \sum_{i=1}^{5} (a + t_i + q_i) = \sum_{i=1}^{5} s_i.$$

Next, we have

$$\sum_{i=1}^{5} p_i^3 + \sum_{i=1}^{5} q_i^3 = \sum_{i=1}^{5} (a + c_i + t_i)^3 + \sum_{i=1}^{5} (-(a + t_i) + s_i)^3.$$

Since $q_i < 0$, the minimum is attained when the q_i's are as disparate as possible, namely one $s_i = 0$ (say $s_1 = 0$) and for the other values of i, $s_i = 1 - d_1 - d_2$ (their upper bound). So,

$$\sum_{i=1}^{5} p_i^3 + \sum_{i=1}^{5} q_i^3 = \sum_{i=1}^{5} (a + c_i + t_i)^3 - (a + t_1)^3 - \sum_{i=2}^{5} (a + t_i - 1 + d_1 + d_2)^3.$$

This expression is a function of ten variables, $f(t_1,\dots,t_5,c_1,\dots,c_5)$, in the compact set C given by $t_i \in [0, 1-a-c_i]$ and $c_i \in [d_1, d_2]$. The partial derivatives with respect to the variables t_i are

$$\frac{\partial f}{\partial t_1} = 3(a+c_1+t_1)^2 - 3(a+t_1)^2,$$

$$\frac{\partial f}{\partial t_i} = 3(a+c_i+t_i)^2 - 3(a+t_i-1+d_1+d_2)^2,\ i=2,\dots,5.$$

Since $c_i > 0$ and $-1+d_i+d_2 < 0$, all these partial derivatives are positive, so there is no local extreme in the interior of the compact set C. As for the frontier of C, it is clear that

$$f(0,\dots,0,c_1,\dots,c_5) \le f(t_1,\dots,t_5,c_1,\dots,c_5),\ \text{ for all }\ (t_1,\dots,t_5),$$

and this fact is sufficient to continue with our argument. So

$$\min\left(\sum_{i=1}^{5} p_i^3 + \sum_{i=1}^{5} q_i^3\right) = \sum_{i=1}^{5}(a+c_i)^3 - a^3 - 4(a-1+d_1+d_2)^3. \tag{2}$$

Of course, the proposed spectrum cannot occur if (2) > (1), that is

$$\sum_{i=1}^{5}(a+c_i)^3 - a^3 - 4(a-1+d_1+d_2)^3 > 4+3a^3-4(a+d_1)^3-4(a+d_2)^3+\sum_{i=1}^{5}(a+c_i)^3$$

and, after algebraic reduction, we obtain

$$(a+d_1)^3+(a+d_2)^3 > 1+a^3+(a+d_1+d_2-1)^3,$$

the same condition as in the case $d_1=d_2=d$ studied in [3], see Theorem 1.

Theorem 3. *Let* $a, d_1 > 0$, $d_2 > d_1$ *satisfy* $a+d_2, d_1+d_2 < 1 < a+d_1+d_2$. *If* $(a+d_1)^3+(a+d_2)^3 > 1+a^3+(a+d_1+d_2-1)^3$, *then* $1, a, a, -(a+d_1), -(a+d_2)$ *are not the eigenvalues of a 5-by-5 symmetric nonnegative matrix.*

Note that the sections for a fixed a in d_1, d_2-space, under the hypothesis of Theorem 3, are:

- If $0 < a < \frac{1}{2}$, the interior of the polygon with vertices (see fig. 2 and fig. 3):

$$(0, 1-a),\left(\frac{1-a}{2},\frac{1-a}{2}\right),\left(\frac{1}{2},\frac{1}{2}\right)\ \text{ and }\ (a, 1-a).$$

- If $\frac{1}{2} \le a < 1$, the interior of the triangle with vertices (see fig. 2 and fig. 3):

$$(0, 1-a),\left(\frac{1-a}{2},\frac{1-a}{2}\right),\ \text{ and }\ (1-a, 1-a).$$

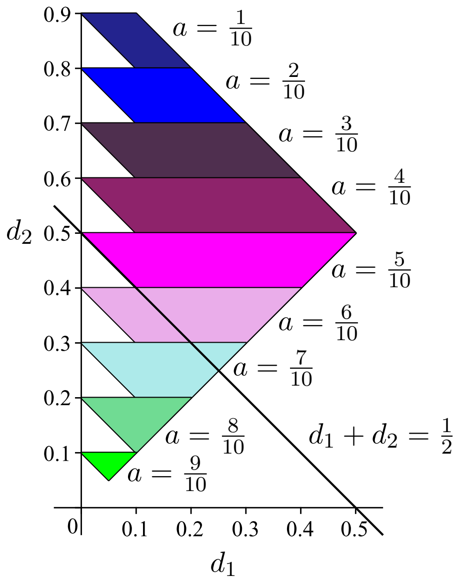

fig. 2: $d_1 d_2$-sections of the domain of Theorem 3, for $a = \frac{i}{10}$, $i = 1, \ldots, 9$.

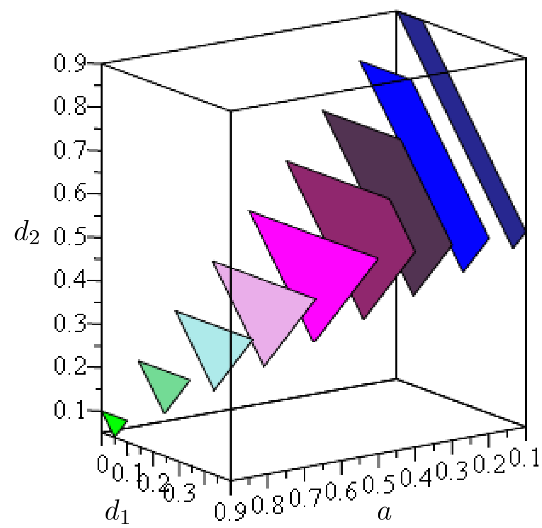

fig. 3: 3D-sections of the domain of Theorem 3, for $a = \frac{i}{10}$, $i = 1, \ldots, 9$.

The spectrum $1, a, a, -(a+d_1), -(a+d_2)$ under the hypothesis of Theorem 3, clearly satisfies conditions 1 and 2 but not 3 from Theorem 2. Note that in this case $\sum_{i=1}^{5} \lambda_i \geq \frac{\lambda_1}{2}$ leads us to $d_1 + d_2 \leq \frac{1}{2}$. Therefore, no spectrum corresponding to points under or on the plane $d_1 + d_2 = \frac{1}{2}$ is symmetrically realizable because of Theorem 2. From the sections in fig. 2, it is clear that for $a \leq \frac{1}{2}$ none of these spectra are in these circumstances, for $a \geq \frac{3}{4}$ none of these spectra are symmetrically realizable and for $\frac{1}{2} < a < \frac{3}{4}$, the ones under or on $d_1 + d_2 = \frac{1}{2}$ are not symmetrically realizable.

The spectrum $1, a, a, -(a+d_1), -(a+d_2)$ is symmetrically realizable with constant diagonal if and only if the translated spectrum, that has trace zero,

$$1 - \frac{1-d_1-d_2}{5}, a - \frac{1-d_1-d_2}{5}, a - \frac{1-d_1-d_2}{5}, -(a+d_1) - \frac{1-d_1-d_2}{5}, -(a+d_2) - \frac{1-d_1-d_2}{5}$$

is symmetrically realizable. The characterization [8] gives $F(a, d_1, d_2) \geq 0$ where

$$F(a, d_1, d_2) = \left(\frac{4+d_1+d_2}{5}\right)^3 + 2\left(\frac{5a-1+d_1+d_2}{5}\right)^3 + \left(\frac{d_2-5a-1-4d_1}{5}\right)^3 + \left(\frac{d_1-5a-1-4d_2}{5}\right)^3.$$

The Perron condition for the translated spectrum when $F(a, d_1, d_2) \geq 0$ is given in Appendix 1. The surface S_{cd} given in fig. 4 is that portion of the surface $S_{cd} \equiv F(a, d_1, d_2) = 0$ lying in the domain of Theorem 3. The points under or on S_{cd} are symmetrically realizable with constant diagonal. Notice then, see fig. 4, that for spectra under the hypothesis of Theorem 3 with $a \geq \frac{4}{10}$ this result is not applicable. In fact, considering the vertices of the 3D-polygonal sections, $\frac{3}{10} < a < \frac{4}{10}$, of the domain of Theorem 3 we have:

$$F(a, 0, 1-a) = -\frac{6a(3a^2+5)}{25} < 0$$

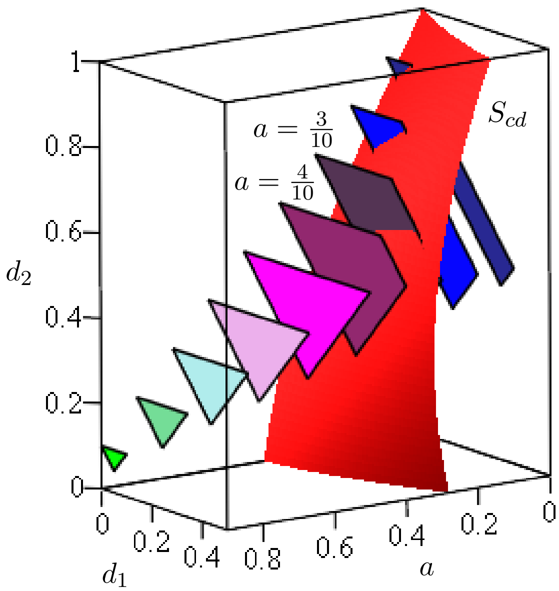

fig. 4: 3D-sections of the domain of Theorem 3, for $a = \frac{i}{10}$, $i = 1, \ldots, 9$ and that portion of S_{cd}, the border surface for constant diagonal symmetric realization, lying in the domain.

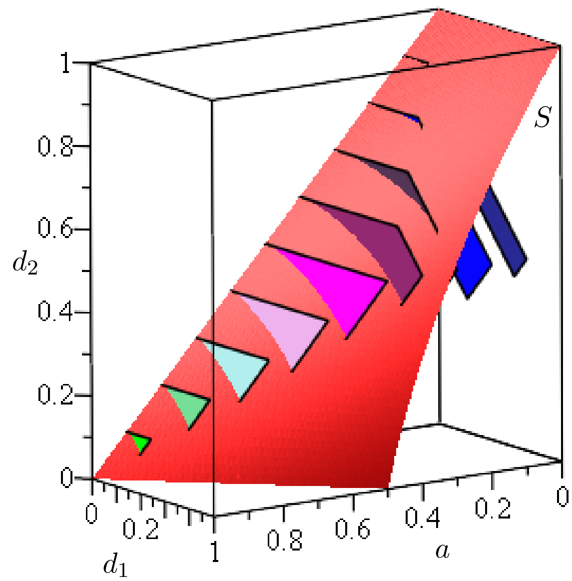

fig. 5: 3D-sections of the domain of Theorem 3, for $a = \frac{i}{10}$, $i = 1, \ldots, 9$ and that portion of the border surface $S \equiv (a+d_1)^3 + (a+d_2)^3 = 1 + a^3 + (a + d_1 + d_2 - 1)^3$ from Theorem 3 lying in the domain.

$$F\left(a, \frac{1-a}{2}, \frac{1-a}{2}\right) = \frac{3(a-5)(11a^2+10a-5)}{100} \begin{cases} > 0 \text{ if } a < \dfrac{4\sqrt{5}-5}{11} \approx 0.3585701734 \\ \leq 0 \text{ if } a \geq \dfrac{4\sqrt{5}-5}{11} \end{cases}$$

$$F\left(a, \frac{1}{2}, \frac{1}{2}\right) = \frac{3-6a-12a^2}{4} \begin{cases} > 0 \text{ if } a < \dfrac{\sqrt{5}-1}{4} \approx 0.3090169942 \\ \leq 0 \text{ if } a \geq \dfrac{\sqrt{5}-1}{4} \end{cases}$$

$$F(a, a, 1-a) = -6a^3 < 0.$$

Therefore for $a \geq \frac{4\sqrt{5}-5}{11}$ none of these spectra are in these circumstances and for $a < \frac{4\sqrt{5}-5}{11}$ the ones under or on S_{cd} are symmetrically realizable. See Appendix 2.

Fig. 5 shows the exclusionary surface S given by Theorem 3, that is that portion of the surface $S \equiv G(a, d_1, d_2) = 0$ lying in the domain of Theorem 3, where

$$G(a, d_1, d_2) = (a+d_1)^3 + (a+d_2)^3 - 1 - a^3 - (a + d_1 + d_2 - 1)^3.$$

No spectrum corresponding to points above it is symmetrically realizable. Note that there are always points of the domain of Theorem 3 above and under it. In fact, for the vertices of the sections of the domain of Theorem 3 we have:

$$G(a, 0, 1-a) = 0$$

$$G\left(a,\frac{1-a}{2},\frac{1-a}{2}\right) = -\frac{3(a+1)(a-1)^2}{4} < 0$$

$$G\left(a,\frac{1}{2},\frac{1}{2}\right) = \frac{12a^2+6a-3}{4}\begin{cases} \leq 0 \text{ if } a \leq \dfrac{\sqrt{5}-1}{4} \approx 0.3090169942 \\ > 0 \text{ if } a > \dfrac{\sqrt{5}-1}{4} \end{cases}$$

$$G(a,a,1-a) = 6a^3 > 0$$

$$G(a,1-a,1-a) = 3a(1-a) > 0.$$

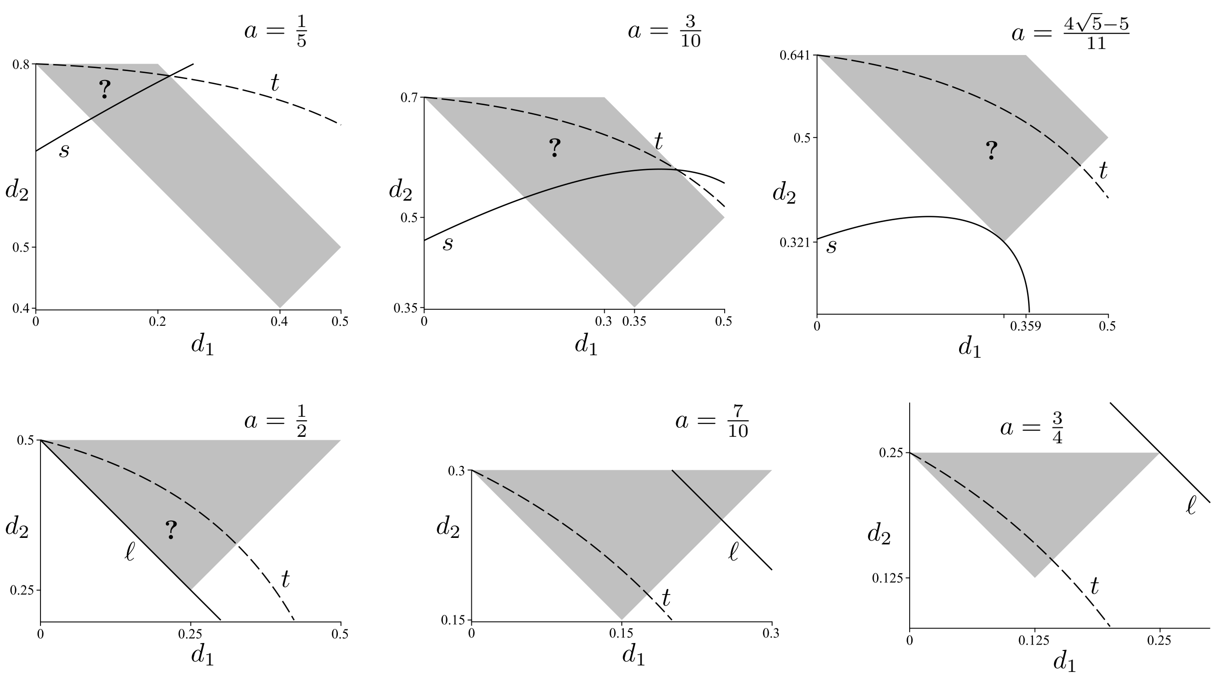

fig. 6: d_1d_2-sections of the domain of Theorem 3 with curve $s = S_{cd} \cap \{X = a\} \equiv F(a, d_1, d_2) = 0$, curve $t = S \cap \{X = a\} \equiv G(a, d_1, d_2) = 0$ and curve $\ell = \{d_1 + d_2 = \frac{1}{2}\} \cap \{X = a\}$ for $a \in \left\{\frac{1}{5}, \frac{3}{10}, \frac{4\sqrt{5}-5}{11}, \frac{1}{2}, \frac{7}{10}, \frac{3}{4}\right\}$.

In summary, for the spectra σ under the hyphotesis of Theorem 3 we have:

• If $a < \dfrac{4\sqrt{5}-5}{11}$, for some (d_1, d_2) the spectrum σ is symmetrically realizable with constant diagonal, those under or on curve s in fig. 6. And for others σ is not symmetrically realizable by Theorem 3, *e.g.* those above curve t in fig. 6. The question mark in fig. 6 means that the region between s and t (including t) is unresolved.

• If $\dfrac{4\sqrt{5}-5}{11} \leq a \leq \dfrac{1}{2}$, for some (d_1, d_2) the spectrum σ is not symmetrically realizable by Theorem 3, those above curve t in fig. 6. The question mark in fig. 6 means that the region under or on t is unresolved.

• If $\dfrac{1}{2} < a < \dfrac{3}{4}$, for some (d_1, d_2) the spectrum σ is not symmetrically realizable by Theorem 3, those above curve t, and for others neither because of Theorem 2, those under or on line ℓ in fig. 6.

Since all the section is covered between both, σ is not symmetrically realizable.

- If $a \geq \frac{3}{4}$, the spectrum σ is not symmetrically realizable by Theorem 2, see fig. 6 and fig. 2.

4 5-Spectra with a Repeated Negative Eigenvalue

Throughout this section, we consider 5-spectra of the form

$$1, a, a-r, -(a+d), -(a+d)$$

with $a > r > 0,\ d > 0,\ a+d < 1,$ and $1 < a+2d,$ as otherwise existence has been characterized [1]. Since the trace is $1-r-2d,$ we have $1 > r+2d,$ and, again the inequality may be taken to be strict, as trace 0 spectra have been characterized [8].

If these are the eigenvalues of a 5-by-5 symmetric nonnegative matrix $A = (a_{ij})$, then we suppose that the 4-by-4 principal submatrix A_i of A, resulting from deletion of row and column i, has eigenvalues

$$p_i, a_i, q_i, -(a+d), \quad i = 1, \dots, 5,$$

in which $p_i,\ 1 \geq p_i \geq a,$ is the Perron root, $a-r \leq a_i \leq a,$ and $-(a+d) \leq q_i < a-r,$ all because of interlacing. By Perron-Frobenius again, $p_i \geq a+d > a.$

We have $4\text{Tr }(A) = \sum_{i=1}^{5} \text{Tr }(A_i),$ and $4\text{Tr }(A^3) \geq \sum_{i=1}^{5} \text{Tr }(A_i^3).$ From the latter, we obtain

$$4(1+a^3+(a-r)^3-2(a+d)^3) \geq \sum_{i=1}^{5} p_i^3 + \sum_{i=1}^{5} a_i^3 + \sum_{i=1}^{5} q_i^3 - 5(a+d)^3$$

which gives

$$\sum_{i=1}^{5} p_i^3 + \sum_{i=1}^{5} q_i^3 \leq 4(1+a^3+(a-r)^3) - \sum_{i=1}^{5} a_i^3 - 3(a+d)^3. \tag{3}$$

Via optimization, we also give a lower bound for $\sum_{i=1}^{5} p_i^3 + \sum_{i=1}^{5} q_i^3,$ so that we can compare it to (3) and reach a contradiction in some cases, thereby ruling such cases out.

We will see that $q_i < 0.$ Since $p_i \geq a+d$ by Perron-Frobenius and since, for a given total weight among the p_i's, $\sum_{i=1}^{5} p_i^3$ is minimized when the p_i's are equal, we assume for minimization that

$$p_i = a+d+t, \ \text{ with } \ t \in [0, 1-a-d]$$

as was done in [3]. Now

$$\text{Tr }(A_i) = t + a_i + q_i \geq 0.$$

Also $0 \leq a_{ii} = \text{Tr }(A) - \text{Tr }(A_i) = 1-r-2d-(t+a_i+q_i)$ from which we obtain

$$-(a_i+t) \leq q_i \leq -(a_i+t)+1-r-2d = 1-a-2d+a-r-a_i-t,$$

so that $q_i < 0$ and

$$q_i = -(a_i+t)+s_i \ \text{ with } \ s_i \in [0, 1-r-2d].$$

From $4\text{Tr }(A) = \sum_{i=1}^{5} \text{Tr }(A_i)$, we obtain

$$4(1-r-2d) = \sum_{i=1}^{5}(t+a_i+q_i) = \sum_{i=1}^{5} s_i.$$

Next, we have

$$\sum_{i=1}^{5} p_i^3 + \sum_{i=1}^{5} q_i^3 = 5(a+d+t)^3 + \sum_{i=1}^{5}(s_i - (a_i+t))^3.$$

Since $q_i < 0$, the minimum is attained when the q_i's are as disparate as possible (as in the prior section), namely one $s_i = 0$ (say $s_1 = 0$) and for the other values of i, $s_i = 1-r-2d$ (their upper bound). So,

$$\sum_{i=1}^{5} p_i^3 + \sum_{i=1}^{5} q_i^3 = 5(a+d+t)^3 - (a_1+t)^3 + \sum_{i=2}^{5}(1-r-2d-(a_i+t))^3. \tag{4}$$

Differentiation with respect to t gives

$$15(a+d+t)^2 - 3(a_1+t)^2 - 3\sum_{i=2}^{5}(1-r-2d-(a_i+t))^2$$

and, since each of the 15 positive terms is greater than each 15 negative terms, the minimum of expression (4) occurs when $t = 0$. So we have

$$\min\left(\sum_{i=1}^{5} p_i^3 + \sum_{i=1}^{5} q_i^3\right) = 5(a+d)^3 - a_1^3 - \sum_{i=2}^{5}(a_i - (1-r-2d))^3. \tag{5}$$

Of course, the proposed spectrum cannot occur if (5) > (3), or, after algebraic reduction

$$8(a+d)^3 - 4\left(1 + a^3 + (a-r)^3\right) + \sum_{i=2}^{5} a_i^3 - \sum_{i=2}^{5}(a_i - (1-r-2d))^3 > 0. \tag{6}$$

Now, viewing the a_i's as variables ($(a-r) \le a_i \le a$) and because $a_i \ge a-r$ and $1 < a+2d$ we have $a_i > 1-r-2d = \text{Tr }(A) > 0$, and so all partial derivatives of (6) with respect to the variables a_i are positive. This means that the expression cannot be less than its evaluation at the left hand endpoint $a_i = a-r$. If it is positive, then nonexistence is clear, independently of the a_i's. This gives

$$2(a+d)^3 - (1 + a^3 + (a-r)^3) + (a-r)^3 - (a-(1-2d))^3 > 0$$

or

$$2(a+d)^3 > 1 + a^3 + (a+2d-1)^3,$$

the same condition as in the case $r = 0$ studied in [3], see Theorem 1.

Theorem 4. *The spectrum* $1, a, a-r, -(a+d), -(a+d)$ *with* $d, r > 0\,, a > r$ *and* $a+d, r+2d < 1 < a+2d$ *is not realizable by a symmetric nonnegative* 5*-by-*5 *matrix if*

$$2(a+d)^3 > 1 + a^3 + (a+2d-1)^3.$$

Note that the sections for a fixed a in d, r-space, under the hypothesis of Theorem 4, are:

- If $0 < a \leq \frac{1}{2}$, the interior of the triangle with vertices (see fig. 7 and fig. 8):

$$\left(\frac{1-a}{2}, 0\right), \left(\frac{1}{2}, 0\right) \quad \text{and} \quad \left(\frac{1-a}{2}, a\right).$$

- If $\frac{1}{2} < a < 1$, the interior of the polygon with vertices (see fig. 7 and fig. 8):

$$\left(\frac{1-a}{2}, 0\right), (1-a, 0), (1-a, 2a-1) \quad \text{and} \quad \left(\frac{1-a}{2}, a\right).$$

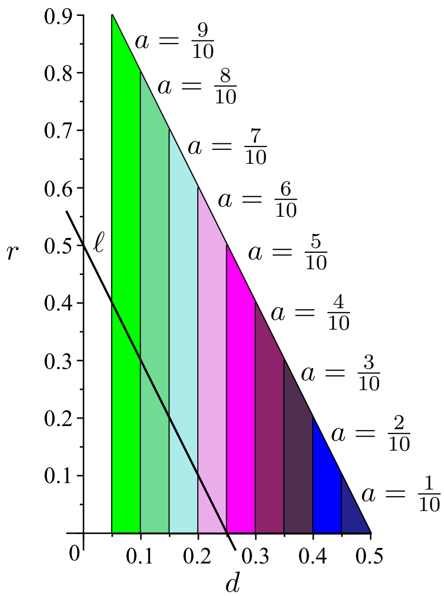

fig. 7: dr-sections of the domain of Theorem 4, for $a = \frac{i}{10}$, $i = 1, \ldots, 9$ and line $\ell \equiv r + 2d = \frac{1}{2}$.

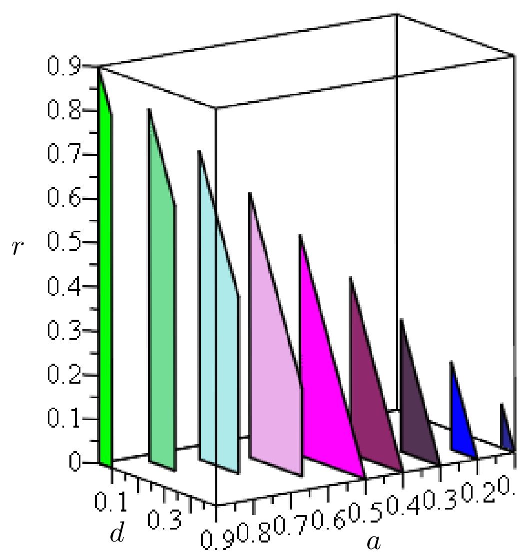

fig. 8: 3D-sections of the domain of Theorem 4, for $a = \frac{i}{10}$, $i = 1, \ldots, 9$.

The spectrum $1, a, a-r, -(a+d), -(a+d)$ under the hypothesis of Theorem 4, clearly satisfies conditions 1 and 2 but not 3 from Theorem 2. Note that in this case $\sum_{i=1}^{5} \lambda_i \geq \frac{\lambda_1}{2}$ leads us to $r + 2d \leq \frac{1}{2}$. Therefore, no spectrum corresponding to points under or on the plane $r + 2d = \frac{1}{2}$ is symmetrically realizable because of Theorem 2. From the sections in fig. 7, it is clear that for $a \leq \frac{1}{2}$ none of these spectra are in these circumstances and for $\frac{1}{2} < a$, the ones under or on $r + 2d = \frac{1}{2}$ are not symmetrically realizable.

The spectrum $1, a, a-r, -(a+d), -(a+d)$ is symmetrically realizable with constant diagonal if and only if the translated spectrum, that has trace zero,

$$1 - \frac{1-r-2d}{5}, a - \frac{1-r-2d}{5}, a - r - \frac{1-r-2d}{5}, -(a+d) - \frac{1-r-2d}{5}, -(a+d) - \frac{1-r-2d}{5}$$

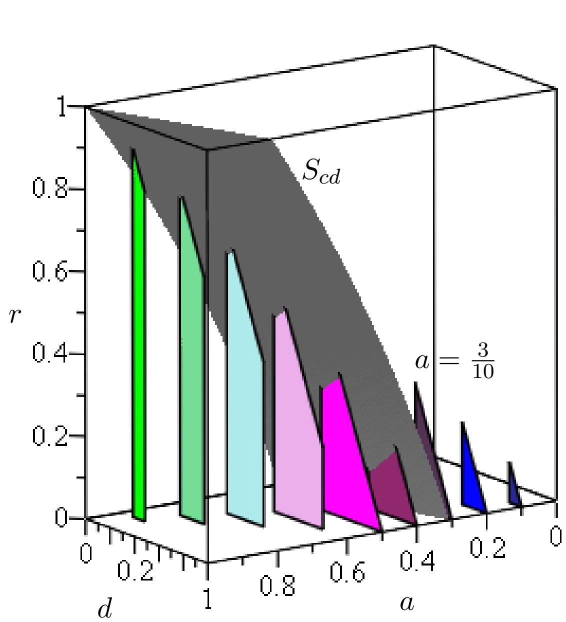

fig. 9: 3D-sections of the domain of Theorem 4, for $a = \frac{i}{10}$, $i = 1, \ldots, 9$ and that portion of S_{cd}, the border surface for constant diagonal symmetric realization, lying in the domain.

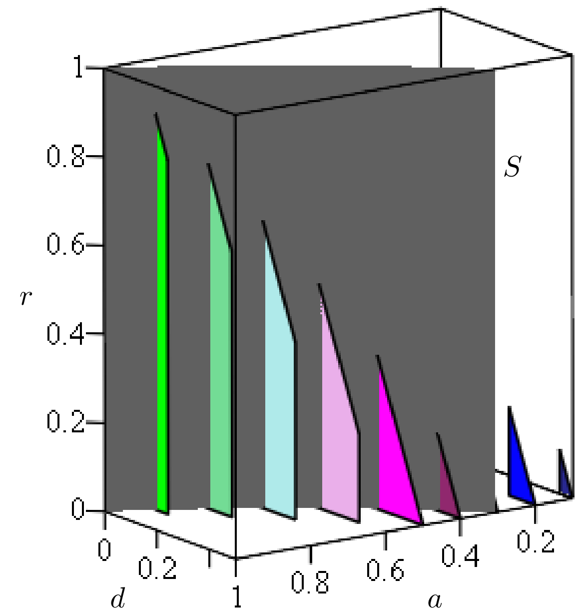

fig. 10: 3D-sections of the domain of Theorem 4, for $a = \frac{i}{10}$, $i = 1, \ldots, 9$ and that portion of the border surface $S \equiv 2(a+d)^3 = 1+a^3+(a+2d-1)^3$, from Theorem 4, lying in the domain.

is symmetrically realizable. The characterization [8] gives $H(a,d,r) \geq 0$ where

$$H(a,d,r) = \left(\frac{4+r+2d}{5}\right)^3 + \left(\frac{5a-1+r+2d}{5}\right)^3 + \left(\frac{5a-4r-1+2d}{5}\right)^3 + 2\left(\frac{r-5a-3d-1}{5}\right)^3.$$

The Perron condition for the translated spectrum when $H(a,d,r) \geq 0$ appears in Appendix 3. The surface S_{cd} given in fig. 9 is that portion of the surface $S_{cd} \equiv H(a,d,r) = 0$ lying in the domain of Theorem 4. The points above or on S_{cd} are symmetrically realizable with constant diagonal. Notice then, see fig. 9, that spectra under the hypothesis of Theorem 4 with $a \leq \frac{3}{10}$ are always symmetrically realizable with constant diagonal and for other a's we always have a region with realizable spectra that decreases as a increases. In fact, considering the vertices of the 3D-polygonal sections of the domain of Theorem 4 we have:

$$H\left(a, \frac{1-a}{2}, 0\right) = \frac{3(a-5)(11a^2+10a-5)}{100} \begin{cases} > 0 \text{ if } a < \dfrac{4\sqrt{5}-5}{11} \approx 0.3585701734 \\ \leq 0 \text{ if } a \geq \dfrac{4\sqrt{5}-5}{11} \end{cases}$$

$$H\left(a, \frac{1}{2}, 0\right) = \frac{3-6a-12a^2}{4} \begin{cases} > 0 \text{ if } a < \dfrac{\sqrt{5}-1}{4} \approx 0.3090169942 \\ \leq 0 \text{ if } a \geq \dfrac{\sqrt{5}-1}{4} \end{cases}$$

(It is a vertex for $a \leq \frac{1}{2}$)

$$
\begin{aligned}
H\left(a, \frac{1-a}{2}, a\right) &= \frac{3(a+1)(a-1)^2}{4} > 0 \\
H(a, 1-a, 0) &= \frac{6(a-3)(a^2+4a-1)}{25} \begin{cases} > 0 \text{ if } a < \sqrt{5}-2 \approx 0.236067977 \\ \leq 0 \text{ if } a \geq \sqrt{5}-2 \end{cases} \\
& \qquad \text{(It is a vertex for } a > \tfrac{1}{2}\text{)}
\end{aligned}
$$

$$
H(a, 1-a, 2a-1) = 3a(a-1) < 0 \qquad \text{(It is a vertex for } a > \tfrac{1}{2}\text{)}.
$$

Therefore the points $(a, \frac{1-a}{2}, a)$ are always above the surface S_{cd}, the points $(a, \frac{1-a}{2}, 0)$are above or on it if and only if $a \leq \frac{4\sqrt{5}-5}{11}$, the points $(a, \frac{1}{2}, 0)$ are above or on it if and only if $a \leq \frac{\sqrt{5}-1}{4}$ and the points $(a, 1-a, 0)$ and $(a, 1-a, 2a-1)$ are always under S_{cd}. So we can conclude that for $a \leq \frac{\sqrt{5}-1}{4}$ all the spectra are symmetrically realizable with constant diagonal. See Appendix 4.

Fig. 10 shows the exclusionary surface S given by Theorem 4, that is that portion of the surface $S \equiv J(a, d, r) = 0$ lying in the domain of Theorem 4, where

$$
J(a, d, r) = 2(a+d)^3 - 1 - a^3 - (a+2d-1)^3.
$$

No spectrum corresponding to points in front of it is symmetrically realizable. Note then, see fig. 10, that for the spectra under the hypothesis of Theorem 4 with $a \leq \frac{3}{10}$ the theorem is not applicable and for $a \geq \frac{4}{10}$ there are always points of the domain behind and in front of S. In fact, for the vertices of the sections of the domain of Theorem 4 we have:

$$
\begin{aligned}
J\left(a, \frac{1-a}{2}, 0\right) &= J\left(a, \frac{1-a}{2}, a\right) = -\frac{3(a+1)(a-1)^2}{4} < 0 \\
J\left(a, \frac{1}{2}, 0\right) &= \frac{12a^2+6a-3}{4} \begin{cases} \leq 0 \text{ if } a \leq \dfrac{\sqrt{5}-1}{4} \approx 0.3090169942 \\ > 0 \text{ if } a > \dfrac{\sqrt{5}-1}{4} \end{cases} \\
& \qquad \text{(It is a vertex for } a \leq \tfrac{1}{2}\text{)} \\
J(a, 1-a, 0) &= J(a, 1-a, 2a-1) = 3a(1-a) > 0 \qquad \text{(It is a vertex for } a > \tfrac{1}{2}\text{)}.
\end{aligned}
$$

Therefore for $a \leq \frac{\sqrt{5}-1}{4}$ none of these spectra satisfy Theorem 4. For $a > \frac{\sqrt{5}-1}{4}$, there are spectra, for which Theorem 4 is applicable, those in front of S. The others, for which it is not applicable, those behind, or on, S. See Appendix 5.

In summary, for the spectra σ under the hyphotesis of Theorem 4 we have:

- If $a \leq \frac{\sqrt{5}-1}{4}$, the spectrum σ is always symmetrically realizable with constant diagonal.
- If $\frac{\sqrt{5}-1}{4} < a \leq \frac{1}{2}$, for some (d, r) the spectrum σ is symmetrically realizable with constant diagonal, those above or on curve s in fig. 11. And for others σ is not symmetrically realizable by Theorem 4, *e.g.* those on the right hand side of curve t in fig. 11. The question mark in fig. 11 means that the region under s and on the left hand side of t (including t) is unresolved.
- If $a > \frac{1}{2}$, for some (d, r) the spectrum σ is symmetrically realizable with constant diagonal, those above or on curve s, for others σ is not symmetrically realizable by Theorem 4, *e.g.* those on

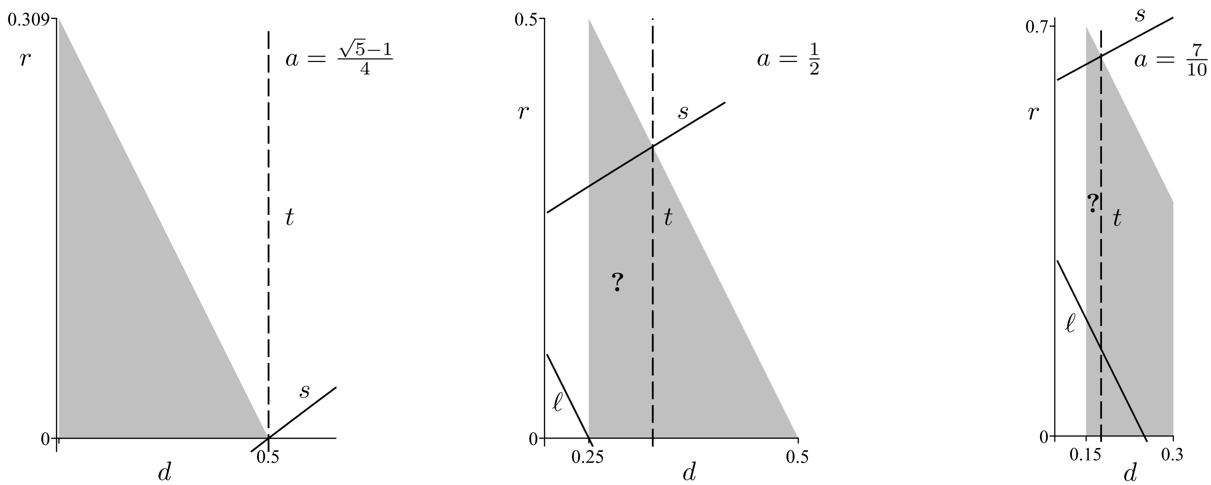

fig. 11: dr-sections of the domain of Theorem 4 with curve $s = S_{cd} \cap \{X = a\} \equiv H(a, d, r) = 0$, curve $t = S \cap \{X = a\} \equiv J(a, d, r) = 0$ and curve $\ell = \{r + 2d = \frac{1}{2}\} \cap \{X = a\}$ for $a \in \left\{\frac{\sqrt{5}-1}{4}, \frac{1}{2}, \frac{7}{10}\right\}$.

the right hand side of curve t, and for others neither because of Theorem 2, *e.g.* those under or on line ℓ in fig. 11. The question mark in fig. 11 means that the region among ℓ, t and s (including only t) is unresolved.

Appendix 1

Let a, d_1 and d_2 satisfy conditions of the domain of Theorem 3. If $F(a, d_1, d_2) \geq 0$, then $\lambda_1 + \lambda_5 = 1 - \frac{1-d_1-d_2}{5} - (a + d_2) - \frac{1-d_1-d_2}{5} = \frac{3-5a+2d_1-3d_2}{5} \geq 0$.

Proof: Observe that

$$\lambda_1 + \lambda_5 = \frac{3}{5} - a + \frac{2}{5}d_1 - \frac{3}{5}d_2 = \frac{3}{5}(1 - a - d_2) + \frac{2}{5}(d_1 - a) \geq 0 \quad \text{if} \quad d_1 \geq a.$$

Suppose then, that $d_1 < a$. Let us take for simplicity $d_1 = d, a = d + x$ and $d_2 = d + y$ with $x, y > 0$. The domain of Theorem 3 with these variables is: $2d + x + y < 1 < 3d + x + y$. If we assume $\lambda_1 + \lambda_5 = \frac{3-6d-5x-3y}{5} < 0$, that is $d > \frac{3-5x-3y}{6}$, we will arrive at the contradiction $F(a, d_1, d_2) = F(d + x, d, d + y) < 0$.

Note that $F(a, d_1, d_2) = F(d + x, d, d + y) = Ad^3 + Bd^2 + Cd + D$ with

$$A = -\frac{66}{25} < 0 \qquad C = -\frac{6\left(12y^2 + 2(5x + 3)y + 5x^2 + 30x - 3\right)}{25}$$

$$B = -\frac{90x + 54y + 126}{25} < 0 \qquad D = -\frac{12y^3 + 3(15x + 3)y^2 + 3(5x^2 + 10x - 3)y + 60x^2 - 12}{25}.$$

If $C \leq 0$ and $3 - 5x - 3y \geq 0$, we have

$$F(d + x, d, d + y) < F\left(\frac{3 - 5x - 3y}{6} + x, \frac{3 - 5x - 3y}{6}, \frac{3 - 5x - 3y}{6} + y\right) = -\frac{(3(1 - x - y) + 2x)^3}{36} < 0.$$

If $C > 0$ and $3 - 5x - 3y \geq 0$, then

$$F(d+x,d,d+y) < A\left(\frac{3-5x-3y}{6}\right)^3 + B\left(\frac{3-5x-3y}{6}\right)^2 + C\left(\frac{1-x-y}{2}\right) + D$$
$$= -\frac{\frac{335}{9}x^3 + 5(11y+53)x^2 + 3(7y^2+66y-33)x + 75(1-y)^3}{100}$$
$$< -\frac{5(11y+53)x^2 + 3(7y^2+66y-33)x + 75(1-y)^3}{100} < -\frac{5(53)x^2 + 3(7y^2+66y-33)x + 75(1-y)^3}{100}.$$

If $7y^2 + 66y - 33 \geq 0$, then $F(d+x,d,d+y) < 0$. Otherway

$$7y^2 + 66y - 33 = \frac{\left(7y+33-2\sqrt{330}\right)\left(7y+33+2\sqrt{330}\right)}{7} < 0 \iff y < \frac{2\sqrt{330}-33}{7} \approx 0.47 < \frac{1}{2},$$

and we have

$$F(d+x,d,d+y) < -\frac{5(53)x^2 + 3(-33)x + 75(1-1/2)^3}{100} = -\frac{265\left(x - \frac{99}{530}\right)^2 + \frac{273}{2120}}{100} < 0.$$

Finally, if $3 - 5x - 3y < 0$, then $C < 0$ and $D < 0$ since $x > 3(1-y)/5 > 0$ implies

$$C < -\frac{6\left(12y^2 + 2\left(5\left(\frac{3(1-y)}{5}\right)+3\right)y + 5\left(\frac{3(1-y)}{5}\right)^2 + 30\left(\frac{3(1-y)}{5}\right) - 3\right)}{25}$$
$$= -\frac{18}{125}\left[13\left(y - \frac{8}{13}\right)^2 + \frac{300}{13}\right] < 0$$

$$D < -\frac{12y^3 + 3\left(15\left(\frac{3(1-y)}{5}\right)+3\right)y^2 + 3\left(5\left(\frac{3(1-y)}{5}\right)^2 + 10\left(\frac{3(1-y)}{5}\right) - 3\right)y + 60\left(\frac{3(1-y)}{5}\right)^2 - 12}{25}$$
$$= -\frac{48(1-y)^3}{125} < 0$$

and hence $F(d+x,d,d+y) < 0$.

Appendix 2

$F(a,d_1,d_2) < 0$, for every d_1 and d_2 under the conditions of the domain of Theorem 3, if and only if $a > \frac{4\sqrt{5}-5}{11}$.

Proof: Let $\frac{1}{2} \leq a < 1$. A point of the domain is in the interior of the triangle with vertices $\left(a, \frac{1-a}{2}, \frac{1-a}{2}\right)$, $(a, 1-a, 1-a)$ and $(a, 0, 1-a)$, *i.e.*, it is a convex combination of its vertices:

$$x\left(a, \frac{1-a}{2}, \frac{1-a}{2}\right) + y(a, 1-a, 1-a) + (1-x-y)(a, 0, 1-a) = \left(a, \frac{(x+2y)(1-a)}{2}, \frac{(2-x)(1-a)}{2}\right)$$

with $0 < x, y < 1$ and $x + y < 1$. It can be seen that $F\left(a, \frac{(x+2y)(1-a)}{2}, \frac{(2-x)(1-a)}{2}\right) = Ax^2 + Bx + C$ with

$$\begin{aligned}
A &= -\frac{3(1-a)^2(5+7a+3(1-a)y)}{20} < 0 \\
B &= \frac{3(1-a)^2(y-1)(3(a-1)y-7a-5)}{10} > 0 \\
C &= \frac{6}{25}\left[(2y^3-9y^2+11y-3)a^3-(6y^3-18y^2+11y)a^2+(6y^3-9y^2-5y-5)a-(2y^3-5y)\right]
\end{aligned}$$

and the discriminant of this polynomial in x is

$$\frac{-27\left((1-a)^2y^2+8a(1-a)y+11a^2+10a-5\right)\left((\frac{7}{3}-y)a+y+\frac{5}{3}\right)(1-a)^2((1-a)y+5-a)}{500} < 0.$$

Because the discriminant is negative, the sign of $Ax^2 + Bx + C$ is the sign of $A < 0$ and we have $F(a, d_1, d_2) < 0$.

Let $0 < a < \frac{1}{2}$. A point of the domain is in the interior of the polygon with vertices $\left(a, \frac{1-a}{2}, \frac{1-a}{2}\right)$, $\left(a, \frac{1}{2}, \frac{1}{2}\right)$, $(a, a, 1-a)$ and $(a, 0, 1-a)$, *i.e.*, it is a convex combination of its vertices:

$$\begin{aligned}
x\left(a, \frac{1-a}{2}, \frac{1-a}{2}\right) + y\left(a, \frac{1}{2}, \frac{1}{2}\right) + z(a, a, 1-a) + (1-x-y-z)(a, 0, 1-a)& \\
= \left(a, \frac{(2z-x)a+x+y}{2}, \frac{(x+2y-2)a-x-y+2}{2}\right)&
\end{aligned}$$

with $0 < x, y, z < 1$ and $x + y + z < 1$. If $a < \frac{4\sqrt{5}-5}{11}$, we have seen that $F\left(a, \frac{1-a}{2}, \frac{1-a}{2}\right) > 0$, so because of the continuity of F there are points of the domain of Theorem 3 with $F(a, d_1, d_2) > 0$. Let $\frac{4\sqrt{5}-5}{11} \leq a < \frac{1}{2}$. It can be seen that $F\left(a, \frac{(2z-x)a+x+y}{2}, \frac{(x+2y-2)a-x-y+2}{2}\right) = Ax^2 + Bx + C$ with

$$\begin{aligned}
A &= -\frac{3(1-a)^2(5+(3y+3z+7)a)}{20} < 0 \\
B &= \frac{3(1-a)(1-y+(y-z-1)a)(5+(3y+3z+7)a)}{10} \\
-\frac{100C}{3} &= a(16a^2-30a+15)y^3 + (12(1-z)a^3+20a^2+15(z-3)a+25)y^2 \\
&\quad -2(2(3z^2+14z+13)a^3-5(3z^2+6z+11)a^2-10(z+2)a+25)y \\
&\quad +8a\left((2z+3)(z^2+3z+1)a^2+5(1-z)\right)
\end{aligned}$$

and the discriminant of this polynomial in x is

$$\frac{-9(5+(y+z-1)a)(5+(3y+3z+7)a)(1-a)^2((y^2+(2z+8)y+z^2+8z+11)a^2+10a-5)}{500}.$$

Therefore the sign of the discriminant is determined by the sign of the last factor

$$(y^2+(2z+8)y+z^2+8z+11)a^2+10a-5 > 11a^2+10a-5 \geq 0 \Longleftrightarrow a \geq \frac{4\sqrt{5}-5}{11}.$$

Then the discriminant is negative if $a \geq \frac{4\sqrt{5}-5}{11}$, the sign of $Ax^2 + Bx + C$ is the sign of $A < 0$ and we have $F(a, d_1, d_2) < 0$.

Appendix 3

Let a, d and r satisfy conditions of the domain of Theorem 4. If $H(a, d, r) \geq 0$, then $\lambda_1 + \lambda_5 = 1 - \frac{1-r-2d}{5} - (a + d) - \frac{1-r-2d}{5} = \frac{3-5a+2r-d}{5} \geq 0$.

Proof: Observe that

$$\lambda_1 + \lambda_5 = \frac{3}{5} - a + \frac{2}{5}r - \frac{1}{5}d = \frac{3}{5}(1 - a - d) + \frac{2}{5}(d - (a - r)) \geq 0 \quad \text{if} \quad d \geq a - r.$$

Suppose then, that $d < a - r$. Let us take for simplicity $x = a - r - d$ and $y = a - d$ with $0 < x < y < 1$. The domain of Theorem 4 with the variables x, y and d is: $2d + y < 1 < 3d + y$. If we assume $\lambda_1 + \lambda_5 = \frac{3-6d-2x-3y}{5} < 0$, that is $d > \frac{3-2x-3y}{6}$, we will arrive at the contradiction $H(a, d, r) = H(y + d, d, y - x) < 0$.

Note that $H(a, d, r) = H(y + d, d, y - x) = Ad^3 + Bd^2 + Cd + D$ with

$$A = -\frac{66}{25} < 0 \qquad C = \frac{3\left(21x^2 - 2(16y + 9)x + y^2 - 42y + 6\right)}{25}$$

$$B = -\frac{9(11y - x + 14)}{25} < 0 \qquad D = \frac{3\left(4x^3 - 3(1 - y)x^2 - (13y^2 + 4y + 3)x + 6y^3 - 13y^2 + 3y + 4\right)}{25}.$$

If $C \leq 0$ and $3 - 2x - 3y \geq 0$ we have

$$\begin{aligned} H(y + d, d, y - x) &< H\left(y + \frac{3 - 2x - 3y}{6}, \frac{3 - 2x - 3y}{6}, y - x\right) \\ &= -\frac{(3 - x)(3 - x + 3(y - x))(3(1 - y) + 2x)}{36} < 0. \end{aligned}$$

If $C > 0$ and $3 - 2x - 3y \geq 0$, or equivalently $y \leq (3 - 2x)/3$ then $x < y \leq (3 - 2x)/3$ implies $x < 3/5$ and we have

$$\begin{aligned} H(y + d, d, y - x) &< A\left(\frac{3 - 2x - 3y}{6}\right)^3 + B\left(\frac{3 - 2x - 3y}{6}\right)^2 + C\left(\frac{1}{2}\right) + D \\ &= \frac{1}{900}\left[54y^3 - 27(71x + 59)y^2 + 54(8x^2 - 71x + 6)y + 556x^3 - 198x^2 + 891x - 675\right] \\ &< \frac{1}{900}\left[54y^3 - 27(71x + 59)y^2 + 54(8x^2 - 71x + 6)y + 556(3/5)^3 - 198x^2 + 891(3/5) - 675\right] \\ &= \frac{1}{12500}\left[250x^2(24y - 11) - 26625xy(y + 2) + 3(250y^3 - 7375y^2 + 1500y - 94)\right] \\ &< \frac{1}{12500}\left[250x^2(24y - 11) - 26625x^2(y + 2) + 3(250y^2 - 7375y^2 + 1500y - 94)\right] \\ &= -\frac{125(165y + 448)x^2 + 21375\left(y - \frac{2}{19}\right)^2 + \frac{858}{19}}{12500} < 0. \end{aligned}$$

Finally, if $3-2x-3y<0$, then $C<0$ since $0<y<1$ and $y>(3-2x)/3>0$ implies

$$C < \frac{3\left(21x^2-2\left(16\left(\frac{3-2x}{3}\right)+9\right)x+1^2-42\left(\frac{3-2x}{3}\right)+6\right)}{25} = \frac{127x^2-66x-105}{25} < 0,$$

for $0<x<1$. Under the hypothesis of Theorem 4 we have $d>(1-y)/3>0$, and $3-2x-3y<0$ is equivalent to $x>3(1-y)/2$, so $3(1-y)/2<x<y$ implies $y>3/5$. Then

$$\begin{aligned}
H(y+d,d,y-x) &< H\left(y+\frac{1-y}{3},\frac{1-y}{3},y-x\right)\\
&= \frac{2\left(54x^3+54(1-y)x^2-9\left(3y^2+14y+13\right)x-(1-y)\left(38y^2+59y-7\right)\right)}{225}\\
&< \frac{2\left(54x^3+54\left(1-\frac{3-2x}{3}\right)x^2-9\left(3\left(\frac{3-2x}{3}\right)^2+14\left(\frac{3-2x}{3}\right)+13\right)x-(1-y)\left(38\left(\frac{3-2x}{3}\right)^2+59\left(\frac{3-2x}{3}\right)-7\right)\right)}{225}\\
&= \frac{4\left(351x^3+4(19y+116)x^2-405(y+2)x-405(1-y)\right)}{2025} < \frac{4x\left(351x^2+4(19y+116)x-405(y+2)\right)}{2025}\\
&< \frac{4x\left(351(1)^2+4(19(1)+116)1-405\left(\frac{3}{5}+2\right)\right)}{2025} = -\frac{8x}{25} < 0.
\end{aligned}$$

Appendix 4

$H(a,d,r)\geq 0$, for every d and r under the conditions of the domain of Theorem 4, if and only if $a\leq \frac{\sqrt{5}-1}{4}$.

Proof: If $\frac{1}{2}<a<1$, we have seen that $H(a,1-a,2a-1)<0$, so, because of the continuity of H, there are points of the domain of Theorem 4 with $H(a,d,r)<0$.

Let $0<a\leq\frac{1}{2}$. A point of the domain is in the interior of the triangle with vertices $\left(a,\frac{1}{2},0\right)$, $\left(a,\frac{1-a}{2},a\right)$ and $\left(a,\frac{1-a}{2},0\right)$, *i.e.*, it is a convex combination of its vertices:

$$x\left(a,\frac{1}{2},0\right)+y\left(a,\frac{1-a}{2},a\right)+(1-x-y)\left(a,\frac{1-a}{2},0\right)=\left(a,\frac{1+(x-1)a}{2},ay\right)$$

with $0<x,y<1$ and $x+y<1$. The minimum of H in the previous triangle is attained at $\left(a,\frac{1}{2},0\right)$ or $\left(a,\frac{1-a}{2},0\right)$ if and only if the minimum of $f_a(x,y)=H\left(a,\frac{1+(x-1)a}{2},ay\right)$ is attained at $(x,y)=(1,0)$ or $(x,y)=(0,0)$. Let us see first that f_a does not have critical points:

$$\begin{aligned}
\frac{\partial f_a}{\partial x}(x,y) &= \frac{3a}{100}\left[12a^2y^2+4a((x-1)a+5)y-(3x^2+14x+3)a^2-10(x+5)a+5\right]\\
\frac{\partial f_a}{\partial y}(x,y) &= \frac{3a}{50}\left[a^2x^2+2a((6y-1)a+5)x-(24y^2-48y+9)a^2+10a+15\right]
\end{aligned}$$

$$\frac{\partial f_a}{\partial x}(x,y)=0 \overset{y>0}{\iff} y=\frac{a(1-x)-5+\sqrt{10}\sqrt{(x^2+4x+1)a^2+2(2x+7)a+1}}{6a}:=y_0$$

$$\frac{\partial f_a}{\partial y}(x,y_0)=0 \overset{x\in\mathbb{R}}{\iff} x=-\frac{\sqrt{3}(1-a)+2(1+a)}{a}<0 \text{ or } x=-\frac{(2+\sqrt{3})a+2-\sqrt{3}}{a}<0.$$

Because both values of x are negative, f_a has no critical points. Now we study f_a on the sides of the triangle. On the one hand,

$$\begin{aligned}\frac{\partial f_a}{\partial y}(0,y) &= \frac{3a}{50}\left[15a^2+10a+15-24a^2(1-y)^2\right] \geq \frac{3a}{50}\left[15-24\left(\frac{1}{2}\right)^2(1-0)^2\right] > 0 \\ \frac{\partial f_a}{\partial x}(x,1-x) &= -\frac{3a}{4}(3ax+a+1)(a(1-x)+1) < 0.\end{aligned}$$

Therefore, the function f_a is a monotonous function on these sides of the triangle: the minimum of $f_a(0,y)$ is attained at $y=0$ and the minimum of $f_a(x,1-x)$ at $x=1$. On the other hand,

$$\frac{\partial f_a}{\partial x}(x,0) = \frac{-3a}{100}\left[3a^2x^2+2a(7a+5)x+3a^2+5(10a-1)\right] = 0 \overset{x>0}{\Longleftrightarrow} x = \frac{2\sqrt{10}-5-(7+2\sqrt{10})a}{3a} := x_0.$$

The function $f_a(x,0)$ has a critical point at x_0 if and only if $a \in \left(\frac{2\sqrt{10}-5}{10+2\sqrt{10}}, \frac{2\sqrt{10}-5}{7+2\sqrt{10}}\right)$, otherwise there is none. But

$$\begin{aligned}f_a(x_0,0)-f_a(0,0) &= \frac{(160\sqrt{10}+497)(-37a+65+16\sqrt{10})(-3a-25+8\sqrt{10})^2}{299700} > 0 \\ f_a(x_0,0)-f_a(1,0) &= \frac{(4\sqrt{10}+5)(-2a+7+2\sqrt{10})(-2a-3+\sqrt{10})^2}{180} > 0,\end{aligned}$$

and

$$\min(f_a(0,0),f_a(1,0)) = \begin{cases} f_a(0,0) & \text{if} \quad 0 < a < \frac{\sqrt{3245}-55}{22} \approx 0.089313703 \\ f_a(1,0) & \text{if} \quad \frac{\sqrt{3245}-55}{22} \leq a \leq \frac{1}{2}. \end{cases}$$

As a conclusion we have

$$H(a,d,r) \geq 0 \quad \forall (d,r) \Longleftrightarrow \begin{cases} H\left(a,\frac{1-a}{2},0\right) \geq 0 & \text{if} \quad 0 < a < \frac{\sqrt{3245}-55}{22} \\ \text{or} & \\ H\left(a,\frac{1}{2},0\right) \geq 0 & \text{if} \quad \frac{\sqrt{3245}-55}{22} \leq a \leq \frac{1}{2} \end{cases}.$$

Note that

$$H\left(a,\frac{1-a}{2},0\right) = \frac{3(a-5)(11a^2+10a-5)}{100} \geq 0 \Longleftrightarrow a \leq \frac{4\sqrt{5}-5}{11} \approx 0.3585701734$$

$$H\left(a,\frac{1}{2},0\right) = \frac{3-6a-12a^2}{4} \geq 0 \Longleftrightarrow a \leq \frac{\sqrt{5}-1}{4} \approx 0.3090169942.$$

Finally, we have

$$H(a,d,r) \geq 0 \quad \forall (d,r) \Longleftrightarrow a \leq \frac{\sqrt{5}-1}{4}.$$

Appendix 5

$J(a,d,r) \leq 0$, for every d and r under the conditions of the domain of Theorem 4, if and only if $a \leq \frac{\sqrt{5}-1}{4}$.

Proof: If $\frac{1}{2} < a < 1$, we have seen that $J(a,1-a,0) = 3a(1-a) > 0$, so, because of the continuity of J, there are points of the domain of Theorem 4 with $J(a,d,r) > 0$.

Let $0 < a \leq \frac{1}{2}$. A point of the domain is in the interior of the triangle with vertices $\left(a, \frac{1}{2}, 0\right)$, $\left(a, \frac{1-a}{2}, a\right)$ and $\left(a, \frac{1-a}{2}, 0\right)$. Let us see that the maximum of J in this triangle is attained at $(d, r) = \left(\frac{1}{2}, 0\right)$. There is no critical points in the interior of the triangle because

$$\frac{\partial J}{\partial d}(a, d, r) \;=\; 18(1-d)\left(d - \frac{1-2a}{3}\right) > 0 \quad \text{for} \quad d \in \left(\frac{1-a}{2}, \frac{1}{2}\right).$$

Now we study J on the sides of the triangle:

$$\begin{aligned} J\left(a, \frac{1-a}{2}, r\right) &= -\frac{3(a+1)(1-a)^2}{4} \qquad \text{it is constant} \\ \frac{\partial J}{\partial d}(a, d, 0) &= \frac{\partial J}{\partial d}(a, d, 1-2d) = 18(1-d)\left(d - \frac{1-2a}{3}\right) > 0 \quad \text{for} \quad d \in \left(\frac{1-a}{2}, \frac{1}{2}\right). \end{aligned}$$

Therefore, we need to compare the values:

$$J\left(a, \frac{1-a}{2}, r\right) = -\frac{3(a+1)(1-a)^2}{4}, \qquad \text{for } 0 \leq r \leq a,$$

and

$$J\left(a, \frac{1}{2}, 0\right) = \frac{12a^2 + 6a - 3}{4}.$$

It is easy to check that

$$-\frac{3(a+1)(1-a)^2}{4} < \frac{12a^2 + 6a - 3}{4}.$$

Then the maximum it is attained at $(d, r) = \left(\frac{1}{2}, 0\right)$. Finally, we have

$$J(a, d, r) \leq 0 \quad \forall (d, r) \Longleftrightarrow J\left(a, \frac{1}{2}, 0\right) \leq 0 \Longleftrightarrow a \leq \frac{\sqrt{5} - 1}{4}.$$

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