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G. Caporossi, D. Cvetković,
P. Rowlinson

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Gilles Caporossi

GERAD & HEC Montréal
Montréal (Québec) Canada, H3T 2A7

gilles.caporossi@gerad.ca

Dragoš Cvetković

Mathematical Institute SANU
11000 Belgrade, Serbia

ecvetkod@etf.rs

Peter Rowlinson

Mathematics and Statistics Group
Institute of Computing Science and Mathematics
University of Stirling
Stirling FK9 4LA, Scotland, UK

p.rowlinson@stirling.ac.uk

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Abstract: The Euclidean distance between the eigenvalue sequences of graphs G and H, on the same number of vertices, is called the *spectral distance* between G and H. This notion is the basis of a heuristic algorithm for reconstructing a graph with prescribed spectrum. By using a graph Γ constructed from cospectral graphs G and H, we can ensure that G and H are isomorphic if and only if the spectral distance between Γ and $G + K_2$ is zero. This construction is exploited to design a heuristic algorithm for testing graph isomorphism. We present preliminary experimental results obtained by implementing these algorithms in conjunction with a meta-heuristic known as a variable neighbourhood search.

Key Words: Spectral distance, graph angles, graph isomorphism, variable neighbourhood search.

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1 Introduction

The paper [8] surveys spectral recognition problems for graphs. Among the topics discussed are the spectral reconstruction problem, based on spectral distances between graphs, and the problem of defining a spectral distance between cospectral graphs.

The present paper offers an optimization approach to spectral distance between cospectral graphs and a heuristic algorithm for testing graph isomorphism. This algorithm and the spectral reconstruction problem are treated here in conjunction with a meta-heuristic known as a variable neighbourhood search (briefly, VNS). We present the first experimental results obtained by using AutoGraphiX (AGX), a programming package for finding graphs with extremal values of a graph invariant chosen by the user.

The rest of the paper is organized as follows. Section 2 discusses the spectral reconstruction problem. Some basic results on graph angles are presented in Section 3, while the graph isomorphism problem is treated in Section 4. Section 5 is devoted to experimental results and Section 6 contains tentative conclusions.

2 Spectral reconstruction

The Euclidean distance between the eigenvalue sequences of graphs G and H, on the same number of vertices, is called the *spectral distance* between G and H. Other spectral distances have also been considered, notably the Manhattan distance (the sum of absolute values of differences between ordered eigenvalues). Usually the eigenvalues are taken to be those of the adjacency matrix, but other graph matrices (such as the Laplacian or signless Laplacian) can be used.

Some mathematical results on the Manhattan spectral distance have been obtained in [16]. An interesting observation from that paper is that the Manhattan distance arises in connection with graph energy, a graph invariant much studied in the literature (see [17]). The *energy* of a graph is the sum of absolute values of its eigenvalues. Thus the energy of a graph is the Manhattan spectral distance of the graph from a graph without edges.

Use of the Laplacian and the signless Laplacian matrix in conjunction with the Manhattan distance seems to be very appropriate when considering subgraphs. By the interlacing theorems for these matrices (see [8, Section 5]), all eigenvalues decrease or remain the same when an edge is deleted from the graph. Hence the Manhattan distance between a graph and any of its edge-deleted subgraphs is equal to the decrement in the trace of the matrix. Since for both matrices the trace is equal to the sum of vertex degrees, we conclude that the distance is equal to the twice the number of deleted edges. None of these properties holds for the adjacency matrix.

If two graphs are at zero distance, they are not necessarily equal (i.e. isomorphic); they are merely cospectral. In the next section we introduce a metric which in some cases can distinguish cospectral graphs because the (new) distance between them is positive.

For several reasons it is of interest to construct or generate a graph with prescribed spectrum: see [5], where an algorithm for such a spectral graph reconstruction is presented. Given the spectrum of a graph, the algorithm starts from a random graph and uses the tabu search to reduce the Euclidean spectral distance between the given and the current spectrum. Both the metric and the meta-heuristic can be varied. One could use the Manhattan distance based on the adjacency matrix or on the signless Laplacian. The tabu search can be replaced by a variable neighbourhood search (see, for example, [3]) or by some other meta-heuristic.

The variable neighbourhood search is exploited in AGX for finding graphs with extremal values of a graph invariant chosen by the user. The system starts from a random graph or from a graph given by the user. This graph is perturbed to some extent using a variable neighbourhood search and a new graph is chosen which optimizes the invariant in question. The system AGX is very useful in formulating conjectures which are treated later by theoretical means. For example, it has generated several conjectures concerning the energy

of a graph [3] and thirty conjectures concerning signless Laplacian eigenvalues [12]. See also [1]. It would be interesting to use AGX to treat some conjectures from [16] concerning spectral distances between graphs.

The system AGX is used here for the spectral reconstruction of graphs. It is sufficient to require that the system minimizes the distance (of any kind) between the current graph and a fixed graph. One could compare the speed of convergence for several distances and for several meta-heuristics. (We do not give running times here since they are not directly relevant to our investigation.) More generally, computer programs for the spectral reconstruction of graphs can be used to generate examples of graphs with prescribed spectral properties.

3 The use of graph angles

Cospectral graphs are at spectral distance 0 and if we wish to define some kind of positive distance between them we can turn to graph invariants other than eigenvalues. Since eigenvectors are not graph invariants it is reasonable to extend eigenvalue based techniques by certain invariants of the eigenspaces called *graph angles*.

Let G be a graph on n vertices with distinct eigenvalues $\mu_1, \mu_2, \ldots, \mu_m$ $(\mu_1 > \mu_2 > \cdots > \mu_m)$ and let $S_1, S_2, \ldots, S_m$ be the corresponding eigenspaces. Let $\{e_1, e_2, \ldots, e_n\}$ be the standard (orthonormal) basis of R^n. The numbers $\alpha_{pq} = \cos\beta_{pq}$ $(p = 1, 2, \ldots, m; q = 1, 2, \ldots, n)$, where β_{pq} is the angle between S_p and e_q, are called *graph angles*. The sequence α_{pq} $(q = 1, 2, \ldots, n)$ is called the *eigenvalue angle sequence* corresponding to the eigenvalue μ_p $(p = 1, 2, \ldots, m)$. We also define the *angle matrix* of G as the $m \times n$ matrix (α_{ij}): here columns are ordered lexicographically, so that the matrix is a graph invariant. The rows of the angle matrix are called the *standard eigenvalue angle sequences*.

Let $x_i = (x_{i1}, x_{i2}, \ldots, x_{in})$ $(i = 1, 2, \ldots, n)$ be orthonormal eigenvectors of G. Define $M_p = \{j \mid Ax_j = \mu_p x_j\}$. We have $\alpha_{pq}^2 = \sum_{j \in M_p} x_{jq}^2$ for squares of angles of G, and this formula holds for any choice of orthonormal eigenvectors of G (cf. [11], p. 76). The angles between the vector $(1, 1, \ldots, 1)^\top \in \mathbf{R}^n$ and the eigenspaces $S_1, S_2, \ldots, S_m$ are called the *main angles* of the graph. Graph angles, like graph eigenvalues, can be computed in polynomial time. An overview of results on graph angles, and their relation to graph structure, is given in [11]. In particular, the number $c_4(G)$ of 4-cycles in G is given by

$$c_4(G) = \frac{1}{8} \sum_{i=1}^{m} \sum_{j=1}^{n} \alpha_{ij}^2 \mu_i^3 (\mu_i^2 + 1 - 2 \sum_{h=1}^{m} \alpha_{hj}^2 \mu_h^2). \tag{1}$$

It was suggested in [7] that cospectral graphs can be ordered by graph angles, in particular, lexicographically by their standard eigenvalue angle sequences. The paper provides an example of 21 cospectral graphs (on 10 vertices with 20 edges) ordered by the first standard eigenvalue angle sequences.

In defining a spectral graph distance we use differences between corresponding eigenvalues of two graphs. For each spectral graph distance we can define a corresponding *cospectral graph distance* by using differences between the corresponding entries of the angle matrix instead of differences between corresponding eigenvalues. For example, the *Manhattan cospectral graph distance* is the sum of absolute values of differences between the corresponding entries of the angle matrices of the graphs [8].

An alternative approach to distances between cospectral graphs will be described in the next section.

4 An optimization approach

Here we use network alignment techniques to define a distance between cospectral graphs. We note first that one can characterize graph isomorphisms in terms of eigenvalues. To be precise, let θ be a bijection $V(G) \to V(H)$, where G, H are disjoint finite graphs and $V(G)$ denotes the vertex-set of G. We define the *recognition graph* $\Gamma(G, \theta, H)$ as the graph consisting of G, H and the edges $\{v,\ \theta(v)\}$ $(v \in V(G))$. (The

terminology is suggested by a graph-theoretical model for pattern recognition formulated in [2].) With a suitable ordering of vertices, $\Gamma(G, \theta, H)$ has adjacency matrix $\begin{pmatrix} A & I \\ I & B \end{pmatrix}$, where A, B are adjacency matrices for G, H respectively. If θ is an isomorphism then $A = B$ and $\Gamma(G, \theta, H)$ has characteristic polynomial

$$\det((x+1)I - A)\det((x-1)I - A);$$

hence if $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of G then those of $\Gamma(G, \theta, H)$ are $\lambda_1 \pm 1,\ \lambda_2 \pm 1, \ldots, \lambda_n \pm 1$. The converse holds for cospectral graphs G, H: a proof of the following result from [19] is reproduced in [11, pp. 52-54].

Theorem. *Suppose that G, H are cospectral graphs, with common eigenvalues $\lambda_1, \ldots, \lambda_n$, and let θ be a bijection $V(G) \to V(H)$. Then θ is an isomorphism if and only if the eigenvalues of $\Gamma(G, \theta, H)$ are $\lambda_1 \pm 1, \ldots, \lambda_n \pm 1$.*

Of course, if G and H are not cospectral then there is no isomorphisim $\theta : V(G) \to V(H)$. We note in passing that if θ is an isomorphism then $\Gamma(G, \theta, H)$ is a NEPS (more precisely, the sum of graphs) as defined in [11].

It follows that if θ is "close" to an isomorphism then the spectral distance between Γ and $G+K_2$ is "small" because eigenvalues are perturbed. Now we can define the *cospectral distance* $\mathrm{cospd}(G, H)$ between cospectral graphs G and H as the minimum over all bijections θ of the spectral distance between $\Gamma(G, \theta, H), G)$ and $G + K_2$, i.e.

$$\mathrm{cospd}(G, H) = \min_{\theta} d(\Gamma(G, \theta, H), G + K_2).$$

Here we can use any "ordinary" spectral graph distance and for each of them we have a cospectral distance $\mathrm{cospd}(G, H)$ between cospectral graphs G and H.

A disadvantage of this definition is that one should solve an optimization problem in order to determine the distance. However, one can use meta-heuristics, and the situation is similar to that in the spectral reconstruction problems described in Section 2. In particular, if the distance $\mathrm{cospd}(G, H)$ is equal to 0, the graphs are isomorphic. Hence we have a heuristic algorithm for checking graph isomorphism.

The algorithm

Given graphs G and H:

- *check whether they are cospectral,*
  - *if no, they are non-isomorphic,*
  - *if yes, with eigenvalues $\lambda_1, \ldots, \lambda_n$, form the recognition graph $\Gamma(G, \theta, H)$ with a random bijection θ, compute its spectrum and the spectral distance from $\lambda_1 \pm 1,\ \lambda_2 \pm 1, \ldots, \lambda_n \pm 1$,*
- *using a meta-heuristic repeatedly change θ to diminish the distance $d(\Gamma(G, \theta, H), G+K_2)$ until it becomes 0 or the program has to be stopped.*

We may refine the algorithm by inserting an additional step to confine the heuristic to cospectral graphs with a common angle matrix. In this case, G and H have the same number of edges, say e, while Equation (1) shows that they have the same number of 4-cycles, say c. Note that if Z is a 4-cycle in $\Gamma(G, \theta, H)$ which does not lie in G or H then Z has two vertices in each of G and H. It follows that the number c_θ of 4-cycles in $\Gamma(G, \theta, H)$ is at most $2c + e$, with equality if and only if θ is an isomorphism. Now we have the option of maximizing c_θ by a variable neighbourhood search, calculating each c_θ from the angles of $\Gamma(G, \theta, H)$. The parameter $2c + e - \max_\theta c_\theta$ is an alternative measure of the "closeness" of G and H.

5 Experimental results

5.1 Spectral reconstruction

The package AGX was used for the reconstruction problem, the objective function being the distance between the spectrum of the current graph and the desired spectrum. The optimization algorithm used in AGX is based upon the VNS metaheuristic [15, 18]. The strategy of VNS is to alternate local searches and perturbations of variable magnitude; however, in AGX the local search is replaced by a learning descent that adapts the neighbourhoods used within the optimization algorithm according to the problem under study [4]. Let G^* be a graph with eigenvalues λ_i^* $(i = 1, \ldots, n)$ in non-increasing order. The spectral reconstruction problem is to find a graph G with eigenvalues $\lambda_1, \ldots, \lambda_n$ such that $\lambda_i^* = \lambda_i$ $(i = 1, \ldots, n)$. It may be formulated in AGX as :

$$\text{Min} \quad d(G^*, G) = (\sum_{i=1}^{n} |\lambda_i^* - \lambda_i|^p)^{\frac{1}{p}}, \tag{2}$$

where p is the Minkowski parameter; thus $p = 1$ for the Manhattan distance and $p = 2$ for the Euclidean distance.

Let M be a symmetric matrix (m_{ij}) with zero diagonal, and let $\Phi(M) = \text{diag}(\phi_1, \ldots, \phi_n)$, where $\phi_i = \sum_j m_{ij}$. We call $\Phi(M) - M$ the Laplacian of M, and $\Phi(M) + M$ the signless Laplacian of M. The Laplacian (or signless Laplacian) matrix of a graph G is just the Laplacian (or signless Laplacian) of the adjacency matrix of G. The distance matrix of G is the matrix $D = \{d_{ij}\}$, where d_{ij} is the geodesic distance between vertices i and j. The eigenvalues λ_i of G are most commonly computed from the adjacency matrix A, the Laplacian matrix L or the signless Laplacian matrix SL. We may also use the distance matrix D, its Laplacian LD or its signless Laplacian SLD.

The algorithm was tested using each of the aforementioned matrices, and with both Euclidean and Manhattan distances, for the graphs described in Table 1. Here, m is the number of edges, δ the minimum degree, Δ the maximum degree, and D the diameter. The path, cycle and star of order n are denoted by P_n, C_n and $K_{1,n-1}$ respectively. Other graphs are: a cubic graph on 12 vertices (Cu12), a 4-regular circulant graph on 12 vertices (R12C4), the hypercube on 16 vertices (H16), a cubic graph on 18 vertices (Cu18), a 4-regular circulant on 18 vertices and degree 4 (R18C4), three random graphs on 10 vertices (G10-1,G10-2, G10-3) and three random graphs on 12 vertices (G12-1, G12-2, G12-3). The lower triangular parts of the adjacency matrices of these random graphs are given in Table 2.

Table 1: Description of the graphs used.

	n	m	δ	Δ	D
P_{10}	10	9	1	2	9
$K_{1,9}$	10	9	1	9	2
C_{10}	10	10	2	2	5
G10-1	10	25	4	6	2
G10-2	10	23	3	6	3
G10-3	10	19	1	7	4
Cu12	12	18	3	3	3
R12C4	12	24	4	4	3
G12-1	12	28	2	8	3
G12-2	12	36	3	10	3
G12-3	12	35	3	8	3
H16	16	32	4	4	4
Cu18	18	27	3	3	5
R18C4	18	36	4	4	5
P_{20}	20	19	1	2	19
$K_{1,19}$	20	19	1	19	2
C_{20}	20	20	2	2	10

Table 2: Description of the random graphs used.

Graph	Adjacency matrix
G10-1	0 11 110 0011 11001 100001 1110101 11101000 000111110
G10-2	1 01 001 1100 01011 101010 0010011 00101011 010101101
G10-3	1 10 001 1010 10001 110000 0000000 10101000 110011111
G12-1	0 01 010 0000 11110 001001 0101100 00111010 100001010 1111011100 00100000101
G12-2	0 10 001 0110 00011 111010 1000010 10110001 110011001 1110100010 11101111111
G12-3	1 11 000 1011 11110 111110 1101110 01010101 000011011 0010101001 10000100100

Table 3: Results with AGX on the spectral reconstruction problem with Euclidean distance.

Euclidean	A	L	SL	D	LD	SLD
P_{10}	100	100	100	100	100	100
$K_{1,9}$	98	100	100	82	100	100
C_{10}	90	100	100	100	100	51
G10-1	96	25	98	81	96	90
G10-2	45	27	80	27	100	34
G10-3	63	97	100	85	73	90
Cu12	5	29	47	8	64	55
R12C4	41	89	100	9	97	78
G12-1	0	1	0	0	0	0
G12-2	0	1	0	0	0	0
G12-3	0	0	0	0	0	0
H16	0	0	20	0	0	0
Cu18	0	0	7	0	0	6
R18C4	0	2	2	0	30	29
P_{20}	100	100	100	100	100	100
$K_{1,19}$	80	100	100	36	35	59
C_{20}	15	100	100	25	3	7

One hundred runs were undertaken, involving 100,000 evaluations of the objective function and starting from a random graph. The number of successes is given in Tables 3 and 4.

5.2 Graph isomorphism

A routine based upon VNS was implemented within AGX to verify isomorphism.

After an appropriate permutation of rows and columns, the adjacency matrix of $\Gamma(G, \theta, H)$ can be written as $M_\Theta = \begin{pmatrix} A & \Theta \\ \Theta^T & B \end{pmatrix}$, where Θ is a permutation matrix. The use of the matrix Θ instead of I is a means of reducing the computations.

The graphs G and H, each with spectrum $\lambda_1, \ldots, \lambda_n$ are isomorphic if and only if there exists a permutation matrix Θ such that the matrix M_Θ has eigenvalues $\lambda_i + 1,\ \lambda_i - 1$ $(i = 1, \ldots, n)$. We order these eigenvalues as $\lambda_1^* \geq \cdots \geq \lambda_{2n}^*$ and denote this sequence by Λ^*. Thus G and H are isomorphic if and only if there exists a permutation matrix Θ such that M_Θ has eigenvalue sequence Λ^*. Thus the optimization problem can be formulated as:

$$\text{Min} \quad Z = (\sum_{i=1}^{2n} |\lambda_i^* - \lambda_i(M_\Theta)|^p)^{\frac{1}{p}}. \tag{3}$$

Table 4: Results with AGX on the spectral reconstruction problem with Manhattan distance.

Manhattan	A	L	SL	D	LD	SLD
P_{10}	100	100	100	100	100	100
$K_{1,9}$	100	100	100	100	100	82
C_{10}	100	100	100	100	100	74
G10-1	98	83	11	100	83	97
G10-2	44	29	69	44	94	40
G10-3	68	100	100	87	90	88
Cu12	2	16	79	1	81	47
R12C4	11	88	99	2	100	56
G12-1	0	0	0	0	0	0
G12-2	0	2	1	0	0	4
G12-3	0	0	0	0	0	0
H16	0	0	18	0	1	1
Cu18	0	0	4	0	0	2
R18C4	0	1	0	0	20	12
P_{20}	100	100	100	100	100	100
$K_{1,19}$	92	100	100	30	31	8
C_{20}	9	96	97	25	4	0

Problem (3) mirrors Problem (2), except that the optimization does not apply to the graph, but to the permutation matrix Θ. To take advantage of this matrix, the transformations to be considered in the optimization need to preserve the structure of a permutation matrix.

We used a local search which implements a variable neighbourhood descent (VND) with the transformation of the matrix Θ to a matrix in one of the 'neighbourhoods' $N_h(\Theta)$ $(h = 1, 2, 3, 4)$ obtained as follows. Each $N_h(\Theta)$ consist of all matrices obtained from Θ by applying a permutation of a certain form π_h to the columns. We take π_1 to be a transposition, π_2 to be the product of two disjoint transpositions. π_3 to be a 3-cycle, and π_4 to be a 4-cycle.

The rules of the routine VND(Θ) are as follows.

Routine VND(Θ)

Initialization:

Take $\Theta = I$.

Let $N_h(\Theta)$ $(h = 1, 2, 3, 4)$ be the set of neighborhoods of the solution Θ as defined above.

Main Step:

Set $h = 1$ and $imp = FALSE$ (improvement indicator);

Until $h = 4$, repeat the following steps :

(a) Find the best neighbour Θ' of Θ in $N_h(\Theta)$.

(b) If Θ' is better than Θ,

set $\Theta \leftarrow \Theta'$ and $imp = TRUE$.

Otherwise set $h \leftarrow h + 1$;

(c) if $h = 4$ and $imp = TRUE$

set $h = 1$ and $imp = FALSE$.

The VND algorithm may converge to a local optimum. To escape a local optimum, VND is used within a VNS scheme. The VNS implementation used was the following, where the perturbation routine PERTURB$_k(\Theta)$ applies k random transpositions of columns of Θ.

VNS implementation of the isomorphism algorithm

Initialization

Let $\Theta = I$ be the initial solution.

Let Z^* the best known objective function, and let Θ^* be the best known solution.

Let $k = 1$, set $k_{max} = 10$.

Let $c = 0$.

Repeat:

$\Theta \leftarrow \text{PERTURB}_k(\Theta^*)$

Apply VND(Θ)

Let Z be the value of the objective function after VND and let Θ be the solution.

If $Z < Z^*$

If $Z = 0$ *STOP*: the graphs are isomorphic

$Z^* \leftarrow Z$,

$\Theta^* \leftarrow \Theta$,

$k \leftarrow 1$

else

$k \leftarrow k + 1$

If $k \geq k_{max}$

$k \leftarrow 1$

$c \leftarrow c + 1$

Until $c = 10$.

A maximum number of evaluations of the objective function is given, so that the algorithm is terminated when the graphs are found to be isomorphic (the objective function value is 0), or when the maximum number of evaluations of the objective function is reached (100,000), or when $c = 10$.

For each graph G from Table 1 the algorithm was applied 100 times on graphs G and H, where H is a random relabelling of G. The results obtained with the algorithm are presented in Table 5. For each graph the number of successful detections of isomorphism is given.

Table 5: Results with AGX on the graph isomorphism problem.

Graph	Successes	Graph	Successes	Graph	Successes
P_{10}	64	Cu12	87	Cu18	13
$K_{1,9}$	100	R12C4	100	R18C4	74
C_{10}	100	G12-1	25	P_{20}	0
G10-1	70	G12-2	31	$K_{1,19}$	100
G10-2	50	G12-3	5	C_{20}	6
G10-3	84	H16	29		

The algorithm was also tested, using Manhattan distance, on pairs of non-isomorphic cospectral graphs G_1, G_2 described in [10] (with labels 164a, 164b etc.), and on pairs of isomorphic graphs (G_1, G_1'). Here G_1' is constructed from G_1 by randomly relabelling vertices (or swapping rows and columns of the adjacency matrix). For each test, the best objective function value (Value) was recorded, together with the number of evaluations of the objective function required to obtain this value. As there is an element of randomness in the algorithm, it was run 100 times on each pair of graphs. The results of these tests are reported in Table 6. The first two columns indicate the reference graphs used, columns 3 to 5 indicate the minimum, average and maximum number of evaluations of the objective function in the case that the test succeeded, and columns 6 to 8 indicate these values in the case of failure of the procedure. In all cases, the best objective function value

proved to be the cospectral distance between the two graphs, i.e. cospd($Graph1, Graph2$). Accordingly, the numbers of successes and failures among the 100 runs used are not provided.

Table 6: Results on isomorphic graphs and non-isomorphic cospectral graphs

Graph 1	Graph 2	Min S	Avg S	Max S	Min F	Avg F	Max F	Value
164a	164b	-	-	-	0	37.25	234	1.55088
164a	164a	9	9408.71	48091	-	-	-	0
165a	165b	-	-	-	9	4401.09	33358	1.94835
165a	165a	14	5527.18	39993	-	-	-	0
166a	166b	-	-	-	3	6813.39	43627	2.14076
166a	166a	19	7836.97	62036	-	-	-	0
167a	167b	-	-	-	16	11772	72180	1.68145
167a	167a	12	4098.77	22782	-	-	-	0
168a	168b	-	-	-	0	247.91	896	2.0721
168a	168a	8	5927	29491	-	-	-	0

The graphs used for these tests are pairs of cospectral graphs described in [10]. They are listed in Table 7, the first column providing the name of the graph, the second specifying the lower triangular part of the adjacency matrix, and the remaining columns giving the spectrum.

Table 7: Description of the graphs used for the results from Table 6.

Graph	Adjacency matrix	Spectrum			
164a	1 10 010 1010 01110 101110 1111011	4.6458	1.7321	0.0000	0.0000
164b	1 10 010 1010 01110 111101 1110110	−0.6458	−1.7321	−2.0000	−2.0000
165a	1 10 010 0010 10110 111101 1111111	5.0884	1.0883	0.2467	0.0000
165b	1 10 010 1000 10111 111101 1111011	−1.0000	−1.6693	−1.7451	−2.0000
166a	1 10 010 1010 01110 101110 1111111	4.9095	1.6093	0.0000	0.0000
166b	1 10 010 1010 11010 111110 1011111	−1.0000	−1.5188	−2.0000	−2.0000
167a	1 10 010 0010 10110 111111 1111111	5.2588	1.0000	0.2518	0.0000
167b	1 10 010 1000 10111 111101 1111111	−1.0000	−1.5106	−2.0000	−2.0000
168a	1 10 010 1011 01110 111111 1111111	5.6056	1.0000	0.0000	0.0000
168b	1 10 010 1011 11011 111110 1111111	−1.0000	−1.6056	−2.0000	−2.0000

6 Conclusions

The tests for spectral reconstruction tend to show that the performance of the adjacency or the distance matrices is rather poor. It seems that the signless Laplacian matrix performs better than the Laplacian matrix, but the Laplacian of the distance matrix performs better than the signless Laplacian of the distance matrix, and the overall best matrix seems to be the Laplacian of the distance matrix. However these conclusions are tentative because results vary from graph to graph. As the complexity of building the distance matrix is higher than that for the adjacency matrix, a reasonable choice for spectral reconstruction seems to be the use of the signless Laplacian matrix. For this matrix, Euclidean distance appears to perform slightly better than Manhattan distance. It is interesting to note that the path P_n and the star $K_{1,n-1}$ seem rather easy to reconstruct, while this is not the case for other graphs.

The results for isomorphism testing are more encouraging. Indeed, in the case of isomorphic graphs, an isomorphism was found in about 5,000–10,000 evaluations of the objective function, and this compares favourably with the 40,320 possible permutations for graphs on 8 vertices, even though the algorithm was not designed to avoid multiple evaluations of the same configuration. We are not surprised to see that graphs with higher symmetry, such as the star $K_{1,n-1}$, are easier to test, since the search space is smaller in this case.

These conclusions are tentative. One should explain theoretically some of the results obtained, and also perform additional experiments.

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