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On the energy of symmetric matrices and Coulson's integral formula

Sobre la energía de matrices simétricas y la fórmula integral de Coulson

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Abstract. We define the *outer energy* of a real *symmetric* matrix M as

$$E_{out}(M) = \sum_{i=1}^{n} \left|\lambda_i - \overline{\lambda}(M)\right|$$

for the eigenvalues $\lambda_1, \ldots, \lambda_n$ of M and their arithmetic mean $\overline{\lambda}(M)$. We discuss the properties of the outer energy in contrast to the *inner energy* defined as $E_{inn}(M) = \sum\limits_{i=1}^{n} |\lambda_i|$. We prove that E_{inn} is the maximum among the energy functions $e : S(n) \to \mathbb{R}$ and E_{out} among functions $f\left(M - \overline{\lambda}(M)1_n\right)$, where f is an energy function. We prove a variant of the Coulson integral formula for the outer energy.

Key words and phrases. Total π-electron energy, Energy of a symmetric matrix, Bounds for energy, Coulson's integral formula.

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Resumen. Definimos la energía exterior de una matriz simétrica real M como

$$E_{out}(M) = \sum_{i=1}^{n} \left|\lambda_i - \overline{\lambda}(M)\right|$$

donde $\lambda_1, \ldots, \lambda_n$ son los autovalores de M y $\overline{\lambda}(M)$ es su media aritmética. Discutimos las propiedades de la energía exterior en contraste con la *energía* *interior* definida como $E_{inn}(M) = \sum_{i=1}^{n} |\lambda_i|$. Demostramos que E_{inn} es máxima entre todas las funciones de energía $e : S(n) \to \mathbb{R}$ y E_{out} entre todas las funciones $f\left(M - \overline{\lambda}(M)1_n\right)$, donde f es una función de energía. Demostramos una variante de la fórmula integral de Coulson para la energía exterior.

Palabras y frases clave. Energía π-electrón total, Energía de una matriz simétrica, Cotas para la energía, Fórmula integral de Coulson.

1. Introduction

Research on *energy of a graph* goes back to the work of Erich Hückel on the approximate solution of the Schrödinger equation of certain organic molecules. Generalizing from facts observed in this molecular theory, Gutman introduced in [7] the definition of the *energy of a graph* G as

$$E(G) = \sum_{i=1}^{n} |\lambda_i|$$

where n is the number of vertices and $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix $A(G) = (a_{ij})$, defined as $a_{ij} = 1$ if there is an edge between i and j and 0 otherwise. Details on the development of the mathematical concept and its associated chemistry applications can be seen in the recent book [14].

We denote by $\varphi_G(x)$ (or simply $\varphi(x)$ when no confusion arises) the *characteristic polynomial* of the graph G defined as

$$\varphi(x) = det\,(x1_n - A(G))$$

which is a monic polynomial of degree n whose roots are the eigenvalues $\lambda_1, \ldots, \lambda_n$ of the adjacency matrix $A(G)$. In the theory of graph energy a prominent role is played by the Coulson integral formula

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \left(n - \frac{ix\varphi'(ix)}{\varphi(ix)} dx \right)$$

where $\varphi'(x) = \left(\frac{d}{dx}\right)\varphi(x)$ is the first derivative of $\varphi(x)$. A derivation of the integral formula as well as several of its chemical applications can be seen in [14] (see also [10]).

In 2006 Gutman and Zhou [11] introduced a new energy based on the Laplacian matrix of a graph G, defined as $L = D - A$, where $D = diag\,(d_1, \ldots, d_n)$ is the diagonal matrix of vertex degrees and A is the adjacency matrix of G. Note that if $\mu_1, \ldots, \mu_n$ are the eigenvalues of L then $\sum_{i=1}^{n} |\mu_i| = 2m$, where m is the number of edges of G, and thus is trivial. With the intention to conceive a graph-energy-like quantity that preserves the main features of the original graph energy, Gutman and Zhou defined the Laplacian energy of a graph G with n vertices and m edges as $LE\left(G\right)=\sum_{i=1}^{n}\left|\mu_i-\frac{2m}{n}\right|$.

Later Consonni and Todeschini [6] used the expression $E\left(M\right)=\sum_{i=1}^{n}\left|\xi_i-\overline{\xi}\right|$, where $\xi_1,\ldots,\xi_n$ are the eigenvalues of a molecular matrix and $\overline{\xi}$ is their arithmetic mean, for designing quantitative structure-property relations for a variety of physical-chemical properties of a number of classes of organic compounds. Note that in the case of the Laplacian matrix L, the arithmetic mean of its eigenvalues is precisely $\frac{2m}{n}$, so the Laplacian energy of a graph is a particular case of this expression.

After this a large number of energies appeared in the mathematical and mathematico-chemical literature, which were based on the eigenvalues of matrices associated to the graph. For example, the signless Laplacian energy ([1],[26]), the normalized Laplacian energy [5], the distance energy ([13],[25]), also generalizations to digraphs ([18],[19],[20],[21],[22],[23],[24]) and ([2],[3],[4]), among others. Motivated by the analogous forms of various graph energies, Gutman [8] proposed an ultimate extension of the graph-energy concept as

$$E_X=\sum_{i=1}^{n}\left|x_i-\overline{x}\right|$$

for numbers $x_1,\ldots,x_n$ and $\overline{x}$ their arithmetic mean value. For more details on energies of graphs and digraphs we refer to ([9],[15],[17]).

In this paper we refer to the energy conceived by Consonni and Todeschini as to the *outer energy* of a real *symmetric* matrix M as

$$E_{out}\left(M\right)=\sum_{i=1}^{n}\left|\lambda_i-\overline{\lambda}\left(M\right)\right|$$

for the eigenvalues $\lambda_1,\ldots,\lambda_n$ of M and their arithmetic mean $\overline{\lambda}\left(M\right)$. In this paper we discuss the properties of this "energy" in contrast to the *inner energy* defined as

$$E_{inn}\left(M\right)=\sum_{i=1}^{n}\left|\lambda_i\right|$$

Observe that these quantities coincide in case $tr(M)=0$, as happens for the adjacency matrix of a graph.

Let $S(n)$ be the space of real symmetric $n\times n$-matrices. For $M\in S(n)$ we denote by $M^{(j)}\in S(n-1)$ the matrix o btained from M by deleting the *j-th* row and column, and $M_0^{(j)}\in S(n)$ is the matrix formed from M by replacing the *j-th* row and column by zeroes.

We shall say that $f_n:S(n)\longrightarrow\mathbb{R}$ is an *energy function* if it satisfies the following conditions for every $n\geq 1$:

(E0) f_n is non-negative, unitarily invariant and $f_1(1) = 1$;

(E1) if $M, N \in S(n)$ then $f_n(M+N) \leq f_n(M) + f_n(N)$ and for r any scalar we have $f_n(rM) = |r|\, f_n(M)$;

(E2) if $M \in S(n)$ has a *j-th* row and column of zeroes then $f_n(M) = f_{n-1}\left(M^{(j)}\right)$, for all $n \geq 2$.

Theorem 1.1. *The inner energy $E_{inn} : S(n) \longrightarrow \mathbb{R}$ is the maximal function among the energy functions $f_n : S(n) \longrightarrow \mathbb{R}$.*

We say that $f_n : S(n) \longrightarrow \mathbb{R}$ is an *affine-energy function* if $f_n(M) = e_n\left(M - \overline{\lambda}(M)1_n\right)$ for an energy function e_n and the linear function $\frac{1}{n}tr = \overline{\lambda} : S(n) \longrightarrow \mathbb{R}$.

Theorem 1.2. *The outer energy $E_{out} : S(n) \longrightarrow \mathbb{R}$ is the maximal function among the affine-energy functions $f_n : S(n) \longrightarrow \mathbb{R}$.*

We denote $\varphi_M(x)$ (or simply $\varphi(x)$ when no confusion arises) the *characteristic polynomial* of the real symmetric $n \times n$-matrix M defined as $\varphi(x) = det\,(x1_n - M)$. This a a monic polynomial of degree n whose roots are the eigenvalues $\lambda_1, \ldots, \lambda_n$ of M. Let $\overline{\lambda}$ be the arithmetic mean of the λ_i. We consider the associated *affine polynomial*

$$\psi\,(x) = \varphi\left(x - \overline{\lambda}\right)$$

whose roots are of the form $\overline{\lambda} - \lambda_i$. We prove the following variant of Coulson integral formula:

Theorem 1.3. *Let M be a real symmetric $n \times n$-matrix. The following holds:*

$$E_{out}(M) = \frac{1}{\pi} \int_{-\infty}^{\infty} \left(n - \frac{ix\psi'(ix)}{\psi(ix)} dx \right).$$

We mention some applications of this formula.

2. The (outer) energy of a matrix

(1) Examples:

(a) For $1 \leq k \leq n$, define $p_k : S(n) \longrightarrow \mathbb{R}$ by $p_k(M) = \sum_{i=1}^{k} |\lambda_i|$, where the eigenvalues of M are ordered as $|\lambda_1(M)| \geq |\lambda_2(M)| \geq \cdots \geq |\lambda_n(M)|$. p_k is an energy function for each $1 \leq k \leq n$. In particular, $E_{inn} : S(n) \longrightarrow \mathbb{R}$ is an energy function.

(b) For $M = (m_{ij}) \in S(n)$ define $f_n(M) = \left(\frac{1}{n}\sum\limits_{i=1}^{n} |m_{ij}|^2\right)^{\frac{1}{2}}$. Then f_n is an energy function.

(2) Let $\lambda_n, \ldots, \lambda_{s+1} \le \overline{\lambda} \le \lambda_s, \ldots, \lambda_1$ be the eigenvalues of a matrix M. We assume that the arithmetic mean $\overline{\lambda} \ge 0$. Observe that $E_{inn}(M) \ge n\overline{\lambda} \ge 0$ and

$$\left(1 + \frac{n-s}{n}\right)\sum_{i=1}^{s} \lambda_i \ge E_{inn}(M) = \sum_{i=1}^{s} \lambda_i + \sum_{j=s+1}^{n} |\lambda_j| \ge \sum_{i=1}^{s} \lambda_i - (n-s)\overline{\lambda}$$

Moreover

$$E_{out}(M) = \sum_{i=1}^{n} \left|\lambda_i - \overline{\lambda}\right| = \sum_{j=1}^{s} \lambda_j + (n-2s)\overline{\lambda} - \sum_{i=s+1}^{n} \lambda_i = \sum_{j=1}^{s} \lambda_j - \sum_{i=s+1}^{n} \lambda_i + ni(M)\overline{\lambda}$$

where $i(M) = 1 - \frac{2s}{n} < 1$ is the balance index of the matrix M.

Proposition 2.1. *Let $M = (a_{ij})$ be a matrix with eigenvalues λ_i with $\lambda_n, \ldots, \lambda_{s+1} \le \overline{\lambda} \le \lambda_s, \ldots, \lambda_1$, where $0 \le \overline{\lambda}$ is the mean value of the λ_i. Then*

(a) $0 \le i(M) < 1$;

(b) $\frac{1}{2}E_{out}(M) = \sum\limits_{j=1}^{s} \left(\lambda_j - \overline{\lambda}\right) = \sum\limits_{j=s+1}^{n} \left(\overline{\lambda} - \lambda_j\right)$.

If moreover all $\lambda_i \ge 0$ then

(c) $2E_{inn}(M) - E_{out}(M) = 2s(M)\overline{\lambda} > 0$.

Proof. For (a), observe that $s > \frac{n}{2}$ implies

$$0 \le \sum_{j=1}^{s} \lambda_j - s\overline{\lambda} = \sum_{j=1}^{s} \left(\lambda_j - \overline{\lambda}\right) = \sum_{j=s+1}^{n} \left(\overline{\lambda} - \lambda_j\right) = \overline{\lambda} + (n - sj)\,\overline{\lambda} - \sum_{j=s+1}^{n} \lambda_j < \overline{\lambda} - \sum_{j=s+1}^{n} \lambda_j$$

and

$$n\overline{\lambda} < (s+1)\,\overline{\lambda} \le n\overline{\lambda}$$

a contradiction showing that $s \le \frac{n}{2}$ and $i(M) \ge 0$.

For (b), observe that the inequality

$$s\overline{\lambda} + \sum_{i=s+1}^{n} \lambda_i \le \sum_{i=1}^{s} \lambda_i + \sum_{j=s+1}^{n} \lambda_j = n\overline{\lambda} \le \sum_{j=1}^{s} \lambda_j + (n-s)\overline{\lambda}$$

written as $a + A \leq B + b$ has the property that the sum of the first and last terms, a and b, respectively, equals the sum of the second and third terms, A and B, respectively. That is, $a + b = A + B$. Therefore,

$$0 \leq b - A = B - a = \sum_{j=1}^{s} \left(\lambda_j - \overline{\lambda}\right) = \sum_{j=s+1}^{n} \left(\overline{\lambda} - \lambda_j\right) = \frac{1}{2} E_{out}(M)$$

since

$$\sum_{i=1}^{s} \lambda_i - \sum_{j=s+1}^{n} \lambda_j + (n - 2s)\,\overline{\lambda} = E_{out}(M) = \sum_{i \in G} \left|\lambda_i - \overline{\lambda}\right| \geq 0$$

This shows (b).

For (c), asume that $0 \leq \lambda_n, \ldots, \lambda_{s+1} \leq \overline{\lambda} \leq \lambda_s, \ldots, \lambda_1$ such that

$$E_{inn}(M) = \sum_{i=1}^{s} \lambda_i + \sum_{j=s+1}^{n} \lambda_j = n\overline{\lambda} \geq 0$$

Then

$$E_{inn}(M) - E_{out}(M) = \sum_{i=s+1}^{n} \lambda_i - (n - 2s)\overline{\lambda} = -\frac{1}{2} E_{out}(M) + s(M)\overline{\lambda}.$$

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Proposition 2.2. *Let $M = (a_{ij})$ be a matrix with eigenvalues λ_i with $\lambda_n, \ldots, \lambda_{s+1} \leq \overline{\lambda} \leq \lambda_s, \ldots, \lambda_1$, where $0 \leq \overline{\lambda}$ is the mean value of the λ_i. Then the following assertions are equivalent:*

(a) $E_{inn}\,(M) = E_{out}\,(M)$;

(b) $tr\,(M) = 0$;

(c) $\overline{\lambda} = 0$.

Proof. Only that (a) implies (b) is not clear. Assume that $E_{inn}(M) = E_{out}\,(M)$ and let

$$\lambda_n \leq \cdots \leq \lambda_{t+1} \leq 0 \leq \lambda_t \leq \cdots \leq \lambda_{s+1} \leq \overline{\lambda} \leq \lambda_s, \ldots, \lambda_1$$

Then

$$\sum_{i=1}^{s} \lambda_i - \sum_{j=s+1}^{n} \lambda_j + (n-2s)\overline{\lambda} = \sum_{i} \left|\lambda_i - \overline{\lambda}\right| = E_{out}(M) = E_{inn}(M) = \sum_{i=1}^{t} \lambda_i - \sum_{j=t+1}^{n} \lambda_j$$

Hence

$$(1 - i(M)) \sum_{i=1}^{n} \lambda_i = (n - 2s)\,\overline{\lambda} = 2 \sum_{i=s+1}^{t} \lambda_i \le 2\,(t - s)\,\overline{\lambda}.$$

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(3) Proof of Theorem 1.1: First, observe that E_{inn} is an energy function (see Examples). We show our result by induction, being the case $n = 1$ trivial. Let $f_n : S(n) \longrightarrow \mathbb{R}$ be an energy function and $M \in S(n)$. Find a diagonal matrix $D = diag\,(\lambda_1, \dots, \lambda_n)$ equivalent to M, then

$$\begin{aligned} f_n(M) = f_n(D) = f_n\left(\frac{1}{n-1}\sum_{j=1}^{n} D_0^{(j)}\right) &\le \frac{1}{n-1}\sum_{j=1}^{n} f_n\left(D_0^{(j)}\right) \\ = \frac{1}{n-1}\sum_{j=1}^{n} f_{n-1}\left(D^{(j)}\right) &\le \frac{1}{n-1}\sum_{j=1}^{n} E_{inn}(n-1)\left(D^{(j)}\right) \\ = \frac{1}{n-1}\sum_{j=1}^{n}\sum_{j\neq i} |\lambda_i| = E_{inn}(M). \end{aligned}$$

(4) Let $\sigma_1(M) \ge \sigma_2(M) \ge \cdots \ge \sigma_n(M)$ be the singular values of M and $\overline{\sigma}(M)$ the arithmetic mean, that is, $\sigma_j(M)$ are the square roots of the eigenvalues of $MM^\top$.

Observe that the symmetric matrix $N = M - \overline{\lambda}(M)1_n$ has singular values $\left|\lambda_i(M) - \overline{\lambda}(M)\right|$. Therefore

$$E_{out}(M) = \sum_{i=1}^{n} \left|\lambda_i(M) - \overline{\lambda}(M)\right| = \sum_{i=1}^{n} \sigma_i(N).$$

In other words, $E_{out}(M)$ is equal to Nikiforov's energy of $N = M - \overline{\lambda}(M)1_n$ (see [16]). It follows from [12, Corollary 3.4.4] that E_{out} satisfies (E1).

Proposition 2.3. *Let $M \in S(n)$ be a real symmetric matrix. Then $E_{out}(M) = 0$ if and only if $M = a1_n$ for some scalar a.*

Proof. Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of M. Observe that $E_{out}(M) = 0$ implies that the mean value $\overline{\lambda} = \lambda_i$ for all i and therefore $M = \overline{\lambda}1_n$. ☑

(5) Proof of Theorem 1.2: Note that $E_{inn}\left(M - \overline{\lambda}(M)1_n\right) = \sum_{i=1}^{n} \left|\lambda_i - \overline{\lambda}(M)\right| = E_{out}(M)$ so E_{out} is a affine energy function. To check maximality, let $f_n : S(n) \longrightarrow \mathbb{R}$ be any affine-energy function and $M \in S(n)$. Then $f_n(M) = e_n\left(M - \overline{\lambda}(M)1_n\right)$ for any energy function e_n and so by Theorem 1.1

$$f_n(M) = e_n\left(M - \overline{\lambda}(M)1_n\right) \le E_{nn}\left(M - \overline{\lambda}(M)1_n\right) = E_{out}(M).$$

3. Some special classes of matrices

(1) Inverse matrices

Let M be a real symmetric $n \times n$-matrix. Denote by $\varphi_M(x)$ the characteristic polynomial of degree n whose roots are the eigenvalues $\lambda_1, \dots, \lambda_n$ of M. Let $\overline{\lambda}$ be the arithmetic mean of the λ_i. Suppose M is invertible, then all $\lambda_i \neq 0$ and $\lambda_1^{-1}, \dots, \lambda_n^{-1}$ are the eigenvalues of M^{-1} with mean value

$$\overline{\lambda^{-1}} = \frac{1}{n}\sum_{i=1}^{n} \lambda_i^{-1} = H\left(\lambda_1, \dots, \lambda_n\right)^{-1}$$

where $H\left(\lambda_1, \dots, \lambda_n\right)$ is the harmonic mean of the eigenvalues. The harmonic-arithmetic means inequality states that

$$1 \leq H\left(\lambda_1, \dots, \lambda_n\right)^{-1} \overline{\lambda} = \overline{\lambda^{-1}}\overline{\lambda}.$$

More precise information may be obtained as the following result shows:

Proposition 3.1. *Let M be a non-singular real symmetric $n \times n$-matrix. Then*

(a) $s(M) + s\left(M^{-1}\right) \leq n$;

(b) $\overline{\lambda^{-1}} = \overline{\lambda}^{-1}$;

(c) $E_{out}\left(M^{-1}\right) = \frac{1}{\overline{\lambda}^2} E_{out}(M)$.

Proof. Write $\mu_i = \lambda_i^{-1}$ and $\overline{\mu} = \overline{\lambda^{-1}}$. Then $\overline{\lambda} \leq \lambda_i$ implies $\mu_i \leq \overline{\lambda}^{-1} \leq \overline{\mu}$. Therefore

$$s(M) \leq n - s\left(M^{-1}\right)$$

which yields (a). Calculate

$$E_{out}\left(M^{-1}\right) = 2\sum_{i=s(M^{-1})+1}^{n} \left(\overline{\mu} - \mu_i\right) = 2\sum_{i=1}^{s(M)} \left(\frac{\lambda_i - \overline{\lambda}}{\lambda_i \overline{\lambda}}\right) \leq \frac{2}{\overline{\lambda}^2}\sum_{i=1}^{s(M)} \left(\lambda_i - \overline{\lambda}\right) = \frac{1}{\overline{\lambda}^2} E_{out}(M)$$

Moreover,

$$E_{out}\left(M\right) \leq \frac{1}{\overline{\mu}^2} E_{out}\left(M^{-1}\right) \leq \frac{1}{\overline{\mu}^2 \overline{\lambda}^2} E_{out}\left(M\right) \leq E_{out}\left(M\right)$$

which yields equalities (b) and (c). ☑

(2) Exponential matrices

Let M be a matrix with eigenvalues

$$\lambda_n \leq \cdots \leq \lambda_{t+1} \leq 0 < \lambda_t \leq \cdots \leq \lambda_{s+1} < \overline{\lambda} \leq \lambda_s \leq \cdots \leq \lambda_1$$

and whose arithmetic mean is $\overline{\lambda} \geq 0$. We consider the exponential matrix e^M with eigenvalues

$$0 < e^{\lambda_n} \leq \cdots \leq e^{\lambda_{t+1}} \leq e^{\lambda_t} \leq \cdots \leq e^{\lambda_1}$$

and whose arithmetic mean $\overline{\lambda}\left(e^M\right) > 0$ satisfies $e^{\lambda_{t+1}} \leq \overline{\lambda}\left(e^M\right) \leq e^{e^{\lambda_t}}$.

Proposition 3.2. *With the notation above we have:*

(a) $e^{\overline{\lambda}} \leq \overline{\lambda}\left(e^M\right)$, *with equality if and only if* $\lambda_n = \cdots = \lambda_1$;

(b) $s\left(e^M\right) \leq s(M)$ *and* $i(M) \leq i\left(e^M\right)$;

(c) $E_{out}\left(e^M\right) \geq 2\,(n-t)$.

Proof. Observe that the arithmetic mean-geometric mean inequality yields

$$e^{\overline{\lambda}} = \left(\prod_{i=1}^{n} e^{\lambda_i}\right)^{\frac{1}{n}} \leq \frac{1}{n}\sum_{i=1}^{n} e^{\lambda_i} = \overline{\lambda}\left(e^M\right)$$

That is inequality (a). For (b), observe that

$$\lambda_n \leq \cdots \leq \lambda_{m+1} < 0 \leq \lambda_m \leq \cdots \leq \lambda_{s+1} < \overline{\lambda} \leq \lambda_s \leq \cdots \lambda_{t+1} < ln\overline{\lambda}\left(e^M\right) \leq \lambda_t \leq \cdots \leq \lambda_1$$

and $t = s\left(e^M\right) \leq s(M) = s \leq m$.

For (c), consider

$$\begin{aligned} E_{out}\left(e^M\right) &= \sum_{i=1}^{t}\left(e^{\lambda_i} - \overline{\lambda}\left(e^M\right)\right) + \sum_{i=t+1}^{n}\left(\overline{\lambda}\left(e^M\right) - e^{\lambda_i}\right) \\ &\geq \frac{1}{2}E_{out}\left(e^M\right) + \sum_{i=t+1}^{s}\left(\overline{\lambda}\left(e^M\right) - e^{\lambda_i}\right) + \sum_{i=s+1}^{n}\left(e^{\overline{\lambda}} - e^{\lambda_i}\right) \end{aligned}$$

Hence

$$\frac{1}{2}E_{out}\left(e^M\right) \geq \sum_{i=t+1}^{s}\left(\overline{\lambda}\left(e^M\right) - e^{\lambda_i}\right) + \sum_{i=s+1}^{m}\left(e^{\overline{\lambda}-\lambda_i}\right) + \sum_{i=m+1}^{n}\left(e^{\overline{\lambda}} - e^{\lambda_i}\right)$$

the last inequality due to the fact that, for each $t+1 \leq i \leq m$, we have $\overline{\lambda} - \lambda_i = c_i \geq 0$ and $\lambda_i \geq 0$. Then for $k \geq 1$,

$$\overline{\lambda}^k - \lambda_i^k = (\lambda_i + c_i)^k - \lambda_i^k \geq c_i^k$$

Therefore $e^{\overline{\lambda}} - e^{\lambda_i} \geq\ e^{\left(\overline{\lambda}-\lambda_i\right)}$ and $\sum\limits_{i=s+1}^{m} e^{\left(\overline{\lambda}-\lambda_i\right)} \geq (m-s)$.

Moreover,

$$\sum_{i=t+1}^{s}\left(\overline{\lambda}\left(e^{M}\right)-e^{\lambda_i}\right)\geq\sum_{i=t+1}^{s}\left(e^{\lambda_{t+1}}-e^{\lambda_t}\right)\geq(s-t)$$

and

$$\sum_{i=m+1}^{n}\left(e^{\overline{\lambda}}-e^{\lambda_i}\right)\geq(n-m)$$

In conclusion

$$E_{out}\left(e^{M}\right)\geq 2\,(n-t)$$

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A simple example will illustrate the last statement. Consider the matrix

$$M=\begin{pmatrix}0&1\\1&0\end{pmatrix}$$

with eigenvalues $\lambda_1=1$ and $\lambda_2=-1$. Then $E_{out}(M)=2$. Moreover, $m=t=s=1$.

The eigenvalues of e^M are e and e^{-1} with mean $\mu=\frac{e+e^{-1}}{2}$ and

$$E_{out}\left(e^{M}\right)=e-e^{-1}\approx 2.35$$

while the estimated lower bound is 2.

4. On Coulson-like formulas

(1) Let M be a real symmetric $n\times n$-matrix. Denote by $\varphi_M(x)$ (or simply $\varphi(x)$ when no confusion arises) the characteristic polynomial defined as

$$\varphi(x)=det\,(x1_n-M)\,.$$

This is a monic polynomial of degree n whose roots are the eigenvalues $\lambda_1,\ldots,\lambda_n$ of M. Let $\overline{\lambda}$ be the arithmetic mean of the λ_i. We consider the associated affine polynomial

$$\psi(x)=\varphi\left(x-\overline{\lambda}\right),$$

whose roots are of the form $\overline{\lambda}-\lambda_i$.

Let $\psi(x)=b_nx^n-b_{n-1}x^{n-1}+\cdots+(-1)^{n-1}b_1x+(-1)^n b_0$ and consider for $1\leq k\leq n$,

$$s_k=\sum_{i=1}^{n}\left(\overline{\lambda}-\lambda_i\right)^k$$

These coefficients satisfy:

(i) $b_n = 1$;
(ii) $b_1 = 0 = s_1$;
(iii) Newton's identities hold, namely:
$s_2 = b_1\, s_1 - 2b_2$,
$s_3 = b_2\, s_1 - b_1\, s_2 + 3b_3$,
$s_4 = b_3\, s_1 - b_2\, s_2 + b_1\, s_3 - 4b_4$,
etc ...

(2) Proof of Theorem 1.3: Let $\lambda_j = \lambda_j\,(M)$ be the eigenvalues of M. Define

$$f\,(z) = \frac{z\varphi'\left(z - \overline{\lambda}\right)}{\varphi\left(z - \overline{\lambda}\right)} = \frac{z\psi'\,(z)}{\psi\,(z)}$$

Since

$$\frac{\psi'\,(z)}{\psi\,(z)} = \sum_{j=1}^{n} \frac{1}{z - \overline{\lambda} + \lambda_j}$$

then

$$\frac{z\psi'\,(z)}{\psi\,(z)} = n - \sum_{j=1}^{n} \frac{\lambda_j - \overline{\lambda}}{z - \overline{\lambda} + \lambda_j}$$

Take any closed contour Γ containing in its interior exactly those $\lambda_j - \overline{\lambda} \geq 0$. The well-known Cauchy formula in complex calculus yields

$$\frac{1}{2\pi i} \oint_{\Gamma} (f(z) - n)\, dz = \sum_{\overline{\lambda} < \lambda_j} \left(\lambda_j - \overline{\lambda}\right) = \frac{1}{2} E_{out}$$

the last equality due to Proposition 2.1. Observe that the actual form of the contour Γ is unimportant. Therefore we can inflate it as indicated in [7] to obtain

$$\frac{1}{\pi} \int_{-\infty}^{\infty} \left(n - \frac{ix\psi'\,(ix)}{\psi\,(ix)}\right) dx = \frac{1}{\pi i} \oint_{\Gamma} (f(z) - n)\, dz = E_{out}$$

as desired.

(3) Following [7], we establish some direct consequences of the Coulson-like result just proved.

Corollary 4.1. *Let M be a real symmetric $n \times n$-matrix. Denote by $\varphi\,(x)$ its characteristic polynomial and $\psi\,(x) = \varphi\left(x - \overline{\lambda}\right)$ the associated affine polynomial. Then*

$$E_{out}\,(M) = \frac{1}{\pi} \int_{-\infty}^{\infty} \left(n - x\frac{d}{dx} ln\psi\,(ix)\right) dx$$

Corollary 4.2. *Let M_1, M_2 be two real symmetric $n \times n$-matrices. Denote by $\psi_k(x) = \varphi_k\left(x - \overline{\lambda}_k\right)$ the associated afffine polynomials, $k = 1, 2$. Then*

$$E_{out}(M_1) - E_{out}(M_2) = \frac{1}{\pi} \int\limits_{-\infty}^{\infty} \ln \frac{\psi_1(ix)}{\psi_2(ix)} dx.$$

Applying the ordinary Coulson integral formula and Theorem 1.3, we get:

Corollary 4.3. *Let M be a real symmetric $n \times n$-matrix. Denote by $\varphi(x)$ its characteristic polynomial and $\psi(x) = \varphi\left(x - \overline{\lambda}\right)$ the associated affine polynomial. Then*

$$E_{out}(M) - E_{inn}(M) = \frac{1}{\pi} \int\limits_{-\infty}^{\infty} \ln \frac{\psi(ix)}{\varphi(ix)} dx.$$

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