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Calculating the characteristic polynomial and the eigenvectors of a tree

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Abstract

We give in this paper an algorithm **T** based on a general graph theoretical procedure for solving systems of linear equations (see [18]).
T allows the eigenvalues and eigenspaces of any tree to be simultaneously calculated. Some nice results for caterpillars and cospectral trees are described.

1 Introduction

1.1 Definitions and notation

Let G be a finite graph (without loops and multiple edges) with non-empty vertex set $V = V(G)$ and edge set $E = E(G)$ which has $n = n(G)$ $(= |V(G)|)$ vertices; let $\mathbf{A} = \mathbf{A}(G)$ denote the $0-1$ adjacency matrix of G and let $\mathbf{I}$ be the $n \times n$ identity matrix. The polynomial $det(\lambda\mathbf{I} - \mathbf{A})$ in λ and its roots are called the **characteristic polynomial** of G, denoted by $P_G(\lambda)$, and the **eigenvalues** of G, respectively. Let λ^o be an eigenvalue of G and let $\mathbf{0}$ denote the zero vector on n components. The set $\mathbf{X}^o = \mathbf{X}(\lambda^o)$ of all solutions $\mathbf{x}$ of the equation

$$(\lambda^o \cdot \mathbf{I} - \mathbf{A}) \cdot \mathbf{x} = \mathbf{0}$$

forms the eigenspace of G belonging to λ^o and every non-zero $\mathbf{x}^o \in \mathbf{X}^o$ (with $|\mathbf{x}^o| = 1$) is a (normalized) **eigenvector** of G belonging to λ^o. (In Hückel theory, these vectors are called "molecular orbitals" by chemists.)

A **tree** T is a connected graph that has no cycle.

A **forest** F is a graph whose components are trees.

The number of edges of a Graph G which are incident with a vertex v of G is called the **valency** of v, denoted by $val(v, G)$.

Vertex $v \in V(T)$ is called an **isolated vertex**, **pendent vertex** or **branching vertex** of T if and only if $val(v,T) = 0$, $val(v,T) = 1$ or $val(v,T) \geq 3$, respectively (Figure 1).

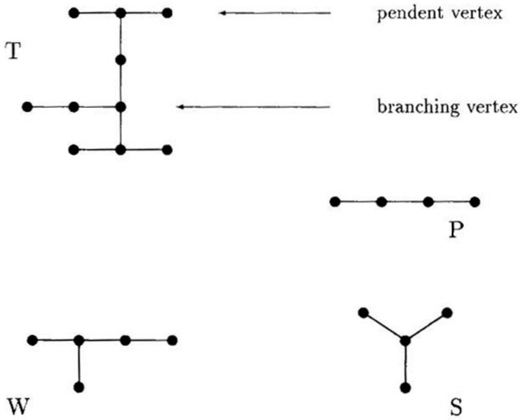


Figure 1

A **whirl** W is a tree with at most one branching vertex. A **star** S is a whirl with exactly one branching vertex v^* and no vertices of valency 2. A **path** P is a whirl without branching vertex (Figure 1).
The **trivial graph** is the graph with only one vertex (and no edges).

1.2 Chemical connection and literature

The interesting eigenvalue-eigenvector problem of a tree has attracted the attention of many theoretical chemists over a long period of time. First results for simple polyenes (paths with even numbers of vertices, see Fig. 2) are given by E. Hückel [1], W.G. Penney [2], J.E. Lennard-Jones [3], C.A. Coulson [4], G.W. Wheland [5] and R.S. Mulliken and C.A. Rieke [6]. H.H. Günthard and H. Primas [7] and U. Wild, J. Keller and H.H. Günthard [8] showed that the eigenvalue-eigenvector problem is of interest in Hückels theory [1]. Much information about the early approaches to Hückel theory of organic compounds are contained in the classical books of C.A. Coulson and A. Streitwieser, Jr. [9], and C.A. Coulson, B.O. Leary and R.B. Mallion [10]. For more details concerning eigenvalues and eigenvectors of a graph see the

mathematical monographs of D.M. Cvetković, M. Doob and H. Sachs [11], and D.M. Cvetković, M. Doob, I. Gutman and A. Torgašev [12].
For trees T, recursive formulas for calculating $P_T(\lambda)$ were developed by E. Heilbronner [13] and F. Harary, C. King, A. Mowshowitz and R.C. Read [14]. A table of all eigenvalues for all trees with no more than 10 vertices is contained in [11].
For paths and stars there are explicit formulas for $P_T(\lambda)$, $T \in \{P, S\}$, [3, 9, 15, 16] for all eigenvalues [3, 9, 16, ?] and for all eigenvectors [3, 9, 16].
In this paper an algorithm **T** based on a general graphentheoretical procedure for solving systems of linear equations, see [18], is developed. **T** allows the eigenvalues and eigenspaces of any tree to be simultaneously calculated.

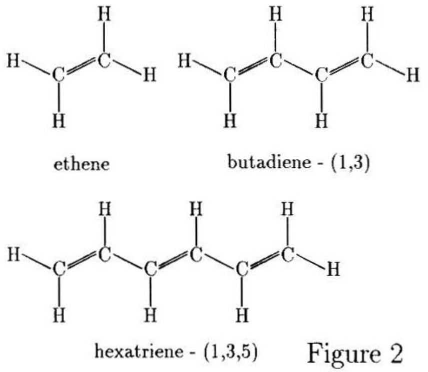


Figure 2

2 Path systems of a tree

Let T be a tree.
If $n = 1$ then T is called a **trivial tree** (or **trivial path**).

If $n > 1$, put $V_1 = V_1(T) := \{v \mid v \in V(T) \text{ and } \mathrm{val}(v,T) = 1\}$, $V_b = V_b(T) := \{v \mid v \in V(T) \text{ and } \mathrm{val}(v,T) \geq 3\}$ and $n_1 = n_1(T) :=\mid V_1 \mid, n_b = n_b(T) :=\mid V_b \mid$. Clearly, $n_b(P) = 0$ for every path P.
The following fact is well known and easy provable (see [19]).

Observation 1:
Let u and v be distinct vertices of a tree T. Then there exists in T exactly one path $P(u, v)$ with end vertices u, v (immediate). □

A **path system** (PS) of T is a set of pairwise (vertex) disjoint paths of T (trivial paths being admitted).

A **complete path system** (CPS) $\mathbf{P} = \mathbf{P}(T)$ of T is a PS which covers all vertices of T (Figure 3).

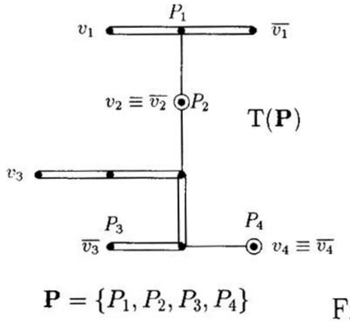


Figure 3

Let $\mathbf{\Pi} = \mathbf{\Pi}(T)$ denote the set of all CPSs of T. For $\mathbf{P} \in \mathbf{\Pi}$, put $p = p(\mathbf{P}) := \mid \mathbf{P} \mid$.

Observation 2:
For every tree T and every $\mathbf{P} \in \mathbf{\Pi}$,

$$\left\lceil \frac{n_1}{2} \right\rceil \leq p \leq n,$$

where $\lceil x \rceil$ is the least integer not less than x.
The proof is simple. □

The elements of $\mathbf{P}$ are denoted by $P_k = P(v_k, \overline{v}_k), k = 1, 2, ..., p$ (Figure 3).

3 The algorithm

Let T be a tree and $\mathbf{P} \in \mathbf{\Pi}$. Let $T(\mathbf{P})$ be a drawing of T in which the edges of $\mathbf{P}$ are fat (Figure 3).
For $k = 1, 2, ..., p$, direct all edges of $P_k = P(v_k, \overline{v}_k)$ towards vertex $\overline{v}_k$. Thus $T(\mathbf{P})$ is turned into a partially directed tree $\overrightarrow{T} = \overrightarrow{T}(\mathbf{P})$ (with directed paths $\overrightarrow{P_k}$) (Figure 4).

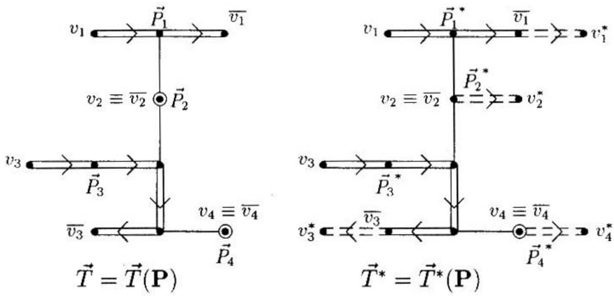


Figure 4

The points v_k are called the **sources** of $\overrightarrow{T}$. Every oriented path $\overrightarrow{P_k}$ of $\overrightarrow{T}$ is prolonged beyond its point $\overline{v}_k$ by one directed edge $\overrightarrow{e_k}^*$ connecting $\overline{v}_k$ with an additional „virtual" vertex v_k^*, thus $\overrightarrow{T}$ is turned into a figure $\overrightarrow{T}^* = \overrightarrow{T}^*(\mathbf{P})$ (Figure 4).
The points v_k^* are called the **sinks** of $\overrightarrow{T}^*$. For any vertex v of $\overrightarrow{T}^*$ which is not a source let v^+ be its unique predecessor and let $N^+(v) := N(v^+) - \{v\}$ be the set of neighbours of v^+ which are different from v (Figure 5).

Algorithm T

To every vertex v of $\overrightarrow{T}^*$ assign a vector $\mathbf{d}(v, \lambda) = (d_1(v,\lambda), d_2(v,\lambda), ..., d_p(v,\lambda))$ accordings to the following rules.

(**T**.1) For a source v_k put $\mathbf{d}(v_k, \lambda) = (\delta_{1k}, \delta_{2k}, ..., \delta_{pk})$, where $\delta_{ii} = 1$ and $\delta_{ik} = 0$ for $i \neq k \quad (i, k = 1, 2, ..., p)$;

(**T**.2) for any vertex v of $\overrightarrow{T}^*$ which is not a source, put
$\mathbf{d}(v, \lambda) = \lambda \cdot \mathbf{d}(v^+, \lambda) - \sum\limits_{v' \in N^+(v)} \mathbf{d}(v', \lambda)$.

It is easy to see that, running through $\overrightarrow{T}^*$ from the sources to the sinks, we have no difficulty in successively calculating the vectors $\mathbf{d}(v, \lambda)$ which are thus uniquely determined by (**T**.1) and (**T**.2). Label the vertices of $\overrightarrow{T}^*$ which are distinct from the sources and sinks in any order as $v_{p+1}, v_{p+2}, ..., v_n$. Form the $n \times p$ matrix

$$\mathbf{D}(T(\mathbf{P}), \lambda) = (\mathbf{d}^{\mathrm{T}}(v_1, \lambda), \mathbf{d}^{\mathrm{T}}(v_2, \lambda), ..., \mathbf{d}^{\mathrm{T}}(v_n, \lambda))^{\mathrm{T}} = (d_k(v_i, \lambda))$$

$(i = 1, 2, ..., n; k = 1, 2, ..., p)$

and die $p \times p$ matrix

$$\mathbf{D}^*(T(\mathbf{P}),\lambda) = (\mathbf{d}^{\mathrm{T}}(v_1^*,\lambda), \mathbf{d}^{\mathrm{T}}(v_2^*,\lambda), ..., \mathbf{d}^{\mathrm{T}}(v_p^*,\lambda))^{\mathrm{T}} = (d_k(v_j^*,\lambda))$$

$(k, j = 1, 2, ..., p)$.

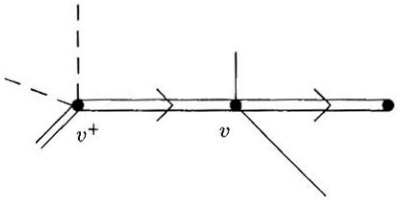


Figure 5

Theorem 1:
$P_T(\lambda) = det\underline{D}^*(T(\mathbf{P}),\lambda)$.

Theorem 2:
Let λ^0 be an eigenvalue of T, let $\mathbf{y}^0$ be a non-trivial solution of
(*) $\mathbf{D}^*(T(\mathbf{P}),\lambda^0) \cdot \mathbf{y}^0 = \mathbf{0}$
and put
(**) $\mathbf{x}^0 = \mathbf{D}(T(\mathbf{P},\lambda^0) \cdot \mathbf{y}^0$.

Then the vector $\mathbf{x}^0$ is an eigenvector of T belonging to λ^0, and all eigenvectors belonging to λ^0 can be obtained this way.

Both theorems follow from theorems in [18]. □

Example 1:
For the tree T in Figure 1 (see Figure 6 with labelled vertices) we obtain the following matrices:

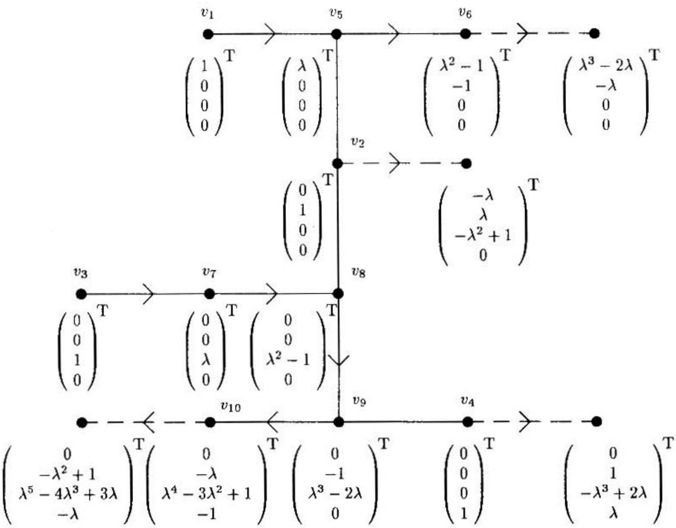


Figure 6

$$\mathbf{D}(T(\mathbf{P}),\lambda)=\begin{pmatrix} 1 & 0 & 0 & 0 & \lambda & \lambda^2-1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & -\lambda \\ 0 & 0 & 1 & 0 & 0 & 0 & \lambda & \lambda^2-1 & \lambda^3-2\lambda & \lambda^4-3\lambda^2+1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}^{\mathrm{T}}$$

and

$$\mathbf{D}^*(T(\mathbf{P}),\lambda)=\begin{pmatrix} \lambda^3-2\lambda & -\lambda & 0 & 0 \\ -\lambda & \lambda & -\lambda^2+1 & 1 \\ 0 & -\lambda^2+1 & \lambda^5-4\lambda^3+3\lambda & -\lambda^3+2\lambda \\ 0 & 0 & -\lambda & \lambda \end{pmatrix}^{\mathrm{T}}.$$

Thus

$$P_T(\lambda)=\varepsilon\cdot det\mathbf{D}^*(T(\mathbf{P}),\lambda)=\lambda^{10}-9\lambda^8+25\lambda^6-23\lambda^4+4\lambda^2.$$

$\lambda^0=0$ is a double root of $P_T(\lambda)$, $\mathbf{y}_1^0=(1,0,0,0)$, $\mathbf{y}_2^0=(0,0,0,1)$ are linearly independent solutions to (*) and the vectors $\mathbf{x}_1^0$, $\mathbf{x}_2^0$ corresponding to $\mathbf{y}_1^0$, $\mathbf{y}_2^0$ by (**) are eigenvectors of T belonging to λ^0; their components x_{1i}^0, x_{2i}^0 are given in Figure 7, close to vertex v_i.

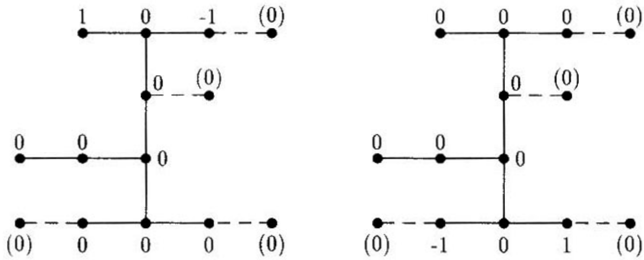


Figure 7

The zeros in the brackets only serve for checking the correctness of the calculation. For the application of the algorithm to be developed, it is very desirable to have a CPS with minimal number of paths.

4 Whirls and minimal complete path systems

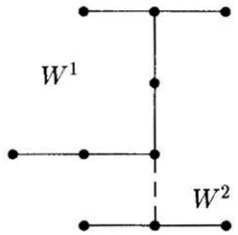
Let T be a tree and $\mathbf{P} \in \mathbf{\Pi}$. A **minimal complete path system** (MCPS) $\overline{\mathbf{P}}$ of T is a CPS with a minimal number of paths $\overline{p} =| \overline{\mathbf{P}} |= min\{| \mathbf{P} | \mid \mathbf{P} \in \mathbf{\Pi}\}$. We need some further notations.

A CPS of a forest F is the disjoint union of the CPSs of all components of F.

A **whirl system** (WS) of T is a set of pairwise (vertex) disjoint whirls of T (also trivial whirls are allowed).

A **complete whirl system** (CWS) $\mathbf{W} = \mathbf{W}(T)$ of T is a WS which covers all vertices of T (Figure 8).

Let $\mathbf{\Omega} = \mathbf{\Omega}(T)$ denote the set of all CWSs of T. For $\mathbf{W} \in \mathbf{\Omega}$ let $w = w(\mathbf{W}) =| \mathbf{W} |$ denote the number of whirls in $\mathbf{W}$.



$\mathbf{W} = \mathbf{W}(T) = \{W^1, W^2\}$

Figure 8

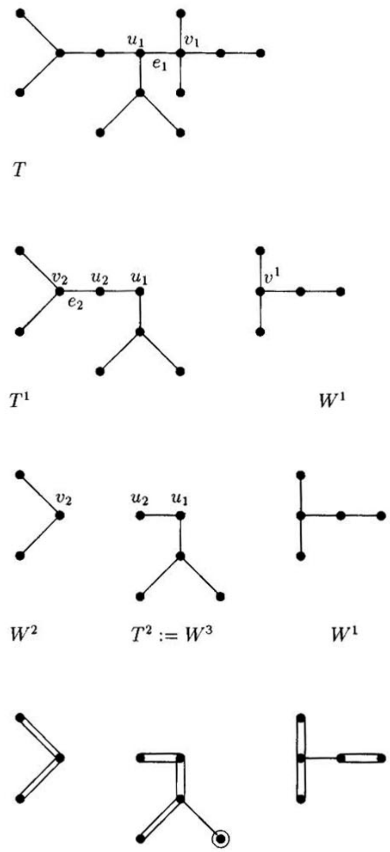
Observation 3:
For every (branched) tree T and every $\mathbf{W} \in \mathbf{\Omega}(T)$,

$$\left\lceil \frac{n_b + 2}{3} \right\rceil \leq w \leq n.$$

Proof:
Let E and $\mathbf{E}$ denote the edge set of T and of $\mathbf{W}$, respectively. Every $W \in \mathbf{W}$ has at most one branching vertex and every edge from the difference set $E - \mathbf{E}$ is incident with at most two branching vertices of T which are not branching vertices of the whirls of $\mathbf{W}$. Therefore
$n_b \leq w + 2 \mid E - \mathbf{E} \mid = w + 2(w-1) = 3w - 2.$ □

Next we give a sketch of an algorithm finding a MCPS of a (branched) tree T. First we construct a sequence $\mathbf{W} = (W^1, W^2, ..., W^W)$ of whirls $W^i \subseteq T$, forming a CWS in the following way.

If T itself is a whirl then set $\mathbf{W} = \{W^1\}$. Otherwise find a branching vertex v_1 and an edge $e_1 = (u_1, v_1)$ in T such that after removing e_1 tree T decomposes into a whirl W^1 containing v^1 and a subtree T^1 of T containing u_1 (Figure 9).



$\mathbf{P^2} = \mathbf{P}(W^2) = \{P_1^2\}$ $\quad$ $\mathbf{P^3} = \mathbf{P}(W^3) = \{P_1^3, P_2^3\}$ $\quad$ $\mathbf{P^1} = \mathbf{P}(W^1) = \{P_1^1, P_2^1\}$

$$\mathbf{P} = \mathbf{P}^1 \cup \mathbf{P}^2 \cup \mathbf{P}^3$$

Figure 9

One can easily check that such an edge e_1 exists. If T^1 is not a whirl then repeat this procedure in order to get an edge $e_2 = (u_2, v_2)$ of T^1 such that $T^1 - e_2$ consists of a whirl W^2 (containing v_2) and a tree T^2 (containing u_2). Continue until a tree T^{w-1} is found which is itself a whirl: $T^{w-1} = W^w$. A sequence $(W^1, W^2, ..., W^w)$ of a tree T constructed this way will be called an **outer whirl sequence** (OWS) of T, denoted by OWS(T).

Let $n_1^i = n_1(W^i)$ be the number of pendent vertices of W^i, $i = 1, 2, ..., w$. For every whirl W^i there is a CPS $\mathbf{P}^i = \{P_1^i, P_2^i, ..., P_p^i\}$ with exactly $P^i = n_1^i - 1$ paths (Figure 9); such a system can be found by the following procedure. Connect two arbitrary pendent vertices of W^i by the path P_1^i. Removing the edges and vertices of p_1^i from W^i results in a graph consisting of paths $P_2^i, P_3^i, ..., P_{n_1^i-1}^i$. It is easy to see that $\mathbf{p}^i$ is an MCPS for W^i. The path system $\mathbf{P} = \mathbf{P}^1 \cup \mathbf{P}^2 \cup ... \cup \mathbf{P}^w$ is a CPS of T and it consists of exactly $n_1^1 + n_1^2 + ... + n_1^w - w$ paths. $\mathbf{P}$ is, in fact, a MCPS; this follows from the next theorem.

Theorem 3:
Any CPS of T has no less than $n_1^1 + n_1^2 + ... + n_1^w - w$ paths.

Proof by induction on the number w of whirls. If $w = 1$, the statement is evidently true. Now assume that it is true for all trees having an outer whirl sequence with no more than w whirls and let T be a tree with OWS$(T) = (W^1, W^2, ..., W^{w+1})$. The tree T^1 has the OWS$(W^2, W^3, ..., W^{w+1})$. Let $\mathbf{P}$ be a CPS of T. The deletion of all edges and vertices of W^1 and of e_1 from the paths of $\mathbf{P}$ results in a CPS $\mathbf{P}'$ of T^1, and removing all edges and vertices of T^1. Except u_1 from the paths of $\mathbf{P}$ we obtain a CPS $\mathbf{P}^*$ of the whirl $W^1 \cup e_1$ (Figure 10). Exactly one path of $\mathbf{P}$ has vertices both in $\mathbf{P}^*$ and $\mathbf{P}'$ that is the path containing u_1.

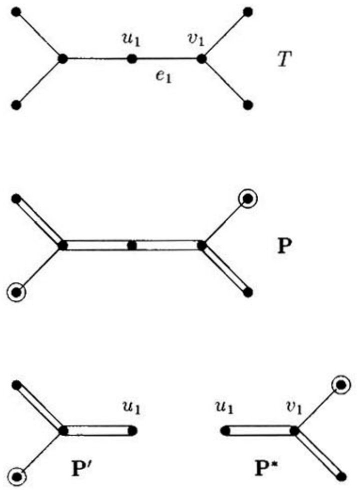


Figure 10

Therefore we get
$| \mathbf{P} |=| \mathbf{P}^* | + | \mathbf{P}' | -1.$
By induction assumption
$| \mathbf{P}' | \geq n_1^2 + n_1^3 + ... + n_1^{w+1} - w$ and
$| \mathbf{P}^* | \geq n_1^1.$
Combeing these equations and inequalities we obtain
$| \mathbf{P} | \geq n_1^1 + n_1^2 + ... + n_1^{w+1} - (w+1)$
proving the assertion. □

Remark: The problem of minimizing the number of paths in a CPS of a tree is equivalent to the problem of maximizing a set in an intersection of two matroids (see [20]).
This problem having a good solution algorithm (i.e., being solvable in polynomial time), it is conceivable that there are also other simple algorithms for finding a MCPS.

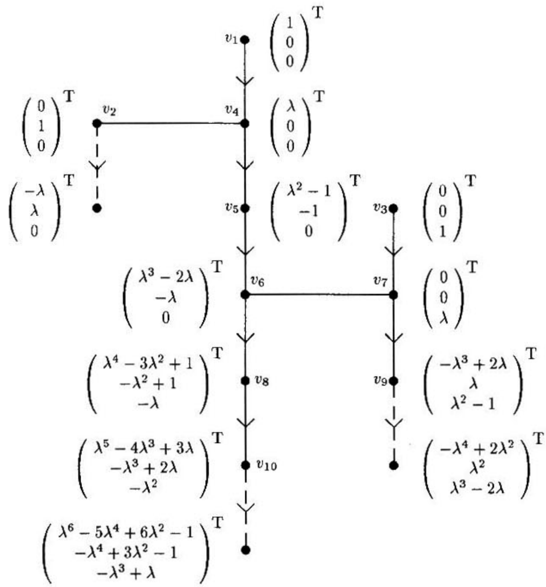


Figure 11

Example 2:
For the tree T in Figure 1 (see Figure 11 with labelled vertices) we obtain the following matrices:

$$\mathbf{D}(T(\overline{\mathbf{P}}),\lambda) = \begin{pmatrix} 1 & 0 & 0 & \lambda & \lambda^2-1 & 0 & \lambda^4-3\lambda^2+1 & -\lambda^3+2\lambda & \lambda^5-4\lambda^3+3\lambda \\ 0 & 1 & 0 & 0 & -1 & 0 & -\lambda^2+1 & \lambda & -\lambda^3+2\lambda \\ 0 & 0 & 1 & 0 & 0 & \lambda & -\lambda & \lambda^2-1 & -\lambda^2 \end{pmatrix}^T$$

and

$$\mathbf{D}^*(T(\overline{\mathbf{P}}),\lambda) = \begin{pmatrix} -\lambda & \lambda^6-5\lambda^4+6\lambda^2-1 & -\lambda^4+2\lambda^2 \\ \lambda & -\lambda^4+3\lambda^2-1 & \lambda^2 \\ 0 & -\lambda^3+\lambda & \lambda^3-2\lambda \end{pmatrix}^T.$$

Thus $P_T(\lambda) = \varepsilon \cdot det\mathbf{D}^*(T(\overline{\mathbf{P}}),\lambda)$ and for the double root $\lambda^0 = 0$ of $P_T(\lambda)$, $\mathbf{y}_1^0 = (1,0,0)$, $\mathbf{y}_2^0 = (1,-1,0)$ are linearly independent solutions to (*) and the vectors $\mathbf{x}_1^0, \mathbf{x}_2^0$ corresponding to $\mathbf{y}_1^0, \mathbf{y}_2^0$ by (**) are eigenvectors of T belonging to λ^0; their components are given in Figure 7.

5 Another algorithm to calculate $P_T(\lambda)$

Let T be a tree with at least 3 vertices and $v" \in V(T)$. Let $val_1(v", T) = | N(v", T) \cap V_1(T) |$ denote the number of pendent vertices of T which are adjacent to vertex $v"$. Assign to every vertex v of T the weight $w(v) = w(v,T) := val_1(v,T)$ and delete all pendent vertices of T. Thus T is turned into a weighted tree which we denote by $H = H(T)$. H is called the **reduced tree** of T (Figure 12). Find an MCPS $\overline{\mathbf{P}}(H)$ of H with q paths and construct $H(\overline{\mathbf{P}})$, $\vec{H}$, $\vec{H}^*$ (Figure 12) as described above for T.

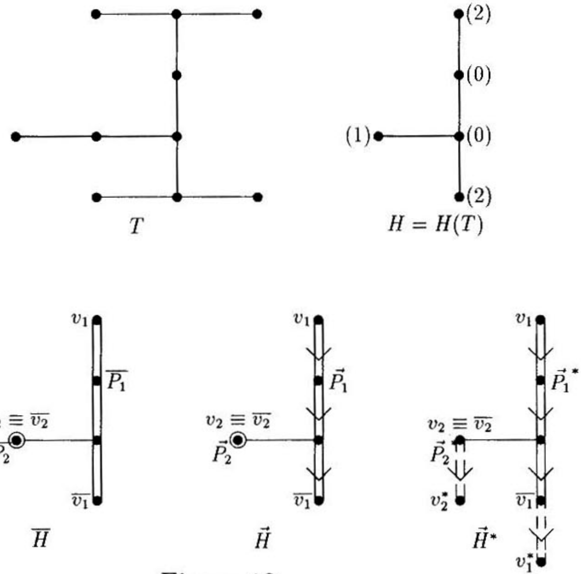


Figure 12

Algorithm H

To every vertex v of $\overrightarrow{H}^{*}$ assign a vector $\mathbf{f}(v,\lambda) = (f_1(v,\lambda), f_2(v,\lambda), ..., f_q(v,\lambda))$ by use of the following rules

(**H**.1) For a source v_k put
$\mathbf{f}(v_k,\lambda) = (\delta_{1k}, \delta_{2k}, ..., \delta_{qk})$,
where $\delta_{ii} = 1$ and $\delta_{ik} = 0$ for $i \neq k$ $(i, k = 1, 2, ..., q)$;

(**H**.2) for any vertex v of $\overrightarrow{H}^{*}$ which is not a source, put
$\mathbf{f}(v,\lambda) = (\lambda - w(v^+)\cdot\mu)\cdot\mathbf{f}(v^+,\lambda) - \sum_{v' \in N^+(v)} \mathbf{f}(v',\lambda)$,
where $\mu := 1/\lambda$.

It is easy to see that the vectors for the sink vertices are uniquely determined by (**H**.1) and (**H**.2). Form the $q \times q$ matrix

$\mathbf{F}^{*}(H(\overline{\mathbf{P}}),\lambda) = (\mathbf{f}^{\mathrm{T}}(v_1^*,\lambda), \mathbf{f}^{\mathrm{T}}(v_2^*,\lambda), ..., f^{\mathrm{T}}(v_q^*,\lambda))^{\mathrm{T}} = (f_k(v_i^*,\lambda))$
$(i, k = 1, 2, ..., q)$.

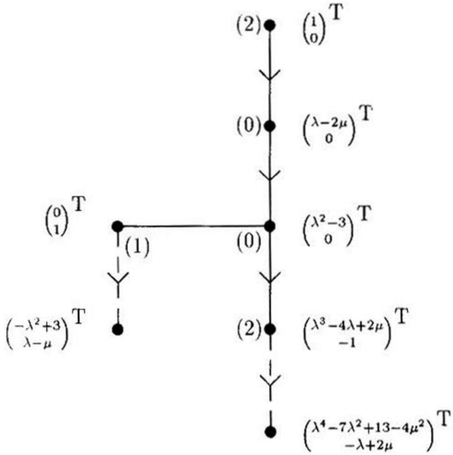
Theorem 4:
$P_T(\lambda) = \lambda^{n_1} \cdot det\mathbf{F}^{*}(H(\overline{\mathbf{P}}),\lambda)$, and $n_1 = n_1(T)$.

Note that this theorem is a modification of a theorem in [18]. □

The polynomial
$f_T(\lambda) := det\mathbf{F}^{*}(H(\overline{\mathbf{P}}),\lambda)$ is called **reduced characteristic polynomial** of T.

Note that this algorithm is also applicable for calculating the eigenvectors of T which belong to an eigenvalue $\lambda \neq 0$ using the procedure described above in slightly modified form.

Example 3:
The simple calculation of $P_T(\lambda)$ is given in Figure 13.



$$\mathbf{F}^*(H(\overline{\mathbf{P}}),\lambda) = \begin{pmatrix} \lambda^4-7\lambda^2+13-4\lambda^{-2} & -\lambda+2\lambda^{-1} \\ -\lambda^2+3 & \lambda+\lambda^{-1} \end{pmatrix},$$

$$f_T(\lambda) = \lambda^5 - 9\lambda^3 + 25\lambda - 23\lambda^{-1} + 4\lambda^{-3}$$

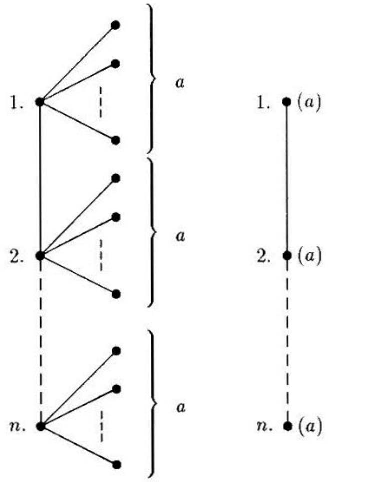
and

$$P_T(\lambda) = \lambda^5 f_T(\lambda)$$

Figure 13

6 Caterpillars

Let $C_n := C(n,a)$ be a caterpillar tree such that the reduced tree $H_n := H(C_n)$ is a weighted path with n vertices and every vertex has weight a (a = 1,2,...) (Figure 14).



$C_n = C(n,a)$ $\quad$ $H_n = H(C_n)$

Figure 14

Note that C_n has $N = n(a+1)$ vertices. In this case,
$P_{C_n}(\lambda) = \lambda^{an} \cdot f_{C_n}(\lambda)$, where $f_{C_n}(\lambda)$ satisfies the recursion

$(\otimes)$ $\quad f_{C_n}(\lambda) = (\lambda - \frac{a}{\lambda}) \cdot f_{C_{n-1}}(\lambda) - f_{C_{n-2}}(\lambda)$ (by use of algorithm **H**).

Thus $(\otimes)$ - in connection with the initial expressions $f_{C_0}(\lambda) := 1,\ f_{C_1}(\lambda) = \lambda - \frac{a}{\lambda}$ - enables $f_{C_n}(\lambda)$ and $P_{C_n}(\lambda)$ to be easily calculated. The result is the formula

$$f_{C_n}(\lambda) = \sum_{i=0}^{n}(-1)^i k_n(i)\lambda^{n-2i}$$

where $k_n(i)$ is the number of matchings with exactly i edges in C_n (see [17]). It is easy to prove (by induction) the validity of the following equations

$$k_n(i) = \begin{cases} 1, & \text{if} \quad n = 0 \\ a^n, & \text{if} \quad n = i > 0 \\ a \cdot k_{n-1}(i-1) + k_{n-2}(i-1) + k_{n-1}(i), & \text{if} \quad n \geq 2 \\ & \text{and} \quad i = 1, 2, ..., n-1, \end{cases}$$

$$k_n(i) = a^{2i-n} \cdot k_n(n-i) \text{ or } a^{n-i} \cdot k_n(i) = a^i \cdot k_n(n-i)$$

and

$$k_n(i) = \sum_{j=0}^{i} \alpha_n(i,j) a^{i-j},$$

where $\alpha_n(i,j) = \binom{n-j}{i} \cdot \binom{i}{j}$.

Therefore, the explicit formula for the characteristic polynomial of C_n is

$$(\otimes\otimes) P_{C_n}(\lambda) = \lambda^{an} \cdot \sum_{i=0}^{n} (-1)^i \Big\{ \sum_{j=0}^{i} \binom{n-j}{i} \binom{i}{j} a^{i-j} \Big\} \cdot \lambda^{n-2i} = \\ = \sum_{i=0}^{n} (-1)^i \Big\{ \sum_{j=0}^{i} \binom{n-j}{i} \binom{i}{j} a^{i-j} \Big\} \lambda^{N-2i}. \qquad (1)$$

The eigenvalues for C_n are described in the following observation.

Observation 4:
C_n has the eigenvalue 0 with multiplicity $N - 2n = (a-1)n$ (because of $(\otimes\otimes)$). The remaining $2n$ eigenvalues can easily be obtained from $(\otimes)$ by using the trigonometric transformation $\lambda - \frac{a}{\lambda} = 2cos\varphi : \lambda_k^{\pm} = cos\frac{k\pi}{n+1} \pm \sqrt{cos^2\frac{k\pi}{n+1} + a}$ $(k = 1, 2, ..., n)$.
If λ_0 is a root of $P_{C_n}(\lambda)$, then $|\lambda_0| < 1 + \sqrt{a+1}$ and

$$\lim_{n\to\infty} max\{|\lambda| \,|\, P_{C_n}(\lambda) = 0\} = 1 + \sqrt{a+1}.$$

Note that the $\alpha_n(i,j)$ play also a role in the theory of dimer coverings of square lattices, see [21, 22], see also [23].

7 Cospectral trees

Two nonisomorphic graphs G', G'' are called cospectral if $P_{G'}(\lambda) = P_{G''}(\lambda)$.
In 1957 L. Collatz and U. Sinogowitz [24] showed that the two trees $T' = T'(a,b)$ and $T'' = T''(c,d)$ given in Figure 15 are cospectral if $(a,b,c,d) = (3,3,4,1)$.

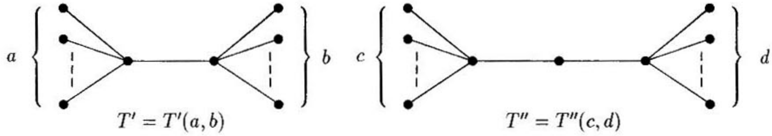


Figure 15

Define

$$\begin{aligned}
\tau_1(k) &:= (k+3, 2k+3, 2k+4, k+1),\\
\tau_2(u) &:= (u^2+u+1, u^2+u+1, (u+1)^2, u^2),\\
\tau_3(u,k) &:= (u^2+(k+1)u+1, u^2+(k+1)(u+1), u^2+(k+2)u+k+1, u^2+ku)
\end{aligned}$$

where k and u are integers. Note that $\tau_1(0) = \tau_2(1) = \tau_3(1,0) = (3,3,4,1)$. Trees T' and T'' are cospectral if $(a,b,c,d) = \tau_1(k),\ k \geq 0$, and if $(a,b,c,d) = \tau_2(u),\ u \geq 1$; this was shown by Mowshowitz [15] (1972) and by Schwenk [25] (1973), respectively. Using algorithm H we find that T' and T'' are also cospectral if and only if $(a,b,c,d) = \tau_3(u,k),\ k \geq 0,\ u \geq 1$.

8 Concluding remark

Note that Algorithm **T** can be applied in modified form (see, e.g., [26]) also for edge and vertex weighted trees.

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