Reconstruction of weighted graphs by their spectrum

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Abstract

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 nonisomorphic 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 adjacency matrix, and where the mass matrix $M = \mathrm{diag}(m_1, \dots, m_n)$ 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 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 $(u_1, \ldots, u_n)$. In other words the negative squares $-\omega^2 = \lambda$ of the eigenfrequences 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 short look at the case of simple graphs when all m_i and all nonzero 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. [2] as a main reference). Nonisomorphic 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 famous Matrix-Tree Theorem of G. Kirchhoff). In how far the spectrum of L reflects the spectral properties of molecules is discussed in [3], [5] and [8]. The relation between a simple graph and its Laplace spectrum is studied e.g. in [6], [7], [15] and [13]. As a general reference for recent results on spectral graph theory see [4]. 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 nonisomorphic trees on n vertices and s_n the number of such trees T for which there exists a nonisomorphic 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 to generate 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 $M(m) = \mathrm{diag}(m)$. 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 $A = (A_{ij})$, $0 \leq A_{ij} \in \mathcal{A}$, and we will say G is a graph over $\mathcal{A}$ and $M(m)$.

In this paper we look at the following problem: Given $m = (m_1, \dots, m_n) \in \mathbb{R}^n_+$, $\mathcal{A} \subset \mathbb{R}$ 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. But 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 a first part 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 a second part 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. So, 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 Laplacian spectrum of weighted graphs

In this section all nonzero 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 to decide which masses are linked in a graph whose Laplace spectrum is known.

Theorem 2 *There exist mass matrices $M_0 = \mathrm{diag}(m_1, \ldots, m_n)$ 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. $q_i \geq s q_{i-1}$ 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. $\square$

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 $i = 1, \ldots, n$. 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 $2^l + 2^m - 2^i - 2^j \neq 0$. But this follows from Lemma 1 since $2^l + 2^m = 2^i + 2^j$ would imply $\{l,m\} = \{i,j\}$ which contradicts the assumption. $\square$

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

$$\begin{aligned}
\det(L - xM) &= \begin{vmatrix} -d_1 - xm_1 & A_{12} & A_{13} & \ldots & A_{1n} \\ A_{21} & -d_2 - xm_2 & A_{23} & \ldots & A_{2n} \\ \vdots & \vdots & \ddots & & \vdots \\ A_{n1} & A_{n2} & \ldots & \ldots & -d_n - xm_n \end{vmatrix} = \qquad (5) \\
&= (-1)^n x^n \prod_{i=1}^{n} m_i + (-1)^n x^{n-1} \sum_{i=1}^{n} d_i \prod_{j \neq i} m_j + \\
&\qquad + (-1)^n x^{n-2} \sum_{i<j} (d_i d_j - A_{ij}^2) \prod_{k \notin \{i,j\}} m_k + \ldots + \det(L).
\end{aligned}$$

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

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

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 $d_i \in \{0, 1, \ldots, n-1\}$. Notice 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. $\square$

Up to now, we consider 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 Laplacian 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* $m_i = n^{(2^i)}$, $i = 1, \ldots, n$. *Then the roots of the characteristic polynomial* $\det(L - xM(m))$ *are simple.*

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

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

From (1) we get for $k = 0, \ldots, n$

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

where the sum is taken over all ordered subsets I of $\{1, \ldots, n\}$ 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 in 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 (9), (10) and (8)

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

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

$$n^{n-k}\binom{n}{k}\frac{1}{m_{n-k}^2} \leq \frac{1}{n^2} \,. \qquad (12)$$

Inserting (12) in (11) yields

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

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

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

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 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 Laplacian 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 Laplacian 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.

$\square$

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}. (Notice 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 has also 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:

$$\sum_{i \in \mathbb{N}_0^n, |i| \le p} q_i m^i = 0 \text{ and } q_i \in Q \text{ for all } i \in \mathbb{N}_0^n, |i| \le p \implies$$

$$\implies q_i = 0 \text{ for all } i \in \mathbb{N}_0^n, |i| \le p. \quad (15)$$

Notice 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 $p \in \mathbb{N}_0$. So, 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 meager and Lebesgue measure zero set in $\mathbb{R}^n$.*

Proof
For a fixed $m = (m_1, \dots, m_{n-1}) \in \mathbb{R}^{n-1}$ let F_m be the set of all not identically vanishing polynomials $f(x)$ with coefficients in $Q \cup \{m_1, \dots, m_{n-1}\}$ of degree at most p. Because the set $Q \cup \{m_1, \dots, m_{n-1}\}$ 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 meager and Lebesgue measure zero set in $\mathbb{R}$ and by the theorems of Kuratowski–Ulam and Fubini (see, e.g., [14] or [10]) we get that the set $\{m \in \mathbb{R}^n : m \text{ not } p\text{-independent over } Q\}$ is a meager and Lebesgue measure zero set in $\mathbb{R}^n$. □

Remember that there exist meager sets which do not have Lebesgue measure zero and vice versa. Moreover, one can cover the real line with a meager 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 countable as well. We show that if the set of masses $m \in \mathbb{R}^n_+$ fulfills 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 meager 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 $0 \le A_{ij} \in \mathcal{A}$.

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 $p(x) = (-1)^n \det(L(G) - xM) = a_n x^n + \ldots + a_2 x^2 + a_1 x + a_0$ 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. □

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*

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

be polynomials with coefficients $c_{i_1\ldots i_j} \in K \setminus \{0\}$. Then, $(p_1(m_1,\ldots,m_n), \ldots, p_n(m_1, \ldots, m_n)) \in \mathbb{R}^n$ 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

$$\max\deg F := \max_{1\leq i\leq n} \deg_t F(x_1,\ldots,tx_i,\ldots,x_n),$$

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

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

after expanding all products but before eliminating terms which cancel. We order the m-monomials in X according to the lexicographical order relation. E.g., $m_1^2 m_2^0 m_3^7 <$

$m_1^2 m_2^1 m_3^1$. This ordering is compatible with multiplication of the monomials. A lexicographically largest m-monomial in X appears while expanding a term

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

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

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

(and all exponents here are less than or equal to nq). By inspection of this last expression it is clear that the exponent $(b_1, \ldots, b_n)$ 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 $F\big(p_1(m_1, \ldots, m_n), \ldots, p_n(m_1, \ldots, m_n)\big) = 0$. 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 $(m_1, \ldots, m_n)$ 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 $n \geq 2$ 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 reminders 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. □

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 $p(x) = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_1 x^1$ 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 get 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

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 meager 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 meager 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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References

[1] P. Botti, R. Merris: Almost all trees share a complete set of immanental polynomials. Journal of graph theory **17** (1993), p. 468ff

[2] D. M. Cvetković, M. Doob, H. Sachs: Spectras of graphs. Academic press, New York (1979)

[3] B. Eichinger: Configuration statistics of Gaussian molecules. Macromolecules **13** (1980), p. 1–11

[4] F. R. K. Chung: Spectral graph theory. CBMS Regional conference series in mathematics; no. 92. American Mathematical Society, Providence, Rhode Island (1997)

[5] W. Forsman: Graph theory and the statistics of polymer chains. J. Chemical Phys. **65** (1976), p. 4111–4115

[6] R. Grone, R. Merris, V. S. Sunder: The Laplacian spectrum of a graph. SIAM Journal on matrix analysis and applications **11** (1990), p. 218

[7] R. Grone, R. Merris: The Laplacian spectrum of a graph II. SIAM Journal on discrete mathematics **7** (1994), p. 221

[8] I. Gutman: Graph-theoretical formulation of Forsman's equation. J. Chem. Phys. **68** (1978), p. 1321–1322

[9] L. Halbeisen, N. Hungerbühler: Generation of isospectral graphs. J. Graph Theory, to appear

[10] A. S. Kechris: Classical descriptive set theory. Springer, New York (1995)

[11] D. C. Kurtz: A sufficient condition for all the roots of a polynomial to be real. Amer. Math. Monthly **99** (1992), p. 259–263

[12] B. D. McKay: On the spectral characteristics of trees. Ars Combinat. **3** (1977), p. 219–232

[13] B. Mohar: The Laplacian spectrum of graphs. Preprint series, Dep. of Math. University of Ljubliana, Yugoslavia, **26** (1988), p. 353–384

[14] J. C. Oxtoby: Measure and category: a survey of the analogies between topological and measure spaces. Springer, New York (1980)

[15] P. Rowlinson: The spectrum of a graph modified by the addition of a vertex. Publikacije Elektrotehnickog fakulteta **3** (1992), p. 67ff

[16] A. J. Schwenk: Almost all trees are cospectral. New directions in the theory of graphs. Academic press, New York (1973), p. 275–307

[17] J. Turner: Generalized matrix functions and the graph isomorhism problem. SIAM J. Appl. Math. **16** (1968), p. 520–536

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