

Seidel Switching and Graph Energy

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(Received March 23, 2012)

Abstract

The energy of a graph Γ is the sum of the absolute values of the eigenvalues of the adjacency matrix of Γ . Seidel switching is an operation on the edge set of Γ . In some special cases Seidel switching does not change the spectrum, and therefore the energy. Here we investigate when Seidel switching changes the spectrum, but not the energy. We present an infinite family of examples with very large (possibly maximal) energy.

The Seidel energy $\mathcal{S}(\Gamma)$ of Γ is defined to be the sum of the absolute values of the eigenvalues of the Seidel matrix of Γ . It follows that $\mathcal{S}(\Gamma)$ is invariant under Seidel switching and taking complements. We obtain upper and lower bounds for $\mathcal{S}(\Gamma)$, characterize equality for the upper bound, and formulate a conjecture for the lower bound.

1 Energy

Suppose Γ is a graph on n vertices with adjacency matrix A . Let $\lambda_1 \geq \dots \geq \lambda_n$ be the eigenvalues of A . The energy $\mathcal{E}(\Gamma)$ of Γ is defined by $\mathcal{E}(\Gamma) = \sum_{i=1}^n |\lambda_i|$, and $\mathcal{E}_{\max}(n)$ is defined to be the maximal energy over all graphs on n vertices. See [3] for more about graph energy. It follows that the energy of an induced subgraph of Γ is at most $\mathcal{E}(\Gamma)$, and that $\mathcal{E}_{\max}(n)$ is monotonically increasing in n . The value of $\mathcal{E}_{\max}(n)$, and the structure of the graphs reaching it, is an important issue in the study of graph energy. Koolen and Moulton [6] proved that $\mathcal{E}(\Gamma) \leq n(1 + \sqrt{n})/2$ with equality if and only if Γ is a strongly regular graph with parameters $(n, (n + \sqrt{n})/2, (n + 2\sqrt{n})/4, (n + 2\sqrt{n})/4)$ (if $n = 4$, $\Gamma = K_4$, which is strictly speaking not strongly regular). Such strongly regular

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graphs are equivalent to regular graphical Hadamard matrices of negative type, which are known to exist for many values of n , for example if n is a power of 4, and if $n = 36$, $n = 100$, or $n = 196$. An obvious necessary condition is that n is an even square, and it is believed that this condition is also sufficient. See [4] and [5] for more about maximal energy graphs. For the necessary background on graph spectra, strongly regular graphs and Seidel switching we refer to [2]. In this note we present examples of pairs of graphs on n vertices with the same energy, where one is regular and the other one is not. The construction works when $n + 1$ is the order of a regular graphical Hadamard matrix. These graphs have energy very close to the Koolen-Moulton bound, and we conjecture that it equals $\mathcal{E}_{\max}(n)$.

2 Equitable partitions

Consider a symmetric matrix A with rows and columns indexed by a set V . Assume V is partitioned into m classes V_1, \dots, V_m . Thus, with a suitable ordering of V we may write

$$A = \begin{bmatrix} A_{1,1} & \cdots & A_{1,m} \\ \vdots & & \vdots \\ A_{m,1} & \cdots & A_{m,m} \end{bmatrix},$$

where each diagonal block $A_{i,i}$ is symmetric. Such a matrix partition is called *equitable* whenever each block $A_{i,j}$ has constant row and column sum. Let $b_{i,j}$ denote the row sum of $A_{i,j}$ then the $m \times m$ matrix $B = (b_{ij})$ is called the *quotient matrix* of A with respect to the given partition. It is well-known (see for example [2]) that the spectrum of B is a sub(multi)set of the spectrum of A , and that the corresponding eigenvectors lie in the space W spanned by the characteristic vectors of V_1, \dots, V_m . The other eigenvalues of A have eigenvectors orthogonal to W , and therefore these eigenvalues and eigenvectors remain unchanged if a multiple of the all-one matrix J is added to some of the blocks $A_{i,j}$. Note that in general B is not symmetric, but B is similar to a symmetric matrix $\tilde{B} = D^{-1}BD$, where $D = \text{diag}(\sqrt{|V_1|}, \dots, \sqrt{|V_m|})$.

Let V be the vertex set of Γ , and assume V is partitioned into two subsets U_1 and U_2 . *Seidel switching* with respect to $\{U_1, U_2\}$ is the operation on Γ that leaves V and the subgraphs induced by U_1 and U_2 unchanged, but deletes all edges between U_1 and U_2 , and inserts all edges between U_1 and U_2 that were not present in Γ . Thus, if

$$A = \begin{bmatrix} A_1 & A_2 \\ A_2^\top & A_3 \end{bmatrix}$$

is the adjacency matrix of Γ , then Seidel switching changes A into

$$A' = \begin{bmatrix} A_1 & J - A_2 \\ J - A_2^\top & A_3 \end{bmatrix}.$$

It easily follows that Seidel switching defines an equivalence relation on graphs.

Assume the partition $\{U_1, U_2\}$ is equitable. Then A and A' have the same eigenvalues for the eigenvectors in W (see the proof of the next theorem for an explanation). Therefore A and A' have the same spectrum if the quotient matrices B and B' are equal, which is the case if every vertex in U_1 is adjacent to exactly half of the vertices in U_2 . If this is the case, then the two graphs obviously have the same energy. The following theorem generalizes this idea to make graphs with the same energy, but not necessarily the same spectrum.

Theorem 2.1 *Let Γ be a graph with an equitable partition with quotient matrix B . Let Γ' be the graph obtained from Γ by Seidel switching with respect to a union of classes of the partition, and let B' be the quotient matrix after switching. If B has no negative eigenvalues, then $\mathcal{E}(\Gamma) \leq \mathcal{E}(\Gamma')$ with equality if and only if B' has no negative eigenvalues.*

Proof. Assume the equitable partition is given by V_1, \dots, V_m , and the switching goes with respect to $\{U_1, U_2\}$, where $U_1 = V_1 \cup \dots \cup V_k$ and $U_2 = V_{k+1} \cup \dots \cup V_m$. Let W be the space spanned by the characteristic vectors of V_1, \dots, V_m , and let A and A' be the adjacency matrices of Γ and Γ' , respectively. Then

$$A = \begin{bmatrix} A_1 & A_2 \\ A_2^\top & A_3 \end{bmatrix} = \left[\begin{array}{ccc|ccc} A_{1,1} & \cdots & A_{1,k} & A_{1,k+1} & \cdots & A_{1,m} \\ \vdots & & \vdots & \vdots & & \vdots \\ A_{k,1} & \cdots & A_{k,k} & A_{k,k+1} & \cdots & A_{k,m} \\ \hline A_{k+1,1} & \cdots & A_{k+1,k} & A_{k+1,k+1} & \cdots & A_{k+1,m} \\ \vdots & & \vdots & \vdots & & \vdots \\ A_{m,1} & \cdots & A_{m,k} & A_{m,k+1} & \cdots & A_{m,m} \end{array} \right]$$

and

$$A' = \begin{bmatrix} A_1 & J - A_2 \\ J - A_2^\top & A_3 \end{bmatrix}.$$

First consider the eigenvalues of A' orthogonal to W . These eigenvalues remain unchanged if one subtracts J from some of the blocks of the partition, so they are eigenvalues of

$$E = \begin{bmatrix} A_1 & -A_2 \\ -A_2^\top & A_3 \end{bmatrix}.$$

Now $E = D^{-1}AD$, where $D = D^{-1}$ is a diagonal matrix with diagonal entries ± 1 . Thus A and E are similar, and therefore A and A' have the same eigenvalues for the eigenvectors in W^\perp .

Let μ_1, \dots, μ_m be the eigenvalues of B and let μ'_1, \dots, μ'_m be the eigenvalues of B' . Then μ_1, \dots, μ_m and μ'_1, \dots, μ'_m are the eigenvalues of A and A' , respectively, with eigenvectors in W . Clearly B and B' have the same diagonal entries, so $\text{trace } B = \text{trace } B'$, and because B has no negative eigenvalues it follows that

$$\sum_{i=1}^m |\mu_i| = \sum_{i=1}^m \mu_i = \sum_{i=1}^m \mu'_i \leq \sum_{i=1}^m |\mu'_i|$$

with equality if and only if $\mu'_i \geq 0$ for $i = 1, \dots, m$. □

Example 1. Consider a graph Γ on n vertices with adjacency matrix A , and let m be an odd integer greater than n . Construct an adjacency matrix M of a graph Δ of order mn as follows. Replace every entry $a_{i,j}$ of A with $i > j$ by a square $(0, 1)$ -matrix $A_{i,j}$ (say) of order m with constant row and column sums equal to $a_{i,j} + \frac{m-1}{2}$, replace $a_{i,j}$ by $A_{j,i}^T$ if $i < j$, and replace $a_{i,i}$ by $J - I$ for $i = 1, \dots, n$. Then M has an equitable partition with quotient matrix $B = \frac{m-1}{2}J + A + \frac{m-1}{2}I$, which is positive semi-definite (indeed, J is positive semi-definite, and so is $A + \frac{m-1}{2}I$, since the smallest eigenvalue of A is least $-\frac{n}{2} \geq -\frac{m-1}{2}$). Take any partition $\{U_1, U_2\}$ of the vertex set of Γ , and let Γ' with adjacency matrix A' be the graph obtained by Seidel switching with respect to $\{U_1, U_2\}$, and let Δ' be the graph obtained by switching from Δ with respect to the corresponding bipartition of the classes. Then Δ' has quotient matrix $B' = \frac{m-1}{2}J + A' + \frac{m-1}{2}I$, which is again positive semi-definite. Therefore Δ and Δ' have the same energy by Theorem 2.1. It easily follows that Δ and Δ' are cospectral if and only if Γ and Γ' are, and that Δ and Δ' poses the same number of edges if and only if Γ and Γ' do. This construction provides a large number of pairs of graphs with different spectrum but equal energy. For many pairs the two graphs poses the same number of edges, and for many pairs they don't.

Example 2. A rather interesting example can be obtained from a strongly regular graph with parameters $(4m^2, 2m^2 + m, m^2 + m, m^2 + m)$ ($m \geq 2$), that is, a graph with maximal energy. By definition, the distance partition with respect to any vertex of such a strongly regular graph is equitable with quotient matrix

$$\begin{bmatrix} 0 & 2m^2 + m & 0 \\ 1 & m^2 + m & m^2 - 1 \\ 0 & m^2 + m & m^2 \end{bmatrix}.$$

Deleting the vertex gives a graph Γ on $n = 4m^2 - 1$ vertices with an equitable partition with quotient matrix

$$B = \begin{bmatrix} m^2 + m & m^2 - 1 \\ m^2 + m & m^2 \end{bmatrix}.$$

This matrix B has no negative eigenvalues (the trace and the determinant are positive), and the same is true for the quotient matrix

$$B' = \begin{bmatrix} m^2 + m & m^2 - m \\ m^2 & m^2 \end{bmatrix}.$$

corresponding to the graph Γ' obtained from Γ by Seidel switching. It is easy to check, and well known from the theory of Seidel switching (see for example [2]) that the graph Γ' is a strongly regular graph with parameters $(4m^2 - 1, 2m^2, m^2, m^2)$. The eigenvalues of Γ' are $2m^2$ (with multiplicity 1) and $\pm m$ (with total multiplicity $4m^2 - 2$), and therefore

$$\mathcal{E}(\Gamma) = \mathcal{E}(\Gamma') = 4m^3 + 2m^2 - 2m.$$

The bound of Koolen-Moulton gives

$$\mathcal{E}_{\max}(4m^2 - 1) < \frac{1}{2}(4m^2 - 1)(1 + \sqrt{4m^2 - 1}) = 4m^3 + 2m^2 - \frac{3}{2}m - \frac{1}{2} + o(1).$$

So the energy of Γ and Γ' is very close to the maximum energy. We conjecture that there exists no graph on $4m^2 - 1$ vertices with larger energy. If this conjecture is true, then we have an infinite family of pairs of maximal energy graphs, where for each pair, one graph is regular and the other one is not. Notice that Γ and Γ' are not cospectral. In fact Γ' has integral eigenvalues, whilst switching changes two eigenvalues $2m^2$ and m into $\frac{1}{2}(2m^2 + m \pm \sqrt{4m^4 + 4m^3 - 3m^2 - 4m})$. The example also shows pairs of graphs with the same (integral) energy, where one graph has integral spectrum and the other one not.

3 Seidel matrix

The algebraic properties of Seidel switching become smooth if one considers the Seidel matrix S of a graph. If A is the adjacency matrix of a graph Γ , then the *Seidel matrix* S of Γ is defined by $S = J - 2A - I$. Thus S has 0 on the diagonal and ± 1 off diagonal, where -1 indicates adjacency. Note that $-S$ is the Seidel matrix of the complement of Γ . In terms of the Seidel matrix, Seidel switching with respect to $\{U_1, U_2\}$ multiplies the rows and columns of U_1 by -1 . If S' is the Seidel matrix after switching, then $S' = DSD$, where D is a diagonal matrix with diagonal entries ± 1 . Clearly $D = D^{-1}$, so S and S' are similar, and therefore S and S' have the same spectrum.

Similar to the normal energy, we define the *Seidel energy* $\mathcal{S}(\Gamma)$ of Γ to be the sum of the absolute values of the eigenvalues of the Seidel matrix. Like for the normal energy,

the Seidel energy is monotonic under taking induced subgraphs. By the above we see that the Seidel energy is invariant under Seidel switching and taking complements. The maximal possible Seidel energy for a graph on n vertices is denoted by $\mathcal{S}_{\max}(n)$.

A *conference matrix* is a square matrix S of order n with zero diagonal and ± 1 off diagonal, such that $SS^T = (n - 1)I$. If S is symmetric, S is the Seidel matrix of a graph, called a *conference graph*. Conference graphs exist for many values of n , for example when $n \equiv 2 \pmod{4}$ and $n - 1$ is a prime power. A necessary condition is that $n \equiv 2 \pmod{4}$ and $n - 1$ is the sum of two squares (see for example [2]). It turns out that conference graphs have maximal Seidel energy.

Theorem 3.1 *Let Γ be a graph with n vertices, then $\mathcal{S}(\Gamma) \leq n\sqrt{n - 1}$, and equality holds if and only if Γ is a conference graph.*

Proof. Let $\sigma_1, \dots, \sigma_n$ be the eigenvalues of the Seidel matrix S of Γ . We have $\text{trace } S^2 = n(n - 1) = \sum_i \sigma_i^2$. With Cauchy-Schwartz we get $\sum_i |\sigma_i| \leq n\sqrt{n - 1}$ with equality if and only if $|\sigma_i| = \sqrt{n - 1}$ for $i = 1, \dots, n$. Moreover, if each eigenvalue equals $\pm\sqrt{n - 1}$, then $S^2 = (n - 1)I$, which means that S is a symmetric conference matrix. □

This theorem says $\mathcal{S}_{\max}(n) \leq n\sqrt{n - 1}$. Using the existing results for conference matrices, it follows that this bound is asymptotically tight.

Corollary 3.2 $\mathcal{S}_{\max}(n) = n\sqrt{n}(1 + o(n))$.

Proof. Let p be the largest prime smaller than \sqrt{n} . If n is sufficiently large, then (see [1]) $p \geq \sqrt{n} - \sqrt{n}^{21/40}$. Since $p^2 \equiv 1 \pmod{4}$, there exists a graph Γ' of order $p^2 + 1$ with energy $\mathcal{S}(\Gamma') = p(p^2 + 1)$. Construct Γ by adding $n - p^2 - 1$ isolated vertices to Γ' . Then $\mathcal{S}(\Gamma) \geq p(p^2 + 1) > (\sqrt{n} - n^{21/80})(n - 2n^{61/80}) = n\sqrt{n}(1 + o(n))$, and therefore $\mathcal{S}_{\max}(n) = n\sqrt{n}(1 + o(n))$. □

Finding asymptotically tight lower bounds for the Seidel energy turns out to be more complicated. The next theorem gives a lower bound, but it is never tight if $n > 2$.

Theorem 3.3 *If Γ is a graph with $n > 2$ vertices, then $\mathcal{S}(\Gamma) > \sqrt{2n(n - 1)}$.*

Proof. Let S be the Seidel matrix of Γ . If $\sigma_1, \dots, \sigma_n$ are the eigenvalues of S , then $\sum_i \sigma_i = 0$ and $\sum_i \sigma_i^2 = n(n - 1)$. Suppose $\sigma_1 \geq \dots \geq \sigma_n$ minimizes $\sum_i |\sigma_i|$ subject to these two constraints. We claim that $\sigma_i = 0$ for all but two values of i . Suppose not,

then without loss of generality we have $\sigma_1 \geq \sigma_2 > 0 > \sigma_n$. Choose x and y ($x \geq y$) such that $x + y = \sigma_1 + \sigma_2 + \sigma_n$ and $x^2 + y^2 = \sigma_1^2 + \sigma_2^2 + \sigma_n^2$. This leads to a quadratic equation with real roots x and y satisfying $x - y = \sqrt{(\sigma_1 + \sigma_2 - \sigma_n)^2 - 4\sigma_1\sigma_2} < \sigma_1 + \sigma_2 - \sigma_n$. Note that also $x + y$ and $-x - y$ are less than $\sigma_1 + \sigma_2 - \sigma_n$. Redefine $\sigma_1 = x$, $\sigma_2 = 0$ and $\sigma_n = y$. Then $\sigma_1, \dots, \sigma_n$ still satisfy the mentioned constraints, but the objective value is decreased by $\sigma_1 + \sigma_2 - \sigma_n - |x| - |y| > 0$, contradiction. This proves the claim. The only solution satisfying the claim is $\sigma_1 = -\sigma_n = \sqrt{n(n-1)/2}$ and $\sigma_i = 0$ for $i = 2, \dots, n-1$. Hence $\mathcal{S}(\Gamma) \geq \sqrt{2n(n-1)}$.

Every Seidel matrix S of order n satisfies $\det S \equiv \det(J - I) \equiv n - 1 \pmod{2}$, so if n is even, $\text{rank } S = n$, and if n is odd, $\text{rank } S \geq n - 1$. This implies that the multiplicity of an eigenvalue 0 is at most 1, hence no graph with at least 4 vertices can have $\mathcal{S}(\Gamma) = \sqrt{2n(n-1)}$. Also if $n = 3$ the inequality is strict, because $\mathcal{S}(\Gamma) = 4$ for all graphs Γ on 3 vertices. \square

If Γ or the complement is switching equivalent to the complete graph K_n , then $\mathcal{S}(\Gamma) = 2(n-1)$. We know of no graph with n vertices whose Seidel energy is smaller than $2(n-1)$, and conjecture that $2(n-1)$ is the minimum value of $\mathcal{S}(\Gamma)$ over all graphs on n vertices. This conjecture has been verified for $n \leq 10$ by Robin Swinkels (private communication).

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