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Energy of Graphs with Multiple Self-Loops

Rajesh Kanna M. R. [1] , Roopa S. [2], Sowmya Prabha B. C.[3]

[1] Maharani's Science College for Women (Autonomous) Mysore-570005, Karnataka, India.

e-mail: mr.rajeshkanna@gmail.com

[2] Government College for Women Maddur–571428, Karnataka, India.

e-mail: rooopa.s.kumar@gmail.com

[3] Research Scholar,

Sri D. Devaraja Urs Government First Grade College (Recognized Research Centre, University of Mysore), Hunsur–571105, Karnataka, India.

e-mail: sowmyaprabha0@gmail.com

Abstract

Building on the foundational work of Professor Ivan Gut- man and collaborators, who introduced the concept of graph energy for graphs with self-loops, this study extends the notion to graphs containing multiple self-loops. For a simple graph G with n vertices and m edges, the modified graph G_M is formed by adding $r_1, r_2, \ldots, r_n$ self-loops to vertices $v_1, v_2, \ldots, v_n$, respectively. The energy of G_M is defined as:

$$E(G_M) = \sum_{i=1}^{n} \lambda_i(G_M) - \frac{\sigma_M}{n},$$

where $\sigma_M = \sum_{i=1}^{n} r_i$ represents the total number of self-loops, and $\lambda_1(G_M), \lambda_2(G_M), \ldots, \lambda_n(G_M)$ are the eigenval- ues of the adjacency matrix of G_M. This work investigates the spectral properties of G_M and derives bounds for its en- ergy, $E(G_M)$. This study focuses on deriving bounds anal- ogous to those of $E(G)$, while highlighting notable differ- ences and identifying opportunities for discovering sharper bounds. The results contribute to advancing the theoret- ical understanding of spectral graph properties, especially for graphs augmented with multiple self-loops.

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Key Words and Phrases: Graph energy, self-loop, eigen- value, adjacency matrix, spectral graph theory.

1 Introduction

The concept of graph energy is a fundamental topic in spectral graph theory, with

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its origins in mathematical chemistry, where it was introduced to estimate the total π-electron energy of molecules. For a simple graph G with n vertices, its adjacency matrix $A(G)$ is defined such that its $(i, j)^{th}$ entry is 1 if vertices v_i and v_j are adjacent, and 0 otherwise. The energy [1] of a graph $E(G)$, introduced by I. Gutman in 1978, is defined as the sum of the absolute values of the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of the adjacency matrix $A(G)$, given by:

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

This measure has been extensively studied, leading to significant applications in both theoretical graph theory and mathematical chemistry, as documented in various works, including [2, 3, 4].

While the energy of simple graphs is well-documented, the study of graphs with self-loops has received limited attention despite its importance. Self-loops naturally arise in mathematical modelling, where they can represent heteroatoms in molecular graphs or other structural features in physical or network systems [5, 6, 7, 8]. Let $S \subseteq V$ with $|S| = \sigma$. A graph with self-loops G_S, with vertex set V and edge set $K(G_S)$, is obtained from the simple graph G by attaching a self-loop to each of its vertices belonging to S. Since graphs with self-loops find applications in chemistry, Gutman et al. defined the adjacency matrix $A(G_S)$ [10] of the graph G_S in 2021. The matrix $A(G_S)$ is a symmetric matrix of order n, whose $(i, j)^{th}$ element is defined as:

$$A(G_S)_{ij} = \begin{cases} 1 & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent,} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ are not adjacent,} \\ 1 & \text{if } i = j \text{ and } v_i \in S, \\ 0 & \text{if } i = j \text{ and } v_i \notin S. \end{cases}$$

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The energy $E(G_S)$ of the graph G_S is defined as [10]:

$$E(G_S) = \sum_{i=1}^{n} \lambda_i(G_S) - \frac{\bar{\sigma}}{n} \qquad (2)$$

where $\lambda_1(G_S)$, $\lambda_2(G_S)$, . . . , $\lambda_n(G_S)$ are the eigenvalues of $A(G_S)$. For more information on energy of graphs with self-loops, Laplacian energy of graphs with self-loops, refer to [11, 12, 13].

The concept of multiple self-loops in graph theory holds signif- icant importance in various fields, including applied mathematics, chemistry, and computer science. In graph spectral theory, they alter eigenvalues and affect the graph's energy. In Markov chains and random walks, multiple self-loops increase the probability of re- maining in the same state, modeling delays or persistent behaviors. In control systems and feedback loops, they represent strong self- reinforcement mechanisms, ensuring stability in dynamic systems.

Electrical and flow networks utilize multiple self-loops to represent parallel resistances or multiple waiting queues at a single node. In neural networks and machine learning, particularly in recurrent models, they enhance memory persistence and sequence learning. Computational chemistry applies multiple self-loops to represent resonance structures or localized electron densities in molecular graphs. In quantum mechanics and quantum graphs, they influ- ence energy levels and quantum state transitions. These applica- tions demonstrate the crucial role of multiple self-loops in modeling complex systems where self-reinforcement and persistence are key factors. It is noteworthy that the energy of graphs with multiple self-loops has not been explored previously. In this paper, we aim to examine the energy of graphs featuring multiple self-loops.

G_M is a graph obtained from a simple graph G by attaching r_1 self-loops to the first vertex v_1, r_2 self-loops to the second vertex v_2, etc., and $\sigma_M = \sum_{i=1}^{n} r_i$ is the total number of self-loops added to the vertices of G. Then adjacency matrix $A(G_M)$ of the graph G_M is a symmetric matrix of order n, whose $(i, j)^{th}$ element is defined as:

$$A(G_M)_{ij} = \begin{cases} 1, & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent and } i \neq j, \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ are not adjacent and } i \neq j, \\ r_i & \text{if } i = j. \end{cases}$$

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Let $\lambda_1(G_M), \lambda_2(G_M), \ldots, \lambda_n(G_M)$ be the eigenvalues of $A(G_M)$. These eigenvalues are all real valued and

$$\lambda_i(G_M) = \sigma_M \sum_{i=1}^{n} \qquad (3)$$

Therefore, the energy of G_M (to account for the contribution of these multiple self-loops) is defined as :

$$E(G_M) = \sum_{i=1} \lambda_i(G_M) - \frac{\sigma_M}{n}, \qquad (4)$$

The energy $E(G_M)$ depends on both the total number of self-loops σ_M and their distribution $r_1, r_2, \ldots, r_n$. Some basic examples that illustrate the definition are gathered in the following example.

Example 1. *Consider the cycle graph C_4 with the vertex set v_1, v_2, v_3, v_4 , where each vertex has a self-loop of weights 4, 2, 3, and 1, respectively as shown in the following figure.*

The adjacency matrix of C_4 is given by

$$A(G) = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$

The eigenvalues of C_4 are

$$\lambda_1 = 2, \quad \lambda_2 = -2, \quad \lambda_3 = 0, \quad \lambda_4 = 0.$$

The energy of C_4 is computed as

$$E(G) = |2| + |-2| + |0| + |0| = 4.$$

Now, consider the adjacency matrix of C_4 with multiple self-loops:

$$\begin{bmatrix} 4 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{bmatrix}$$

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$$A(G_M) = \begin{matrix} & & & \\ & & & \\ 1 & 0 & 1 & 1 \end{matrix} \qquad \begin{matrix} & & & \\ & & & \\ 0 & 1 & 3 & 1 \end{matrix}$$

The eigenvalues of C_4 with multiple self-loops are approximately:
$\lambda_1 \approx 4.88736$, $\lambda_2 \approx 3.39471$, $\lambda_3 \approx 1.60529$, $\lambda_4 \approx 0.11264$.
The energy of C_4 with multiple self-loops is given by:

$$E(G_M) = 4.88736 - \frac{4}{10} + 3.39471 - \frac{4}{10} + 1.60529 - \frac{4}{10} + 0.11264 - \frac{4}{10} = 6.56414.$$

The introduction of self-loops affects the eigenvalues of the ad- jacency matrix, presenting intriguing questions regarding their im- pact on graph energy. Extending this idea, graphs with multiple self-loops at each vertex allow for further generalization. Here, a vertex v_i may have r_i self-loops, resulting in a modified adjacency matrix that includes these contributions. Interestingly, if additional self-loops are uniformly added to all vertices, the adjacency matrix undergoes a uniform transformation, yet the graph energy remains invariant under certain conditions. This invariance underscores the robust nature of energy as a spectral property.

This work aims to explore the energy of graphs with multiple self-loops, focusing on their spectral properties and the invariance of energy under specific transformations. Such investigations not only extend the theoretical framework of graph energy but also open new pathways for applications in mathematical chemistry, network analysis, and beyond.

2 Fundamental properties of the energy of graphs containing multiple self-loops

To begin, we present a fundamental result:

Lemma 1. *Let G be a simple graph of order n, and G_M the graph obtained by adding $r_1, r_2, \ldots, r_n$ self-loops at vertices $v_1, v_2, \ldots, v_n$, respectively. Denote the total number of self-loops as*

$\sigma_M = \sum_{i=1}^{n} r_i$. *Then:*

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1. *If* $\sigma_M = 0$ *(i.e.,* $r_1 = r_2 = \cdots = r_n = 0$*), then* $E(G_M) = E(G)$*.*
2. *If* $r_1 = r_2 = \cdots = r_n = k$*, then* $E(G_M) = E(G)$*.*
3. *For general* $r_1, r_2, \ldots, r_n$*, the energy of* G_M *is given by:*

$$E(G_M) = \sum_{i=1}^{n} \left| \lambda_i(G) + r_i - \frac{\sigma_M}{n} \right|,$$

where $\lambda_i(G)$ *are the eigenvalues of the adjacency matrix* $A(G)$*.*

Proof. **Case (a):** $\sigma_M = \sum_{i=1}^{n} r_i = 0$

If $\sigma_M = 0$ (i.e., $r_1 = r_2 = \cdots = r_n = 0$), then no self-loops are added, and the diagonal matrix $\text{diag}(r_1, r_2, \ldots, r_n) = 0$. Thus, $A(G_M) = A(G)$, and the eigenvalues remain unchanged:

$\lambda_i(G_M) = \lambda_i(G), \qquad \forall i.$

The energy becomes:

$$E(G_M) = \sum_{i=1}^{n} \left| \lambda_i(G_M) - \frac{\sigma_M}{n} \right| = \sum_{i=1}^{n} \left| \lambda_i(G) - \frac{0}{n} \right| = \sum_{i=1}^{n} |\lambda_i(G)| = E(G).$$

Hence, $E(G_M) = E(G)$.

Case (b): If $r_1 = r_2 = \cdots = r_n = k$

If $r_1 = r_2 = \cdots = r_n = k$, then adding k self loops to every vertex modifies the diagonal matrix to $\text{diag}(r_1, r_2, \ldots, r_n) = kI_n$, where I_n is the identity matrix of order n. The modified adjacency matrix becomes:

$$A(G_M) = A(G) + kI_n.$$

Adding kI_n shifts each eigenvalue of $A(G)$ uniformly by k. Thus the eigenvalues of $A(G_M)$ are

$$\lambda_i(G_M) = \lambda_i(G) + k, \quad \forall i.$$

Substituting $\sigma_M = n \cdot k$ in the energy definition:

$$E(G_M) = \sum_{i=1}^{n} \left| \lambda_i(G_M) - \frac{\sigma_M}{n} \right|,$$

$$E(G_M) = \sum_{i=1}^{n} |(\lambda_i(G) + k) - k| = \sum_{i=1}^{n} |\lambda_i(G)| = E(G).$$

Thus, $E(G_M) = E(G)$.

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Case (c): General Distribution of $r_1, r_2, \ldots, r_n$

For a general distribution of self-loops, $r_1, r_2, \ldots, r_n$, the diagonal matrix diag($r_1, r_2, \ldots, r_n$) perturbs the eigenvalues of $A(G)$ non- uniformly. The eigenvalues $\lambda_i(G_M)$ do not simply shift uniformly; instead, they depend on the structure of G and the distribution $r_1, r_2, \ldots, r_n$. In this case, the adjacency matrix is modified to $A(G_M) = A(G) + \text{diag}(r_1, r_2, \ldots, r_n)$, where the diagonal matrix reflects the added self-loops. The eigenvalues of $A(G_M)$ are per- turbed as $\lambda_i(G_M) = \lambda_i(G) + r_i$. Substituting these eigenvalues into the energy formula:

$$E(G_M) = \sum_{i=1}^{n} \lambda_i(G) + \sigma_M - n,$$

where $\sigma_M = \sum_{i=1}^{n} r_i$.

This general form highlights that the energy $E(G_M)$ depends not only on the eigenvalues $\lambda_i(G)$ but also on the distribution of self-loops $r_1, r_2, \ldots, r_n$.

Invariance of Graph Energy Under Uni- form Increment of Self-Loops

The following proof demonstrates that the energy of a graph re- mains invariant under a uniform increment of self-loops, as the shift r cancels out in the calculation of the energy.

Theorem 1. Let G be a graph with n vertices. GM represents the graph obtained by adding r1, r2, . . . , rn self-loops to the vertices v1, v2, . . . , vn of G, respectively. Further, suppose r additional self- loops are added uniformly to each vertex of GM , resulting in a new graph G′ , where the self-loops at the vertices are r1 + r, r2 + r, . . . , rn + r. Then, the energy of G′ remains equal to the energy of GM , i.e.,

E(G′) = E(GM).

Proof. Let λ1(GM), λ2(GM), . . . , λn(GM) denote the eigenvalues of the adjacency matrix A(GM), and let σM = Σn ri represent the sum of all self-loops in GM . The energy of GM is defined as:

E(G) = Σ λ (G) − M .

When r additional self-loops are added to each vertex of GM , the new graph G′ has self-loops given by r1 + r, r2 + r, . . . , rn + r. The sum of all self-loops in G′ becomes:

M = (r1 + r) + (r2 + r) + · · · + (rn + r) = σM + nr,

where σM = Σn ri.

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Adding r self-loops to each vertex modifies the adjacency matrix
A(GM) as follows:
A′(GM) = A(GM) + rI,
where I is the n n identity matrix. The eigenvalues of the modified adjacency matrix A′(GM) are related to the eigenvalues of A(GM) by:
λ′(GM) = λi(GM) + r, for i = 1, 2, . . . , n.
The energy of G′ is defined as:
Σ σ′
Substituting λ′(GM) = λi(GM) + r and σ′ = σM + nr, we get:
i M
′ Σ σM + nr
E(GM) = (λi(GM) + r) − n
i=1
Simplifying the expression inside the absolute value:
σM + nr σM σM
(λ (G) + r) − = λ (G) + r − − r = λ (G) − .
Thus, the energy of G′ becomes:
E(G′) = Σ λ (G) − M .
Since the expression for E(G′) is identical to E(GM), it follows

that:

E(G′

) = E(GM).

Theorem 2. Let G be a bipartite graph of order n, with vertex set V = {v1, v2, . . . , vn}. Let R = (r1, r2, . . . , rn), where ri ≥ 0 represents the number of self-loops added to vertex vi. Define GM as the graph obtained by adding ri self-loops to vi for i = 1, 2, . . . , n. Define R′ = (k−r1, k−r2, . . . , k−rn), where k ≥ max(r1, r2, . . . , rn)
ensures R ≥ 0. Let GM′ be the graph obtained by adding k − ri
self-loops to vertex vi. Then:
E(GM) = E(GM′).
Proof. The adjacency matrix of GM is:
A(GM) = A(G) + JR,
where JR = diag(r1, r2, . . . , rn) is a diagonal matrix containing the self-loop counts.

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The adjacency matrix of $G_{M'}$ is:

$$A(G_{M'}) = A(G) + J_{R'},$$

where $J_{R'} = \text{diag}(k - r_1, k - r_2, \ldots, k - r_n)$.

Since $R' = (k - r_1, k - r_2, \ldots, k - r_n)$, it follows that:

$$J_R + J_{R'} = kI_n,$$

where I_n is the identity matrix of order n. The characteristic polynomial of G_M is:

$\phi(G_M, \lambda) = \det(\lambda I_n - A(G_M)) = \det(\lambda I_n - A(G) - J_R)$.

The characteristic polynomial of $G_{M'}$ is:

$\phi(G_{M'}, \lambda) = \det(\lambda I_n - A(G_{M'})) = \det(\lambda I_n - A(G) - J_{R'})$. Substituting $J_{R'} = kI_n - J_R$ into $\phi(G_{M'}, \lambda)$:

$\phi(G_{M'}, \lambda) = \det(\lambda I_n - A(G) - (kI_n - J_R))$.

Simplifying:

$\phi(G_{M'}, \lambda) = \det((\lambda - k)I_n - A(G) + J_R)$.

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of G_M . For $G_{M'}$, the eigen- values are shifted by k and negated due to the symmetry of bipartite graphs:

Eigenvalues of $G_{M'}$: $\{-\lambda_i + k\}_{i=1}^{n}$.

The energy of G_M is defined as:

$$E(G_M) = \sum_{i=1}^{n} \lambda_i - \frac{\sum_{i=1}^{n} r_i}{n}.$$

The energy of $G_{M'}$ is:

$$E(G_{M'}) = \sum_{i=1}^{n} (-\lambda_i + k) - \frac{\sum_{i=1}^{n} (k - r_i)}{n}.$$

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Substituting $\sum_{i=1}^{n}(k - r_i) = nk - \sum_{i=1}^{n} r_i$:

$$E(G_{M'}) = \sum_{i=1}^{n} -\lambda_i + k - \frac{k - \sum_{i=1}^{n} r_i}{n}.$$

Simplifying:

$$E(G_{M'}) = \sum_{i=1}^{n} -\lambda_i + \frac{\sum_{i=1}^{n} r_i}{n}.$$

i.e.,

$$E(G_{M'}) = \sum_{i=1}^{n} \lambda_i - \frac{\sum_{i=1}^{n} r_i}{n}.$$

Thus:

$E(G_M) = E(G_{M'})$.

□

Counterexample for Non-Bipartite Graphs

Let $G = K_5$ be the complete graph on five vertices with $V = v_1, v_2, v_3, v_4, v_5$. Since K_5 is non-bipartite, the spectral symmetry that underlies the energy invariance for bipartite graphs does not apply.

First Self–Loop Assignment:

Define

$$R = (8, 7, 3, 4, 2).$$

Then the modified graph G_M has the adjacency matrix

$$A(G_M) = A(K_5) + \text{diag}(8, 7, 3, 4, 2).$$

The total number of self-loops is

$$\sigma_M = 8 + 7 + 3 + 4 + 2 = 24,$$

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so that the average self-loop count is

$$\bar{r}_M = \frac{24}{5} = 4.8.$$

Numerical computation (using MATLAB) yields

$$E(G_M) = \sum_{i=1}^{5} \lambda_i(G_M) - 4.8 \approx 13.3995.$$

Complementary Self-Loop Assignment:

Choose

$$k \geq \max\{8, 7, 3, 4, 2\}. \text{ i.e., } k \geq 8. \text{ Let } k = 9$$

and define

$R' = (9-8, 9-7, 9-3, 9-4, 9-2) = (1, 2, 6, 5, 7).$

Then the modified graph $G_{M'}$ has the adjacency matrix

$A(G_{M'}) = A(K_5) + \text{diag}(1, 2, 6, 5, 7).$

Here the total number of self-loops is

$\sigma_{M'} = 1 + 2 + 6 + 5 + 7 = 21,$

so the average self-loop count is

$$\bar{r}_{M'} = \frac{21}{5} = 4.2.$$

A MATLAB eigen analysis yields

$$E(G_{M'}) = \sum_{i=1}^{5} \lambda_i(G_{M'}) - 4.2 \approx 12.7264.$$

Since

$$13.3995 \neq 12.7264,$$

this example shows that

$E(G_M) \neq E(G_{M'}),$

demonstrating that the energy invariance under the complementary self-loop transformation fails for the non–bipartite graph K_5.

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3 McClelland-type upper bound for the energy of graphs with multiple self- loops

In this section, we formulate a McClelland-type upper bound [14] for the energy of graphs with multiple self-loops. Our approach begins with a few fundamental supporting results.

Lemma 2. *Let G be a simple, undirected graph on n ver- tices with m edges, and let r_i denote the number of self-loops added to vertex v_i to form a new graph G_M. Denote by $A(G)$ and $A(G_M)$ the adjacency matrices of G and G_M, respectively. Let $\lambda_1(G_M), \lambda_2(G_M), \ldots, \lambda_n(G_M)$ be the eigenvalues of the adjacency matrix $A(G_M)$. Then:*

$$\sum_{i=1}^{n} \lambda_i^2(G_M) = 2m + \sum_{i=1}^{n} r_i^2,$$

Proof. A well-known linear algebraic identity states that the sum of the squares of the eigenvalues of $A(G_M)^2$ (the squared ad- jacency matrix) is given by:

$$\sum_{i=1}^{n} \lambda_i^2(G_M) = \text{Trace}(A(G_M)^2),$$

The adjacency matrices of G_M and G are related by the expression :

$$A(G_M) = A(G) + J_M,$$

where J_M is the diagonal matrix with $J_M[i, i] = r_i$ representing the number of self-loops at vertex v_i. Substituting $A(G_M) = A(G)+J_M$ into $A(G_M)^2$ we have

$$A(G_M)^2 = (A(G) + J_M)^2 = A(G)^2 + A(G)J_M + J_M A(G) + J_M^2.$$

Computing the trace of each term we have:

$$\text{Trace}(A(G_M)^2) = \text{Trace}(A(G)^2)+\text{Trace}(A(G)J_M)+\text{Trace}(J_M A(G))+\text{Trace}(J_M^2).$$

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- Trace($A(G)^2$) = $2m$: This follows from the definition of $A(G)^2$, where the diagonal entries count twice the number of edges in G.
- Trace($A(G)J_M$) = 0: Since J_M is diagonal and $A(G)$ connects different vertices, their product has zero diagonal entries.
- Trace($J_M A(G)$) = 0: The same reasoning applies here as for $A(G)J_M$.
- Trace(J^2) = $\sum_{i=1}^{n} r_i^2$: Since J_M is diagonal, the square of the diagonal entries contributes r_i^2 for each vertex v_i.

Substituting these values into the trace equation:

$$\text{Trace}(A(G_M)^2) = 2m + 0 + 0 + \sum_{i=1}^{n} r^2 = 2m + \sum_{i=1}^{n} r^2.$$

Thus, the sum of the squares of the eigenvalues of $A(G_M)$ is:

$$\sum_{i=1}^{n} \lambda^2(G_M) = 2m + \sum_{i=1}^{n} r^2.$$

□

Lemma 3. *Let G_M be a graph of order n, with m edges and $r_1, r_2, \ldots, r_n$ self-loops added to vertices $v_1, v_2, \ldots, v_n$, respectively. Let $\lambda_1(G_M), \lambda_2(G_M), \ldots, \lambda_n(G_M)$ be the eigenvalues of the adjacency matrix $A(G_M)$. Then:*

$$\sum_{i=1}^{n} \lambda_i(G_M) = 2m + \sum_{i=1}^{n} r_i - \frac{\sigma_M^2}{n},$$

where $\sigma_M = \sum_{i=1}^{n} r_i$ is the total number of self-loops in G_M.

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Proof. Consider,

$$\sum_{i=1}^{n} \lambda_i(G_M) - \frac{\sigma_M}{n}^2 = \sum_{i=1}^{n} \lambda_i(G_M) - 2\lambda_i(G_M)\frac{\sigma_M}{n} + \frac{\sigma_M}{n}^2$$

$$= \sum_{i=1}^{n} \lambda_i^2(G_M) - 2\frac{\sigma_M}{n}\sum_{i=1}^{n} \lambda_i(G_M) + \frac{\sigma_M^2}{n^2}\sum_{i=1}^{n} 1$$

$$= \sum_{i=1}^{n} \lambda_i^2(G_M) - 2\frac{\sigma_M}{n}\sum_{i=1}^{n} \lambda_i(G_M) + \frac{\sigma_M^2}{n^2}(n)$$

$$= \sum_{i=1}^{n} \lambda_i^2(G_M) - 2\frac{\sigma_M}{n}\text{Trace } A(G_M) + \frac{\sigma_M^2}{n}$$

$$= \sum_{i=1}^{n} \lambda_i^2(G_M) - 2\frac{\sigma_M}{n}\sigma_M + \frac{\sigma_M^2}{n}$$

$$= 2m + \sum_{i=1}^{n} r_i^2 - \frac{\sigma_M^2}{n} + \frac{\sigma_M^2}{n}$$

$$= 2m + \sum_{i=1}^{n} r_i^2 - \frac{\sigma_M^2}{n}.$$

Thus,

$$\sum_{i=1}^{n} \lambda_i(G_M) - \frac{\sigma_M}{n}^2 = 2m + \sum_{i=1}^{n} r_i - \frac{\sigma_M}{n}^2.$$

Since the sum of the eigenvalues equals the trace of $A(G_M)$, we have

$$\sum_{i=1}^{n} \lambda_i(G_M) = \text{Trace } A(G_M) = \sigma_M.$$

and by Lemma 2, the sum of the squares of the eigenvalues is

$$\sum_{i=1}^{n} \lambda_i^2(G_M) = 2m + \sum_{i=1}^{n} r_i^2.$$

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□

This lemma incorporates the effects of varying self-loops distributed across vertices. The term $\sum_{i=1}^{n} r_i^2$ reflects the quadratic contribution of self-loops, and $\frac{\sigma^2}{n}$ accounts for the average shift due to the total self-loop distribution.

Theorem 3. *Let G_M be a graph of order n with m edges, and self-loops such that vertex i has r_i self-loops (i = 1, 2, . . . , n). Then the energy of G_M, denoted $E(G_M)$, satisfies the following inequality:*

$$E(G_M) \leq \sqrt{n\left(2m + \sum_{i=1}^{n} r_i^2 - \frac{\sigma_M^2}{n}\right)},$$

where $\sigma_M = \sum_{i=1}^{n} r_i$ is the total number of self-loops in G_M.

Proof. The energy of the graph G_M is defined as:

$$E(G_M) = \sum_{i=1}^{n} \left|\lambda_i(G_M) - \frac{\sigma_M}{n}\right|,$$

where $\lambda_1(G_M), \lambda_2(G_M), \ldots, \lambda_n(G_M)$ are the eigenvalues of the adjacency matrix of G_M, and $\frac{\sigma_M}{n}$ is the average multiple self-loop contribution. Using the Cauchy-Schwarz inequality:

$$\left(\sum_{i=1}^{n} \left|\lambda_i(G_M) - \frac{\sigma_M}{n}\right|\right)^2 \leq n \cdot \sum_{i=1}^{n} \left|\lambda_i(G_M) - \frac{\sigma_M}{n}\right|^2.$$

Taking the square root on both sides:

$$E(G_M) \leq \sqrt{n \cdot \sum_{i=1}^{n} \left|\lambda_i(G_M) - \frac{\sigma_M}{n}\right|^2}.$$

From the generalized Lemma 3 for graphs with r_i self-loops:

$$\sum_{i=1}^{n} \left|\lambda_i(G_M) - \frac{\sigma_M}{n}\right|^2 = 2m + \sum_{i=1}^{n} r_i^2 - \frac{\sigma_M^2}{n}.$$

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Substitute this into the inequality:

$$E(G_M) \leq \sqrt{n \cdot \left(2m + \sum_{i=1}^{n} r_i^2 - \frac{\sigma_M^2}{n}\right)}.$$

□

Key Insights

1. **Classical McClelland Bound:**
   When $\sigma_M = 0$ (no self-loops), the result reduces to the classical McClelland bound:
   $$E(G) \leq \sqrt{n \cdot 2m}.$$
2. **Interplay Between Edges and Self-Loops:**
   The result reflects a balance between the total number of edges ($2m$) and the contribution of self-loops ($\sum_{i=1}^{n} r_i^2$ and $\frac{\sigma_M^2}{n}$). This balance determines the upper bound on the graph energy.

Conclusion of the Paper

In this paper, we have defined the energy of graphs with multiple self-loops. The equality $E(G_M) = E(G)$ holds for the special cases where $\sigma_M = 0$ or when there is a uniform distribution of self-loops ($r_1 = r_2 = \cdots = r_n$). We have demonstrated that the energy of a graph remains invariant under a uniform increment of self-loops. For a bipartite graph, the energy is invariant under the transformation

$$r_i \to k - r_i,$$

for each vertex, as long as k is chosen appropriately. Addition- ally, we obtained a McClelland–type upper bound for the energy of graphs with multiple self-loops.

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