Acta Math. Hungar., **114 (1–2)** (2007), 91–101.
DOI: 10.1007/s10474-006-0515-9

ON THE MULTIPLICITY OF THE EIGENVALUES OF A GRAPH

J. A. DE LA PEÑA[1] and J. RADA[2] *

[1] Instituto de Matemáticas, UNAM. Cd. Universitaria, México 04510 D.F.
e-mail: jap@matem.unam.mx

[2] Departamento de Matemáticas, Facultad de Ciencias, Universidad de los Andes,
Mérida, Venezuela
e-mail: juanrada@ula.ve

(Received June 20, 2005; revised July 10, 2006; accepted July 12, 2006)

Abstract. Given a graph G with characteristic polynomial $\varphi(t)$, we consider the ML-decomposition $\varphi(t) = q_1(t)q_2(t)^2 \dots q_m(t)^m$, where each $q_i(t)$ is an integral polynomial and the roots of $\varphi(t)$ with multiplicity j are exactly the roots of $q_j(t)$. We give an algorithm to construct the polynomials $q_i(t)$ and describe some relations of their coefficients with other combinatorial invariants of G. In particular, we get new bounds for the energy $E(G) = \sum_{i=1}^{n} |\lambda_i|$ of G, where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of G (with multiplicity). Most of the results are proved for the more general situation of a Hermitian matrix whose characteristic polynomial has integral coefficients.

1. Introduction

Let A be a Hermitian $n \times n$ matrix such that the characteristic polynomial $\varphi_A(t) = \det(tI_n - A)$ has integral coefficients. We consider the *multiplicity layered decomposition* (ML-*decomposition* for short) of $\varphi_A(t)$:

---

*This work was done during a visit of the second named author to UNAM.

Key words and phrases: Hermitian matrix, eigenvalues, characteristic polynomial, energy of a graph.

2000 Mathematics Subject Classification: 05C50, 15A48.

(ML1) $\varphi_A(t) = q_1(t)q_2(t)^2 \dots q_m(t)^m$ with $q_j(t) \in \mathbf{Z}[t]$ and $1 \neq q_m(t)$;

(ML2) $\lambda \in \mathbf{R}$ is a root of $\varphi_A(t)$ with multiplicity j if and only if $q_j(\lambda) = 0$.

Obviously, if $\varphi_A(t)$ has no roots of multiplicity j, then $q_j(t) = 1$. We shall give an algorithmic construction of the polynomials $q_j(t)$ using the Euclidean algorithm in the family of derivatives $\varphi_A^{(j)}(t)$ of $\varphi_A(t)$. We show that the following properties are satisfied by the ML-decomposition.

(ML3) λ is a root of $q_j(t)$ if and only if for every principal $i \times i$ submatrix B of A with $n - j + 1 \leqq i \leqq n$, we have $\varphi_B(\lambda) = 0$ and $\varphi_{B'}(\lambda) \neq 0$ for a principal $(n-j) \times (n-j)$ submatrix B' of A.

(ML4) For $1 \leqq j \leqq m - 1$ the derivative $\varphi_A^{(j)}(t)$ accepts an ML-decomposition $\varphi_A^{(j)}(t) = \hat{q}_{j+1}(t)q_{j+2}(t)^2 \dots q_m(t)^{m-j}$ with $\hat{q}_{j+1}(t) = r_j(t)q_{j+1}(t)$ for some $r_j(t) \in \mathbf{Z}[t]$, such that the simple roots of $\varphi_A^{(j)}(t)$ are exactly the roots of $\hat{q}_{j+1}(t)$.

Motivation for considering the ML-decomposition arises from applications to connected graphs G without loops or multiple edges and its characteristic polynomial $\varphi_G(t) = \varphi_{A(G)}(t)$ where $A(G)$ is the adjacency matrix of G. Multiplicities of roots of $\varphi_G(t)$ are related to symmetries of the graph G [3, Ch. 6], regularity properties [3, Ch. 7] and important structural properties of the graph G. Moreover, in this paper we get further elementary applications of the ML-decomposition for $\varphi_G(t)$. Indeed, let $q_j(t) = t^{n_j} + a_{j1}t^{n_j-1} + \dots + a_{jn_j}$ be the polynomials obtained from the ML-decomposition. We show the following:

(a) $\varphi_G(t) = q_1(t)q_2(t)^2 \dots q_m(t)^m$ with $m = m(G)$ maximal j such that $n_j \geqq 1$.

(b) $n_1 \geqq 1$, since the *spectral radius* $\rho(G) = \max\left\{ \|\lambda\| : \varphi_G(\lambda) = 0 \right\}$ is a simple root of $\varphi_G(t)$.

(c) If $K = G \setminus \{a_1, \dots, a_k\}$ is obtained from G by deleting the vertices $a_1, \dots, a_k$, then $m(G) \leqq m(K) + k$.

(d) $\frac{\varphi'_G(t)}{\varphi_G(t)} = \sum_{j=1}^{m} j \frac{q'_j(t)}{q_j(t)}$; which implies that a real number λ is a root of $\varphi_G(t)$ with multiplicity m_λ if and only if $\lim_{t \to \lambda} \frac{(t-\lambda)\varphi'_G(t)}{\varphi_G(t)} = m_\lambda$.

(e) The *minimal polynomial* of $A(G)$ is $\mu_G(t) = q_1(t)q_2(t) \dots q_m(t)$. In particular, $\sum_{j=1}^{m} n_j \geqq \operatorname{diam}(G) + 1$, where $\operatorname{diam}(G)$ is the *diameter* of the graph G. As a consequence we also get $m(G) \leqq n - \operatorname{diam}(G)$.

For any polynomial $q(t)$ with real roots, define the *energy* of $q(t)$ by $E\big(q(t)\big) = \sum|\lambda|$, where λ runs over the roots of $q(t)$, counting multiplicities.

(f) $E(G) = \sum_{j=1}^{m} jE\big(q_j(t)\big)$, which yields the following McClelland-type bounds for the energy:

$$\sum_{j=1}^{m} j\sqrt{a_{j1}^2 - 2a_{j2} + n_j(n_j-1)|a_{jn_j}|^{2/n_j}} \leqq E(G) \leqq \sum_{j=1}^{m} j\sqrt{n_j(a_{j1}^2 - 2a_{j2})}.$$

2. The multiplicity layered decomposition

2.1. Let A be a Hermitian $n \times n$ matrix such that the characteristic polynomial $\varphi_A(t)$ has integral coefficients. Then the eigenvalues of A are the roots of $\varphi_A(t)$, all of them real $\lambda_1 \leqq \lambda_2 \leqq \dots \leqq \lambda_n$. For any eigenvalue λ of A, we denote by m_λ the multiplicity of λ (writing $m(A,\lambda)$ if some confusion arises).

We shall consider irreducible polynomials in $\mathbf{Z}[t]$ (or equivalently in $\mathbf{Q}[t]$).

LEMMA. *Let λ be an eigenvalue of A with multiplicity m_λ. Let $q(t)$ be an irreducible polynomial such that $q(\lambda) = 0$. Then the following happen:*

(a) *$q(t)$ has minimal degree among those polynomials $p(t) \in \mathbf{Z}[t]$ with $p(\lambda) = 0$.*

(b) *If $q(\lambda') = 0$ for some $\lambda' \in \mathbf{C}$, then λ' is an eigenvalue of A with $m_{\lambda'} = m_\lambda$.*

PROOF. (a) In fact $q(t)$ generates the ideal in $\mathbf{Z}[t]$ of those $p(t)$ with $p(\lambda) = 0$.

(b) $q(t)$ divides $\varphi_A(t)$, hence λ' is an eigenvalue of A. The multiplicity m_λ is the maximal i such that $q(t)^i$ divides $\varphi_A(t)$. Therefore $m_\lambda = m_{\lambda'}$. □

2.2. According to (2.1) we consider irreducible polynomials $p_1(t), \dots, p_s(t) \in \mathbf{Z}[t]$ such that each λ_i is a root of exactly one $p_j(t)$, $1 \leqq i \leqq n$. For each $1 \leqq i \leqq s$, consider $r(j) = \max\big\{k : p_j(t)^k \text{ divides } \varphi_A(t)\big\}$. Set

$$q_i(t) = \prod_{r(j)=i} p_j(t),$$

which yields an ML-decomposition $\varphi_A(t) = q_1(t)q_2(t)^2 \dots q_m(t)^m$.

Since $\varphi_A(t)$ is a monic polynomial, we may assume that each $p_j(t)$ and also $q_j(t)$ are monic polynomials. Set $m(G) = \max\big\{j : q_j(t) \neq 1\big\}$. We shall need the following:

LEMMA (cf. [1]). $\varphi_A^{(k)}(t) = k! \sum_{\mathcal{P}_{n-k}(A)} \varphi_B(t)$, *where the sum runs over the set* $\mathcal{P}_{n-k}(A)$ *of all principal* $(n-k) \times (n-k)$*-submatrices of* A.

PROOF. The proof in [1] considers the case $k = 1$. The general statement follows by induction. □

2.3. PROPOSITION. *For a root* λ *of* $\varphi_A(t)$ *the following are equivalent:*

(a) λ *has multiplicity* k.

(b) $q_k(\lambda) = 0$.

(c) *For any principal* $j \times j$*-submatrix* B *of* A *with* $n - k + 1 \leqq j \leqq n$, *we have* $\varphi_B(\lambda) = 0$ *and* $\varphi_{B'}(\lambda) \neq 0$ *for some* $(n-k) \times (n-k)$*-submatrix* B' *of* A.

PROOF. (a) $\Leftrightarrow$ (b) is clear.

(b) $\Rightarrow$ (c) Let $\lambda_1 \leqq \lambda_2 \leqq \dots \leqq \lambda_n$ be the eigenvalues of A and $\mu_1 \leqq \mu_2 \leqq \dots \leqq \mu_j$ those of a principal $j \times j$-submatrix B of A with $n - k + 1 \leqq j \leqq n$, then by the *interlacing theorem* (see for example [3] for other applications):

$$\lambda_i \leqq \mu_i \leqq \lambda_{n-j+i}, \ (i = 1, \dots, j).$$

If $\lambda_t = \lambda_{t+1} = \dots = \lambda_{t+k-1} = \lambda$, then $\lambda_t \leqq \mu_t \leqq \lambda_{n-j+t}$ with $n - j + t \leqq t + k - 1$ and $\mu_t = \lambda$.

In case λ is a root of all $B \in \mathcal{P}_k(A)$, then by the lemma above, $\varphi_A^{n-k}(\lambda) = 0$ and λ has multiplicity at least $k+1$, a contradiction.

(c) $\Rightarrow$ (a) Apply again the Lemma. □

2.4. Let A be a Hermitian matrix with characteristic polynomial $\varphi_A(t) \in \mathbf{Z}[t]$. Let $\varphi_A(t) = \prod_{j=1}^{m} q_i(t)^i$ the ML-decomposition with $q_m(t) \neq 1$.

LEMMA. $q_m(t) = \operatorname{mcd}\left(\varphi_A(t), \varphi_A^{(1)}(t), \dots, \varphi_A^{(m-1)}(t)\right)$.

PROOF. The claim follows from a straightforward but tedious calculation, we shall illustrate only the case $m = 3$.

$$\varphi_A = q_1 q_2^2 q_3^3 \text{ (omitting the variable } t),$$

$$\varphi_A' = q_1' q_2^2 q_3^3 + 2q_1 q_2 q_2' q_3^3 + 3q_1 q_2^2 q_3^2 q_3' = (q_1' q_2 q_3 + 2q_1 q_2' q_3 + 3q_1 q_2 q_3') q_2 q_3^2,$$

where the polynomial r_1 in parenthesis is not divisible by any q_i, $i = 1, 2, 3$. (Indeed, if p is an irreducible factor of q_1 dividing also r_1, then $p \mid q_1' q_2 q_3$. By (2.1), $p \nmid q_i$, $i = 2, 3$ and therefore $p \mid q_1' = p's + ps'$ where $s \in \mathbf{Z}[t]$ such that $q_1 = ps$. This implies $p \mid p's$ and $p \mid s$, which in turn implies that q_1 has multiple roots, a contradiction. The cases $i = 2, 3$ are similar.) Now, $\varphi_A'' = r_2 q_3$ with $r_2 = r_1' q_2 q_3 + r_1 q_2' q_3 + 2r_1 q_2 q_3'$ is not divisible by any q_i, $i = 1, 2, 3$. Hence $q_3 = \operatorname{mcd}(\varphi_A, \varphi_A', \varphi_A'')$. □

The inductive construction of the polynomials $q_1(t),\dots,q_m(t)$ is easily carried out:

$$q_m(t) = \operatorname{mcd}\big(\varphi_A(t), \varphi_A'(t), \dots, \varphi_A^{(m-1)}(t)\big),$$

$$q_{m-1}(t) = \operatorname{mcd}\left(\frac{\varphi_A(t)}{q_m(t)^m}, \frac{\varphi_A'(t)}{q_m(t)^{m-1}}, \dots, \frac{\varphi_A^{(m-2)}(t)}{q_m(t)^2}\right),$$

$$\vdots$$

$$q_2(t) = \operatorname{mcd}\left(\frac{\varphi_A(t)}{q_3(t)^3 \dots q_m(t)^m}, \frac{\varphi_A'(t)}{q_3(t)^2 \dots q_m(t)^{m-1}}\right),$$

$$q_1(t) = \frac{\varphi_A(t)}{q_2(t)^2 q_3(t)^3 \dots q_m(t)^m}.$$

2.5. To get more precise information on the derivatives of $\varphi_A(t)$ we need some results of elementary analysis.

PROPOSITION. *Let $p(t)$ be a polynomial of degree n whose roots are real. Then the following hold:*

(a) *For every $1 \leqq j \leqq n-1$, $p^{(j)}(t)$ has only real roots.*

(b) *If $\lambda_1 \leqq \lambda_2 \leqq \dots \leqq \lambda_n$ are the roots of $p(t)$ and $\mu_1 \leqq \mu_2 \leqq \dots \leqq \mu_j$ the roots of $p^{(j)}(t)$, then $\lambda_i \leqq \mu_i \leqq \lambda_{n-j+i}$ $(i = 1,\dots,j)$.* □

2.6. Let $\varphi_A(t) = \prod_{i=1}^{m} q_i(t)^i$ be the ML-decomposition as above.

PROPOSITION. *For any $i \geqq 1$, the following is an ML-decomposition:*

$$\varphi_A^{(i)}(t) = \big(r_i(t) q_{i+1}(t)\big)\, q_{i+2}(t)^2 \dots q_m(t)^{m-i},$$

that is, λ is a simple root of $\varphi_A^{(i)}(t)$ if and only if $r_i(\lambda) = 0$ or $q_{i+1}(\lambda) = 0$, where $r_i = r_{i-1}' q_i q_{i+1} \dots q_m + \sum_{j=0}^{m-i} (j+1) r_{i-1} q_i \dots q_{i+j-1} q_{i+j}' q_{i+j+1} \dots q_m$, with $r_0(t) = 1$.

PROOF. The given decomposition follows by induction. It is enough to show that λ is a simple root of $\varphi_A^{(i)}(t)$ if and only if $r_i(\lambda) = 0$ or $q_{i+1}(\lambda) = 0$. We show it by induction on i, the case $i = 0$ being clear.

Assume $q_{i+1}(\lambda) = 0$ and λ is not a simple root of $\varphi_A^{(i)}(t)$. Then by (2.1), $r_i(\lambda) = 0$. Hence $r_{i-1}(\lambda) q_i(\lambda) q_{i+1}'(\lambda) q_{i+1}(\lambda) \dots q_m(\lambda) = 0$ and only $r_{i-1}(\lambda) = 0$ is possible, which contradicts the induction hypothesis.

Assume $r_i(\lambda) = 0$ and λ is not a simple root of $\varphi_A^{(i)}(t)$. By (2.5), λ is also a root of $\varphi_A^{(i-1)}(t) = \big(r_{i-1}(t)q_i(t)\big)\, q_{i+1}(t)^2 \dots q_m(t)^{m-i+1}$.

If $r_{i-1}(\lambda) = 0$, by induction hypothesis, λ is a simple root of $\varphi_A^{(i-1)}(t)$. On the other hand, $r'_{i-1}(\lambda)q_i(\lambda)\dots q_m(\lambda) = 0$ and either $r'_{i-1}(\lambda) = 0$ or $q_{i+j}(\lambda) = 0$ (for any $0 \leqq j \leqq m-i$) yield a contradiction.

If $q_{i+j}(\lambda) = 0$ for some $0 \leqq j \leqq m-i$, we get

$$r_{i-1}(\lambda)q_i(\lambda)\dots q_{i+j-1}(\lambda)q'_{i+j}(\lambda)\dots q_m(\lambda) = 0$$

which also yields a contradiction.

The converse of the claim is clear. □

2.7. The following result shows an interesting relation between the polynomials $r_i(t)$ as defined in (2.6).

PROPOSITION. *For $1 \leqq i \leqq m-1$, and for any $\lambda \in \mathbf{R}$, we have*

$$r_i(\lambda)^2 \geqq r_{i-1}(\lambda)q_i(\lambda)r_{i+1}(\lambda).$$

PROOF. Any polynomial $p(t)$ having only real roots $\mu_1 \leqq \mu_2 \leqq \dots \leqq \mu_n$ satisfies

$$\frac{p'(t)}{p(t)} = \sum_{i=1}^{n} \frac{1}{t-\mu_i} \quad \text{and} \quad \frac{p''(t)p(t) - p'(t)^2}{p(t)^2} = -\sum_{i=1}^{n} \frac{1}{(t-\mu_i)^2}$$

which is negative for any $\lambda \neq \mu_i$ $(1 \leqq i \leqq n)$. Hence

$$p'(\lambda)^2 \geqq p''(\lambda)p(\lambda) \quad \text{for any} \quad \lambda \in \mathbf{R}.$$

Applying this inequality for $p(t) = \varphi_A^{(i)}(t)$ and using (2.6) the result follows.
□

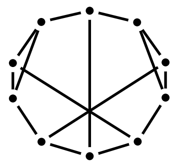
3. ML-decomposition for graphs

3.1. Let G be a connected graph without loops or multiple edges. Let $1, \dots, n$ be the vertices of G and $A = A(G)$ its adjacency matrix. The results of Section 2 apply since A is a symmetric matrix and the characteristic polynomial $\varphi_G(t)$ has integral coefficients. Set $\varphi_G(t) = t^n + a_1 t^{n-1} + \dots + a_n$ and let $\lambda_1 \leqq \lambda_2 \leqq \dots \leqq \lambda_n$ be its (real) roots.

Consider the ML-decomposition $\varphi_G(t) = \prod_{j=1}^{m} q_j(t)^j$ with $n_m \geqq 1$, where n_j is the degree of $q_j(t)$ (write $m(G) := m$). The Perron–Frobenius Theorem (see [4]) says that the spectral radius $\rho(G)$ is a simple root of $\varphi_G(t)$. Therefore $q_1(t) \neq 1$.

The *minimal polynomial* is $\mu_G(t) = \prod_{j=1}^{m} q_j(t)$.

3.2. Examples. (1) Let G be the cubic graph



with 10 vertices and characteristic polynomial

$$\varphi(t) = t^{10} - 15t^8 - 4t^7 + 75t^6 + 24t^5 - 157t^4 - 36t^3 + 144t^2 + 16t - 48.$$

Then

$$q_1(t) = t^2 - 5t + 6 = (t-3)(t-2) \quad \text{and} \quad \rho(G) = 3,$$

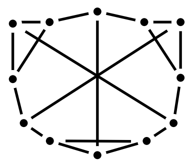
$$q_2(t) = t + 1, \qquad q_3(t) = t^2 + t - 2 = (t-1)(t+2).$$

The ML-decompositions of the derivatives of $\varphi(t)$ are as follows:

$$\varphi'(t) = \left[(5t^4 - 15t^3 - 10t^2 + 36t + 2)(t+1)\right]\left[(t-1)(t+2)\right]^2$$

$$\varphi''(t) = \left[(15t^6 - 15t^5 - 95t^4 + 37t^3 + 148t^2 + 6t - 24)(t-1)(t+2)\right].$$

(2) Let G be the cubic graph



with 12 vertices and with characteristic polynomial

$$\varphi(t) = t^{12} - 18t^{10} - 2t^9 + 117t^8 + 72t^7 - 339t^6$$
$$- 306t^5 + 414t^4 + 532t^3 - 99t^2 - 324t - 108.$$

Then

$$q_1(t) = t - 3 \quad \text{and} \quad \rho(G) = 3,$$

$$q_2(t) = t^3 - t^2 - 5t + 6 = (t-2)(t^2 + t - 3) \quad \text{with roots} \quad -2.3 < 1.3 < 2,$$

$$q_5(t) = t + 1.$$

3.3. Let G be a graph as in (3.1). The principal $(n-k) \times (n-k)$-submatrices of $A(G)$ correspond to the full subgraphs of G obtained by deleting k vertices. Then (2.2) and (2.3) yield:

PROPOSITION. *Let λ be a root of $\varphi_G(t)$. The following are equivalent:*

(a) *λ has multiplicity k.*

(b) $q_k(\lambda) = 0$.

(c) *For any full subgraph $K = G \setminus \{a_1, \dots, a_j\}$ with $n - k + 1 \leqq j \leqq n$ we have $\varphi_K(\lambda) = 0$ and there is a full subgraph $K' = G \setminus \{a_1, \dots, a_{n-k}\}$ with $\varphi_{K'}(\lambda) \neq 0$.* □

COROLLARY. *Let $K = G \setminus \{a_1, \dots, a_k\}$ be a full subgraph of G. Then $m(G) \leqq m(K) + k$.* □

3.4. For any polynomial $p(t)$ with (possibly repeated) real roots $\lambda_1 \leqq \lambda_2 \leqq \dots \leqq \lambda_n$, we have

$$\frac{p'(t)}{p(t)} = \sum_{i=1}^{n} \frac{1}{t - \lambda_i}.$$

Hence for the ML-decomposition we get

$$\frac{\varphi_G'(t)}{\varphi_G(t)} = \sum_{j=1}^{m} j \, \frac{q_j'(t)}{q_j(t)}.$$

There are several uses of these rational functions (see [5, Ch. 2]). Two important facts are the following:

(a) $\lim\limits_{t \to \lambda} \frac{\varphi_G'(t)(t-\lambda)}{\varphi_G(t)} = m_\lambda$ is the multiplicity of λ as a root of $\varphi_G(t)$.

(b) $\frac{\varphi_G'(t)}{\varphi_G(t)} = \sum\limits_{r \geqq 0} \operatorname{tr}\left(A(G)^r\right) x^{-(r+1)}$ is the generating function in the variable x^{-1}.

Note that $\operatorname{tr}\left(A(G)^r\right)$ counts the number of closed walks of length r in G.

For the polynomials $q_j(t) = t^{n_j} + a_{j1}t^{n_j-1} + \dots + a_{jn_j}$ we define the *companion matrix*

$$A_j = \begin{bmatrix} -a_{j1} & -a_{j2} & \dots & -a_{jn_{j-1}} & -a_{jn_j} \\ 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ & & \ddots & \vdots & \vdots \\ & 0 & & 1 & 0 \end{bmatrix}$$

which satisfies $\det(tI_{n_j} - A_j) = q_j(t)$. The trace of the powers A_j^r is easily written as a polynomial in the coefficients $a_{j1}, \dots, a_{jn_j}$. For instance:

$$\operatorname{tr}(A_j) = -a_{j1}, \quad \operatorname{tr}(A_j^2) = a_{j1}^2 - 2a_{j2}, \quad \operatorname{tr}(A_j^3) = -a_{j1}^3 + 3a_{j1}a_{j2} - 2a_{j3}.$$

PROPOSITION. $\operatorname{tr}\big(A(G)^r\big) = \sum_{j=1}^{m} j \operatorname{tr}(A_j^r)$. □

3.5. The *diameter* $\operatorname{diam}(G)$ of G is the longest distance between two vertices of G.

PROPOSITION. (a) $\sum_{j=1}^{m(G)} n_j \geqq \operatorname{diam}(G) + 1$.

(b) $\sum_{j=2}^{m(G)} (j-1)n_j \leqq n - \operatorname{diam}(G) - 1$.

(c) $m(G) \leqq n - \operatorname{diam}(G)$.

PROOF. (a) $\sum_{j=1}^{m(G)} n_j$ is the number of distinct eigenvalues of G. This number is at least $\operatorname{diam}(G) + 1$ (see for example [3, 3.13]).

(b) Since $n = \sum_{j=1}^{m(G)} jn_j$, the inequality follows from (a).

(c) Follows from (b). □

4. The energy of a graph and the ML-decomposition

4.1. The purpose of this section is to obtain McClelland-type bounds for the energy of a graph as an application of the ML-decomposition.

First observe that McClelland's bounds hold for quite general situations namely:

THEOREM (cf. [7]). *Let A be a Hermitian $n \times n$-matrix and let $E(A) = \sum_{i=1}^{n} |\lambda_i|$ be the energy of A, where $\lambda_1 \leqq \lambda_2 \leqq \dots \leqq \lambda_n$ are the eigenvalues of A counted with multiplicities. Then*

$$\sqrt{\operatorname{tr}(A^2) + n(n-1)|\det A|^{2/n}} \leqq E(A) \leqq \sqrt{n \operatorname{tr}(A^2)}.$$

PROOF (cf. [6]). We have

$$E(A)^2 = \sum_{i=1}^{n} |\lambda_i|^2 + 2\sum_{j<k} |\lambda_j|\,|\lambda_k| = \operatorname{tr}(A^2) + n(n-1)\,\mathrm{AM}\left\{ |\lambda_j|\,|\lambda_k| \right\},$$

where AM denotes the arithmetic mean. Let $\mathrm{GM}\left\{ |\lambda_j|\,|\lambda_k| \right\} = |\det A|^{2/n}$ be the geometric mean. Then GM $\leqq$ AM yields the first inequality.

Moreover, the variance of the numbers $|\lambda_j|$, $j = 1, 2, \dots, n$ is:

$$0 \leqq \operatorname{var}\left\{ |\lambda_j| \right\} = \mathrm{AM}\left\{ |\lambda_j|^2 \right\} - \left(\mathrm{AM}\left\{ |\lambda_j| \right\}\right)^2$$

$$= \frac{1}{n}\sum_{j=1}^{n} |\lambda_j|^2 - \left[\frac{1}{n}\sum_{j=1}^{n} |\lambda_j|\right]^2 = \frac{1}{n}\operatorname{tr}(A^2) - \left(\frac{E(A)}{n}\right)^2$$

and the second inequality holds.

4.2. THEOREM. *We have*

$$\sum_{j=1}^{m(G)} j\sqrt{[a_{j1}^2 - 2a_{j2}] + n_j(n_j-1)|a_{jn_j}|^{2/n_j}} \leqq E(G) \leqq \sum_{j=1}^{m(G)} j\sqrt{n_j[a_{j1}^2 - 2a_{j2}]}.$$

PROOF. Using that

$$\frac{\varphi_G'(t)}{\varphi_G(t)} = \sum_{j=1}^{m(G)} j\,\frac{q_j'(t)}{q_j(t)} \quad \text{and} \quad n = \sum_{j=1}^{m(G)} jn_j,$$

and Coulson Theorem [2], we get

$$E(G) = \frac{1}{\pi}\int_{-\infty}^{\infty}\left[n - \frac{it\varphi_G'(it)}{\varphi_G(it)}\right]dt = \sum_{j=1}^{m(G)} \frac{j}{\pi}\int_{-\infty}^{\infty}\left[n_j - \frac{itq_j'(it)}{q_j(it)}\right]dt$$

$$= \sum_{j=1}^{m(G)} jE(A_j),$$

where A_j is the companion matrix of $q_j(t)$. Here $i = \sqrt{-1}$.

By (3.4), $\operatorname{tr}(A_j^2) = a_{j1}^2 - 2a_{j2}$ and $\det A_j = a_{jn_j}$. The result follows from (4.1). □

4.3. As an example we calculate McClelland bounds and the bounds (4.2) for the graph (3.2 (2)):

	lower	$E(G)$	upper
McClelland's bounds	17.94		20.19
		19.2	
(4.2) bounds	19.1		19.48

References

[1] F. Clarke, A graph polynomial and its applications, *Discrete Mathematics,* **3** (1972), 305–313.

[2] C. A. Coulson, On the calculation of the energy in unsaturated hydrocarbon molecules, *Proc. Cambdrigde Phil. Soc.,* **36** (1940), 201–203.

[3] D. Cvetković, M. Doob and H. Sacks, *Spectra of Graphs,* Academic Press (1979).

[4] F. R. Gantmacher, *Matrix Theory,* Vol. II, Chelsea (1974).

[5] C. D. Godsil, *Algebraic Combinatorics,* Chapman and Hall Mathematics (1993).

[6] I. Gutman, The energy of a graph, *10. Steiemarkisches Math. Symposium Graz* (1978).

[7] F. J. McClelland, Properties of the latent roots of a matrix: the estimation of π-electron energies, *J. Chem. Phys.,* **54** (1971), 640–643.