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Reconstruction of Weighted Graphs by their Spectrum

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It will be shown that for almost all weights one can reconstruct a weighted graph from its spectrum. This result is the opposite to the well-known theorem of Botti and Merris which states that reconstruction of non-weighted graphs is, in general, impossible since almost all (non-weighted) trees share their spectrum with another non-isomorphic tree.

1. NOTATIONS AND INTRODUCTION

A weighted graph G is a pair (A, M), where $A = (A_{ij})$ is a symmetric real $n \times n$ matrix with $A_{ii} = 0$, called an adjacency matrix, and where the mass matrix $M = \operatorname{diag}(m_1, \dots, m_n)$ is a real diagonal $n \times n$ matrix. The valence matrix D of G is defined to be the diagonal $n \times n$ matrix with

$$D_{ii} = \sum_{j=1}^{n} A_{ij} =: d_i.$$

If all masses m_i are equal to 1 and if $A_{ij} \in \{0, 1\}$ for all i, j, then G is just a simple graph and D is its vertex degree matrix. If the masses m_i are positive and all $A_{ij} \geq 0$, we consider G as a model for a molecule consisting of n atoms with weights m_i and with A_{ij} being the elasticity constant of the chemical binding between m_i and m_j; that is, if $v_i(t)$ denotes the scalar deviation of m_i at time t from its normal position, we have for every i

$$-m_i \ddot{v}_i = \sum_{j=1}^{n} A_{ij}(v_i - v_j) = v_i D_{ii} - \sum_{j=1}^{n} A_{ij} v_j.$$

Hence, an eigenvibration $v_j(t) = u_j e^{i\omega t}$, $j = 1, \dots, n$, of the molecule satisfies (in matrix notation)

$$\omega^2 M u = Du - Au,$$

where u is the vector $(u_1, \dots, u_n)$. In other words, the negative squares $-\omega^2 = \lambda$ of the eigenfrequencies of the molecule are the spectrum of the (generalized) eigenvalue problem

$$\det(A - D - \lambda M) = 0.$$

Alternatively, we could regard this as a discrete model of an inhomogeneous drum consisting of n vertices bearing weights m_i and with A_{ij} being the elasticity constant between m_i and m_j. Such a discrete model can, for example, arise from discretizing the corresponding continuous problem for a numerical treatment.

Let us have a quick look at the case of simple graphs when all m_i and all non-zero A_{ij} equal 1. The adjacency spectrum of a simple graph G, i.e., the eigenvalue spectrum of the adjacency matrix A, is widely studied (see e.g., [3] as a main reference). Non-isomorphic graphs (i.e., graphs whose adjacency matrices are not permutation similar) affording the same (adjacency) characteristic polynomial are called cospectral. Schwenk showed in [16] that almost all trees are cospectral. On the other hand, the operator $L = L(G) := A - D$ is the so-called Laplace or Kirchhoff operator of G (Laplace operator because it is the discrete analogue of the Laplace differential operator, and Kirchhoff operator since L first occurred in the

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well-known matrix-tree theorem of G. Kirchhoff). In how far the spectrum of L reflects the spectral properties of molecules is discussed in [4,5] and [8]. The relation between a simple graph and its Laplace spectrum is studied, e.g., in [6,7,13] and [15]. As a general reference for recent results on spectral graph theory see [2]. One of the most striking results is the theorem of Botti and Merris (see [1]) which generalizes the results of Schwenk [16], McKay [12] and Turner [17].

THEOREM 1 (BOTTI–MERRIS). *Let t_n be the number of non-isomorphic trees on n vertices and s_n the number of such trees T for which there exists a non-isomorphic tree $\tilde{T}$ such that the polynomial identities*

$$d_\chi(yA(T) + zD(T) - xI) \equiv d_\chi(yA(\tilde{T}) + zD(\tilde{T}) - xI)$$

in the three variables x, y and z hold, simultaneously, for every irreducible character χ of the symmetric group S_n. Then $\lim_{n\to\infty} s_n/t_n = 1$.

Here, I is the identity and d_χ denotes the *immanent*

$$d_\chi(B) = \sum_{p\in S_n} \chi(p) \prod_{i=1}^{n} b_{ip(i)}, \tag{1}$$

where $B = (b_{ij})$ is an $n \times n$ matrix (e.g., for $\chi = \varepsilon$, the alternating character, $d_\chi = \det$).

Techniques which are based on Sunada's trace theorem have recently allowed the generation of isospectral simple graphs which are not necessarily trees, see [9].

The results in [1] and [9] seem to indicate that, in general, it is impossible to reconstruct the structure of a molecule from its spectrum. However, we will see below that the case of weighted graphs offers the possibility of a reconstruction.

We will always identify the vector $m \in \mathbb{R}^n$ with the mass matrix $M(m) = \operatorname{diag}(m)$. For given $m \in \mathbb{R}^n$ and a countable set $\mathcal{A} \subset \mathbb{R}$ we denote by $\mathcal{G}_{\mathcal{A},M(m)}$ the set of weighted graphs $G = (A, M(m))$ with $A = (A_{ij})$, $0 \le A_{ij} \in \mathcal{A}$, and we will say G is a graph over $\mathcal{A}$ and $M(m)$.

In this paper we look at the following problem: given $m = (m_1, \ldots, m_n) \in \mathbb{R}^n_+$, $\mathcal{A} \subset \mathbb{R}$ countable (e.g., $\mathcal{A} = \{0, 1\}$ in the simplest case) and the Laplace spectrum $\{x \in \mathbb{R} : \det(L - xM(m)) = 0\}$ of a graph $(A, M(m)) \in \mathcal{G}_{\mathcal{A},M(m)}$; can you then compute the adjacency matrix A from this information? The naive answer would be just to compare the spectrum of every possible graph with the given spectrum. However, first, this only works for a finite set $\mathcal{A}$, second, the number of simple graphs on n vertices grows superexponentially in n and hence the method is not practicable, and third, it does not answer the question for which set of mass matrices (depending on $\mathcal{A}$) the map $A \mapsto \{x \in \mathbb{R} : \det(L - xM(m)) = 0\}$ is injective. The aim of this paper is to discuss conditions on the mass matrix $M(m)$ such that the answer to this question is affirmative and to describe reconstruction algorithms. In Section 2 we will discuss the case $\mathcal{A} = \{0, 1\}$ with a very strong growth condition on the masses m_i which implies that reconstruction of the graph from its spectrum is possible, and in Section 4 we will consider a general countable set $\mathcal{A}$ and an algebraic condition which shows that for almost all mass matrices (in a sense that will be made precise) reconstruction of the adjacency matrix A is possible.

The conditions we give for reconstructability of weighted graphs are sufficient, but certainly far from being necessary. Therefore—although it seems not to be realistic to apply our results directly to real molecules, since the masses of the atoms of a molecule might not satisfy the growth or the algebraic condition we use—the given reconstruction results at least show that reconstructability is a phenomenon that does occur for weighted graphs. Thus, whether in concrete situations reconstruction is possible or not may be a matter of a more detailed analysis adapted to the case at hand.

2. THE LAPLACE SPECTRUM OF WEIGHTED GRAPHS

In this section all non-zero A_{ij} are assumed to be 1, i.e., we consider the case $\mathcal{A} = \{0, 1\}$, and we ask for a condition on the mass matrix M which allows us to decide which masses are linked in a graph whose Laplace spectrum is known.

THEOREM 2. *There exist mass matrices $M_0 = \operatorname{diag}(m_1, \ldots, m_n)$ such that the following is true: let $G = (A, M)$ and $\tilde{G} = (\tilde{A}, \tilde{M})$ be weighted graphs over $\mathcal{A} = \{0, 1\}$ such that M and $\tilde{M}$ are permutation similar to M_0, then*

$$\det(L(G) - xM) \equiv \det(L(\tilde{G}) - x\tilde{M}) \tag{2}$$

holds if and only if G and $\tilde{G}$ are isomorphic graphs, i.e., $A = P\tilde{A}P^{-1}$ and $M = P\tilde{M}P^{-1}$ holds for a permutation matrix P. A possible choice is $m_i = n^{(2^i)}$.

REMARK. The proof will be constructive and provide an 'algorithm' to reconstruct the adjacency matrix A from the roots of the polynomial $\det(L - xM)$.

The proof of Theorem 2 is based upon the following two elementary lemmas.

LEMMA 1. *Let $q_1, \ldots, q_n$ be a sequence of real numbers of at least geometric growth with constant $s > 1$, i.e., $q_i \geq sq_{i-1}$ for $i = 2, \ldots, n$, and $q_1 > 0$. Then*

$$\sum_{i=1}^{n} \delta_i q_i = \sum_{i=1}^{n} \tilde{\delta}_i q_i \tag{3}$$

implies $\delta_i = \tilde{\delta}_i$ for $i = 1, \ldots, n$, provided that all $\delta_i \in \{0, 1, \ldots, \lfloor s - 1 \rfloor\}$.

PROOF. We proceed by induction: for $n = 1$ the assertion is trivial. On the other hand, using (3) we have for $n > 1$

$$\begin{aligned} (\delta_n - \tilde{\delta}_n)q_n &= \sum_{i=1}^{n-1} (\tilde{\delta}_i - \delta_i)q_i \qquad (4)\\ &\leq (s-1)\sum_{i=1}^{n-1} q_i \\ &\leq (s-1)\sum_{i=1}^{n-1} q_n \frac{1}{s^{n-i}} \\ &= q_n\left(1 - \frac{1}{s^{n-1}}\right) \\ &= q_n\varepsilon \end{aligned}$$

for an $\varepsilon < 1$. We may assume that $\delta_n \geq \tilde{\delta}_n$ and hence we obtain from (4)

$$0 \leq \delta_n - \tilde{\delta}_n < 1.$$

Thus $\delta_n = \tilde{\delta}_n$ and the assertion follows by induction. □

The second lemma we need in the proof of Theorem 2 is the following.

LEMMA 2. *Let* $\mu_i = \nu^{(2^i)}$ *for some* $\nu > 0$ *and for* $i = 1, \dots, n$. *Then the set of the numbers*

$$q_{ij} = \frac{1}{\mu_i \mu_j} \prod_{k=1}^{n} \mu_k$$

with $i \neq j$ *rearranged as a growing sequence has at least geometric growth with constant* ν.

PROOF. Consider $a = \frac{q_{ij}}{q_{lm}}$ for $\{i, j\} \neq \{l, m\}$. We have $a = \frac{\mu_l \mu_m}{\mu_i \mu_j} = \nu^{2^l + 2^m - 2^i - 2^j}$ and therefore the proof is complete if we can show that the exponent $2^l + 2^m - 2^i - 2^j \neq 0$. However, this follows from Lemma 1 since $2^l + 2^m = 2^i + 2^j$ would imply $\{l, m\} = \{i, j\}$ which contradicts the assumption. □

Now we give the proof of Theorem 2.

PROOF. We may assume that the vertex sets of G and $\tilde{G}$ are already renumbered in such a way that $M = \tilde{M} = M_0$. Using (1) we easily find the following expansion

$$\det(L - xM) = \begin{vmatrix} -d_1 - xm_1 & A_{12} & A_{13} & \dots & A_{1n} \\ A_{21} & -d_2 - xm_2 & A_{23} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & & \vdots \\ A_{n1} & A_{n2} & \dots & \dots & -d_n - xm_n \end{vmatrix} \tag{5}$$

$$= (-1)^n x^n \prod_{i=1}^{n} m_i + (-1)^n x^{n-1} \sum_{i=1}^{n} d_i \prod_{j \neq i} m_j$$
$$+ (-1)^n x^{n-2} \sum_{i<j} (d_i d_j - A_{ij}^2) \prod_{k \notin \{i,j\}} m_k + \dots + \det(L).$$

Now we use expansion (5) in identity (2). Comparing the coefficients of x^{n-1} on both sides we conclude by Lemma 1 that

$$d_i = \tilde{d}_i \qquad (i = 1, \dots, n) \tag{6}$$

since by our assumption on the masses m_i the ordered set of numbers $q_i = \prod_{j \neq i} m_j$ is at least of geometric growth with constant n and $d_i \in \{0, 1, \dots, n-1\}$. Note that by the theorem of Botti and Merris this cannot yet imply that the graphs G and $\tilde{G}$ are isomorphic.

Comparing the coefficients of x^{n-2} and using (6) we obtain

$$\sum_{i<j} A_{ij} \prod_{k \notin \{i,j\}} m_k = \sum_{i<j} \tilde{A}_{ij} \prod_{k \notin \{i,j\}} m_k.$$

The numbers $q_{ij} = \prod_{k \notin \{i,j\}} m_k$ obviously satisfy the hypothesis of Lemma 2 with $\nu = n$ and hence we conclude (by applying Lemma 1 once more with $s = 2$) that $A_{ij} = \tilde{A}_{ij}$ and the proof is complete. □

Up to now, we have considered two graphs as isospectral if they share the polynomial $\det(L - xM)$, i.e., the eigenvalues of both graphs coincide *counted with multiplicity*. Now we will show that even if we only require that two graphs have the same spectrum *as sets* they are isomorphic.

Let us consider a connected weighted graph G with masses $m_i = n^{(2^i)}$ as in Theorem 2. Then the following proposition claims that the eigenvalues of the Laplace spectrum of G are simple.

PROPOSITION 1. *Suppose* $\mathcal{A} = \{0, 1\}$ *and let* $G \in \mathcal{G}_{\mathcal{A},M(m)}$ *be a connected weighted graph with masses* $m_i = n^{(2^i)}$, $i = 1, \dots, n$. *Then the roots of the characteristic polynomial* $\det(L - xM(m))$ *are simple.*

PROOF. Let $p(x) = (-1)^n \det(L - xM) = a_n x^n + \cdots + a_2 x^2 + a_1 x + a_0$. Since all roots $\lambda_i = -\omega_i^2$ of p are negative real numbers, we have

$$a_k \geq 0 \qquad \text{for } k = 0, \dots, n. \tag{7}$$

From (1) we obtain for $k = 0, \dots, n$

$$a_k = \sum_{|I|=k} \det(L_I) \prod_{j \in I} m_j, \tag{8}$$

where the sum is taken over all ordered subsets I of $\{1, \dots, n\}$ of cardinality k and where L_I denotes the matrix obtained from L by deleting all rows and columns having a number in I. Of course, since the sum of the rows in L is zero, $a_0 = \det(L) = 0$.

Now, observe first that

$$|\det(L_I)| \leq n^{n-k} \tag{9}$$

for $|I| = k$. This follows from the fact that every column of L_I represents a vector of length at most n. On the other hand, for $1 \leq |I| < n$ we have

$$1 \leq |\det(L_I)| \tag{10}$$

since the graphs under consideration are assumed to be connected, which implies that the matrices L_I are strongly diagonal dominated.

For simplicity we assume $m_i = n^{(3^i)}$ in the proceeding of the proof. The arguments for the case $m_i = n^{(2^i)}$ are similar but more terms have to be taken into consideration. In order to obtain an estimate for the coefficients a_k we proceed as follows: the largest term in $\sum_{|I|=k} \prod_{j \in I} m_j$ is obviously $\Gamma_k := \prod_{j=n-k+1}^{n} m_j$. All other terms are smaller or equal to $\gamma_k := m_{n-k} \prod_{j=n-k+2}^{n} m_j$. The quotient is $\frac{\Gamma_k}{\gamma_k} = m_{n-k}^2$. Since the total number of terms in the sum is $\binom{n}{k}$ we obtain from (8)–(10) that

$$\left(1 - n^{n-k} \binom{n}{k} \frac{1}{m_{n-k}^2}\right) \prod_{j=n-k+1}^{n} m_j < |a_k| < \left(1 + \binom{n}{k} \frac{1}{m_{n-k}^2}\right) n^{n-k} \prod_{j=n-k+1}^{n} m_j. \tag{11}$$

An elementary calculation shows that for $n \geq 1$ and $k = 1, \dots, n$

$$n^{n-k} \binom{n}{k} \frac{1}{m_{n-k}^2} \leq \frac{1}{n^2}. \tag{12}$$

Inserting (12) in (11) yields

$$\left(1 - \frac{1}{n^2}\right) \prod_{j=n-k+1}^{n} m_j < |a_k| < \left(n^{n-k} + \frac{1}{n^2}\right) \prod_{j=n-k+1}^{n} m_j. \tag{13}$$

Using (13) we obtain that for $k = 2, \dots, n-1$

$$a_k^2 - 4a_{k-1}a_{k+1} > 0 \tag{14}$$

provided that $n \geq 3$ (the case $n = 2$ is easily handled separately). Now the claim follows from the criterion of Kurtz on distinct roots of polynomials (see [11]). □

Combining Theorem 2 and Proposition 1 we obtain the following theorem as a corollary.

THEOREM 3. *There exist mass matrices M_0 such that the following is true: let $G = (A, M)$ and $\tilde{G} = (\tilde{A}, \tilde{M})$ be connected graphs over $\mathcal{A} = \{0, 1\}$ such that M and $\tilde{M}$ are permutation similar to M_0. Then G and $\tilde{G}$ are isomorphic if and only if the Laplace spectrum of G and $\tilde{G}$ coincide as sets. A possible choice is $m_i = n^{(2^i)}$, where n is the number of masses.*

PROOF. According to Proposition 1 the Laplace spectrum of both graphs consists of simple eigenvalues. Hence, by Viëta's theorem, we conclude that $\det(L(G) - xM) \equiv \mu \det(L(\tilde{G}) - x\tilde{M})$ for some $\mu \neq 0$. On the other hand, the coefficient of x^n is $(-1)^n \prod_{i=1}^n m_i$ in $\det(L(G) - xM)$ and $(-1)^n \prod_{i=1}^n \tilde{m}_i$ in $\det(L(\tilde{G}) - x\tilde{M})$, which for both cases is the same number since the mass matrices of G and $\tilde{G}$ are permutation similar. Hence $\mu = 1$ and the assertion follows from Theorem 2. □

ALGORITHMIC REMARK. If one starts from the spectrum, the reconstruction algorithm works as follows. First, compute the polynomial $\mu \det(L(G) - xM)$ by Viëta's theorem and normalize it such that the coefficient of x^n is $(-1)^n \prod_{i=1}^n m_i$. Then find the valence matrix D using the coefficient of x^{n-1} as described in the proof of Theorem 2. Finally, use this to compute the adjacency matrix A from the coefficient of x^{n-2}. (Note that the proof of Lemma 1 can be used to determine recursively the values of the δ_i from the value of the sum $\sum_{i=1}^n \delta_i q_i$.)

Inspection of the proof of Theorem 3 shows that the set of masses $m \in \mathbb{R}^n$, for which reconstruction is possible, contains a large open set (all sequences m_i which grow 'fast enough'). However, the set of masses for which reconstruction is possible also has a part with a fine algebraic structure, as we will see in the next section. There, we consider a general countable set $\mathcal{A}$ of possible values of elasticity constants and impose algebraic conditions on the masses to show that for almost all mass matrices, the weighted adjacency matrix of a graph is determined by its Laplace spectrum.

3. p-INDEPENDENT REALS

In order to simplify the formulas, we use a multi-index notation: for $i = (i_1, \ldots, i_n) \in \mathbb{N}_0^n$ we write $|i| := \max(i_1, \ldots, i_n)$ and for $m = (m_1, \ldots, m_n) \in \mathbb{R}^n$ we define $m^i := \prod_{k=1}^n m_k^{i_k}$.

Let Q be a set of real numbers and $p \in \mathbb{N}_0$. We say that $m \in \mathbb{R}^n$ is p-independent over Q if the following implication holds:

$$\sum_{i \in \mathbb{N}_0^n, |i| \leq p} q_i m^i = 0 \text{ and } q_i \in Q \text{ for all } i \in \mathbb{N}_0^n, |i| \leq p$$
$$\Longrightarrow \; q_i = 0 \text{ for all } i \in \mathbb{N}_0^n, |i| \leq p. \quad (15)$$

Note that the set $\{m_1, \ldots, m_n\} \subseteq \mathbb{R}$ is algebraically independent over Q if and only if $m = (m_1, \ldots, m_n) \in \mathbb{R}^n$ is p-independent over Q for every $p \in \mathbb{N}_0$. Thus, the notion of p-independence is weaker than the notion of algebraic independence. For example, $\sqrt[3]{3}$ and $\sqrt[3]{5}$ are 2-independent but not algebraically independent over $\mathbb{Q}$.

LEMMA 3. *If $Q \subset \mathbb{R}$ is countable and $p \in \mathbb{N}_0$, then the set $\{m \in \mathbb{R}^n : m$ not p-independent over $Q\}$ is a meagre and Lebesgue measure zero set in $\mathbb{R}^n$.*

PROOF. For a fixed $m = (m_1, \ldots, m_{n-1}) \in \mathbb{R}^{n-1}$ let F_m be the set of all not identically vanishing polynomials $f(x)$ with coefficients in $Q \cup \{m_1, \ldots, m_{n-1}\}$ of degree at most p. As the set $Q \cup \{m_1, \ldots, m_{n-1}\}$ is countable and p is finite, the set

$$N(m) := \{x \in \mathbb{R} : f \in F_m \wedge f(x) = 0\}$$

is countable. Hence, for every $m \in \mathbb{R}^{n-1}$, the set $N(m)$ is a meagre and Lebesgue measure zero set in $\mathbb{R}$ and by the theorems of Kuratowski–Ulam and Fubini (see, e.g., [14] or [10]) we find that the set $\{m \in \mathbb{R}^n : m \text{ not } p\text{-independent over } Q\}$ is a meagre and Lebesgue measure zero set in $\mathbb{R}^n$. $\square$

Remember that there exist meagre sets which do not have Lebesgue measure zero and vice versa. Moreover, one can cover the real line with a meagre set and a set of Lebesgue measure zero.

4. THE RECONSTRUCTION THEOREM

In this section let C denote an arbitrary but fixed set of countably many real numbers. Then $\mathcal{A} = \mathbb{Q}[C]$, the smallest field containing C and the rational numbers, is also countable. We show that if the set of masses $m \in \mathbb{R}_+^n$ fulfils a suitable algebraic condition with respect to the set $\mathcal{A}$, then the adjacency matrix $A(G)$ of a graph in $\mathcal{G}_{\mathcal{A},M(m)}$ is determined by its Laplace spectrum $\{x \in \mathbb{R} : \det(L(G) - xM(m)) = 0\}$. In particular, we will see that the set of masses $m \in \mathbb{R}_+^n$ for which reconstruction is *not* possible is a meagre and Lebesgue measure zero set in $\mathbb{R}^n$. Remember that for $m \in \mathbb{R}_+^n$, $M(m) = \operatorname{diag}(m)$, and that $\mathcal{G}_{\mathcal{A},M(m)}$ is the set of all weighted graphs $G = (A, M(m))$ with $A = (A_{ij})$ and $0 \leq A_{ij} \in \mathcal{A}$.

THEOREM 4. *Let $m \in \mathbb{R}_+^n$ be 1-independent over $\mathbb{Q}[C]$, and let $G = (A, M)$ and $\tilde{G} = (\tilde{A}, \tilde{M})$ be graphs over $\mathcal{A} = \mathbb{Q}[C]$ of order n such that M and $\tilde{M}$ are permutation similar to $M(m)$. Then G and $\tilde{G}$ are isomorphic if and only if their characteristic polynomials coincide, i.e., if* $\det(L(G) - xM) \equiv \det(L(\tilde{G}) - x\tilde{M})$.

PROOF. It is easy to see that if G and $\tilde{G}$ are isomorphic, then their characteristic polynomials coincide.

For the opposite implication we may assume that the vertex sets of G and $\tilde{G}$ are already renumbered such that $M = \tilde{M} = M(m)$. We recall that $p(x) = (-1)^n \det(L(G) - xM) = a_n x^n + \cdots + a_2 x^2 + a_1 x + a_0$ with $a_0 = 0$ and with $a_{n-1} = \sum_{i=1}^n d_i \prod_{j \neq i} m_j$. If $p(x)$ and $\tilde{p}(x)$ coincide we have in particular $\sum_{i=1}^n d_i \prod_{j \neq i} m_j = \sum_{i=1}^n \tilde{d}_i \prod_{j \neq i} m_j$, hence $\sum_{i=1}^n (d_i - \tilde{d}_i) \prod_{j \neq i} m_j = 0$, and because m is 1-independent over $\mathcal{A}$, we have $d_i = \tilde{d}_i$ for $1 \leq i \leq n$. Thus, the valence matrix is determined by the coefficient a_{n-1}. Comparing the coefficient $a_{n-2} = \sum_{i<j} (d_i d_j - A_{ij}^2) \prod_{k \notin \{i,j\}} m_k$ of x^{n-2}, and using again that m is 1-independent over $\mathcal{A}$ and $d_i = \tilde{d}_i$, we obtain $A_{ij} = \tilde{A}_{ij} \geq 0$ and the proof is complete. $\square$

As in Section 2 in the case $\mathcal{A} = \{0, 1\}$, it turns out that the roots of the polynomial $\det(L(G) - xM)$ are simple, provided the mass matrix is well chosen. In order to prepare the proof, we need the following two lemmas.

LEMMA 4. *Suppose $m = (m_1, \ldots, m_n) \in \mathbb{R}^n$ is nq-independent over a subfield K of the* *real numbers and let*

$$
\begin{aligned}
p_1(x_1, \dots, x_n) &:= \sum_{i=1}^{n} c_i x_i \\
p_2(x_1, \dots, x_n) &:= \sum_{1 \le i_1 < i_2 \le n} c_{i_1 i_2} x_{i_1} x_{i_2} \\
p_3(x_1, \dots, x_n) &:= \sum_{1 \le i_1 < i_2 < i_3 \le n} c_{i_1 i_2 i_3} x_{i_1} x_{i_2} x_{i_3} \\
&\vdots \\
p_n(x_1, \dots, x_n) &:= c_{123\dots n} x_1 x_2 \dots x_n
\end{aligned}
$$

be polynomials with coefficients $c_{i_1 \dots i_j} \in K \setminus \{0\}$. *Then,* $(p_1(m_1, \dots, m_n), \dots, p_n(m_1, \dots, m_n)) \in \mathbb{R}^n$ *is* q*-independent over* K.

PROOF. Let F be a polynomial in n variables with coefficients in K and with maximal degree less than or equal to q. The maximal degree of F is defined by

$$\max\deg F := \max_{1 \le i \le n} \deg_t F(x_1, \dots, t x_i, \dots, x_n),$$

where $\deg_t$ is the usual polynomial degree with respect to the variable t. We assume that F is not the zero polynomial. Now, let us consider the terms in the expression

$$X := F(p_1(m_1, \dots, m_n), \dots, p_n(m_1, \dots, m_n))$$

after expanding all products but before eliminating terms which cancel. We order the m-monomials in X according to the lexicographical order relation. For example, $m_1^2 m_2^0 m_3^7 < m_1^2 m_2^1 m_3^1$. This ordering is compatible with multiplication of the monomials. A lexicographically largest m-monomial in X appears while expanding a term

$$p_1^{b_1} p_2^{b_2} \dots p_n^{b_n} = \left(\sum_{i=1}^{n} c_i x_i \right)^{b_1} \left(\sum_{1 \le i_1 < i_2 \le n} c_{i_1 i_2} x_{i_1} x_{i_2} \right)^{b_2} \cdot \dots \cdot (c_{123\dots n} x_1 x_2 \dots x_n)^{b_n}$$

(where all exponents $b_i \le q$) and is, apparently, the monomial

$$m_1^{b_1 + \dots + b_n} m_2^{b_2 + \dots + b_n} \dots m_n^{b_n}$$

(and all exponents here are less than or equal to nq). By inspection of this last expression it is clear that the exponent $(b_1, \dots, b_n)$ is determined by the lexicographically largest m-monomial in X which therefore cannot cancel with any other (largest) m-monomial in X. Now we assume by contradiction that $F\big(p_1(m_1, \dots, m_n), \dots, p_n(m_1, \dots, m_n)\big) = 0$. Since all appearing m-monomials have maximal degree less than or equal to nq, it follows that all coefficients of the m-monomials must vanish (because $(m_1, \dots, m_n)$ is assumed to be nq-independent over K). This contradicts the fact that the coefficient of the lexicographically largest m-monomial does not vanish. □

LEMMA 5. *If* p *is a polynomial of degree* $n \ge 2$ *such that the set of its coefficients is* $(n^2 - 2n + 2)$*-independent over a subfield* K *of the real numbers, then* p *has only simple roots.*

PROOF. The polynomial p has a multiple root if and only if the greatest common divisor of p and its derivative p' is non-trivial, i.e., if it is a polynomial of degree strictly larger than zero. The greatest common divisor of two polynomials can be determined by the euclidean algorithm. Performing the euclidean algorithm with p and p' and computing the polynomial remainders in each step, it is easy to see that the conditions that p has a multiple root are polynomial equations in the coefficients of p of degree less than or equal to $n^2 - 2n + 2$ and with integer coefficients. Since the coefficients of p are supposed to be $(n^2 - 2n + 2)$-independent over $K \supset \mathbb{Q}$, the claim follows. $\square$

THEOREM 5. *Let $m \in \mathbb{R}_+^n$ be $n(n^2 - 2n + 2)$-independent over $\mathbb{Q}[C]$ and let $G = (A, M)$ be a connected graph over $\mathcal{A} = \mathbb{Q}[C]$ of order n. Then $\det(L(G) - xM(m))$ has only simple roots.*

PROOF. Let $p(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x^1$ be as in the proof of Theorem 4. Recall that

$$a_k = \sum_{|I|=k} \det(L_I) \prod_{j \in I} m_j$$

and that $\det(L_I) \in \mathcal{A} \setminus \{0\}$, since the graph under consideration is supposed to be connected. Thus, by Lemma 4, we find that $(a_1, \ldots, a_n)$ is $(n^2 - 2n + 2)$-independent over $\mathcal{A}$ and the claim follows from Lemma 5. $\square$

Combining Theorem 4 and Theorem 5 we obtain the following theorem.

THEOREM 6. *Let $C \subset \mathbb{R}$ be countable and $\mathcal{A} = \mathbb{Q}[C]$. Let $m \in \mathbb{R}_+^n$ be $n(n^2 - 2n + 2)$-independent over $\mathcal{A}$, and let $G = (A, M)$ and $\tilde{G} = (\tilde{A}, \tilde{M})$ be graphs over $\mathcal{A}$ of order n such that M and $\tilde{M}$ are permutation similar to $M(m)$. Then G and $\tilde{G}$ are isomorphic if and only if their Laplace spectra agree, provided that at least one of the graphs G and $\tilde{G}$ is connected. In particular, the set of masses $m \in \mathbb{R}_+^n$ for which reconstruction is not possible is meagre and has Lebesgue measure zero.*

PROOF. Let $N \subset \mathbb{R}^n$ be the set of all $m \in \mathbb{R}^n$ which are not $n(n^2 - 2n + 2)$-independent over $\mathbb{Q}[C]$. Then, by Lemma 3, we have that N is meagre and has Lebesgue measure zero. We may assume without loss of generality that G is connected. By Theorem 5 we have that the roots of $\det(L(G) - xM(m))$ are all simple. Hence, since the spectra of G and $\tilde{G}$ agree, the roots of $\det(L(\tilde{G}) - x\tilde{M}(m))$ must be simple as well, and the characteristic polynomials of both graphs coincide. Thus, by Theorem 4, the graphs are isomorphic. $\square$

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