

Dinormal graphs

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Abstract A novel type of graph is described, where the graph G has an orientation \vec{G} and reverse orientation \overleftarrow{G} such that $G = \vec{G} \cup \overleftarrow{G}$ and the adjacency matrices $A(\vec{G})$ and $A(\overleftarrow{G})$ of \vec{G} and \overleftarrow{G} commute. Some general characterization and examples are given, e.g., for toroidal graphs.

Keywords Normal matrix · Dinormal graph · Eigenvalue · Square-net toroidal graphs

1 Preliminary comments

Stevanović and Stevanović [1] considered a special class of graphs, manifesting a special type of orientation for its edges, and gave several examples. An orientation \vec{G} of G entails each edge of G being replaced by a directed arc, and $A(\vec{G})$ is such that the (i, j) -entry is 1 iff there is an arc from i to j . Also, \overleftarrow{G} denotes the orientation of G with each arc of \overleftarrow{G} opposite to the corresponding arc of \vec{G} . Then, $A(G) = A(\vec{G}) + A(\overleftarrow{G})$.

Here, we further elaborate the theory of the special class of these graphs (for which $A(\vec{G})$ and $A(\overleftarrow{G})$ commute) described by the Stevanovićs. We start from a slightly different point than they did, leading to a suite of possible equivalent definitions.

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Then, some further results concerning their generation and a relation to “phased” graphs are indicated.

2 General characterization

First, we recall that a square matrix $B = [b_{jk}]_{j,k=1}^n$ is normal iff $BB^\dagger = B^\dagger B$. Here, B^\dagger denotes the Hermitian conjugate of B —i.e., B^\dagger is the transpose complex conjugate of B . Also, B is said to be unitarily diagonalizable iff there exists a unitary matrix U such that UBU^\dagger is diagonal. The characteristic values of an $n \times n$ matrix B are the n roots of $\det(B - \beta I) = 0$. For a square matrix B , the eigenvalues λ_i and eigenvectors \vec{c}_i are solutions to $B\vec{c}_i = \lambda_i\vec{c}_i$ such that \vec{c}_i is not the 0-vector. The multiplicity of an eigenvalue is just the number of associated linearly independent eigenvectors. Recall that for a general square matrix each distinct value of the characteristic roots corresponds to an eigenvalue, but their multiplicities do not necessarily match. See, e.g., Section 1.4.3 of [2].

Theorem 1 *Let B be an $n \times n$ matrix with characteristic roots $\beta_j (1 \leq j \leq n)$. Then, the following are equivalent:*

- (a) B is normal;
- (b) There is an orthonormal set of eigenvectors to B ;
- (c) B is unitarily diagonalizable;
- (d) $\sum_{j,k=1}^n |b_{jk}|^2 = \sum_{j=1}^n |\beta_j|^2$;
- (e) The multiplicity of corresponding eigenvalues and characteristic roots are all the same;
- (f) The eigenvalues of $B + B^\dagger$ are $\beta_j + \beta_j^* (1 \leq j \leq n)$;
- (g) $\text{tr}(B + B^\dagger)^2 = \sum_{j=1}^n (\beta_j + \beta_j^*)^2$.

Proof The equivalence of (a), (b), (c), (d) is given as Theorem 2.5.4 in Horn and Johnson [2]. Condition (e) is seen to be equivalent to condition (c) in Sect. 1.4.3 of [2]. We build on this, first seeking to show that (a) and (c) imply (f). In this case, B and B^\dagger are simultaneously unitarily diagonalizable (via the same unitary transformation, as they have a common set of eigenvectors). Thence, this same unitary transformation also diagonalizes $B + B^\dagger$ to give eigenvalues $\beta_j + \beta_j^* (1 \leq j \leq n)$. As a second step, we seek to show that (f) implies (g). Indeed, this is trivial as the trace of $(B + B^\dagger)^2$ gives just the sum of characteristic roots, which by (f) are $(\beta_j + \beta_j^*)$. As a final step, we seek to show that (g) implies (d). Here, we rewrite (g) as

$$\text{tr}B^2 + 2\text{tr}BB^\dagger + \text{tr}(B^\dagger)^2 = \sum_{j=1}^n \beta_j^2 + 2 \sum_{j=1}^n \beta_j \beta_j^* + \sum (\beta_j^*)^2.$$

Cancellation of the left and right sides of $\text{tr}B^2 = \sum_{j=1}^n \beta_j^2$ and $\text{tr}(B^\dagger)^2 = \sum_{j=1}^n (\beta_j^*)^2$ from the left and right sides leaves $\text{tr}B^\dagger B = \sum_{j=1}^n \beta_j^* \beta_j$, which in fact gives (d). \square

An (undirected) graph G with the adjacency matrix $A = [a_{jk}]_{j,k=1}^n$ is *dinormally partitionable* (or more briefly, just *dinormal*) iff its edges can each be assigned an

orientation to give a directed graph \vec{G} with the adjacency matrix B such that B is normal and $A = B + B^\dagger$.

Now Theorem 1 leads directly to:

Theorem 2 *A graph G is dinormal iff there exists an edge orientation \vec{G} with the adjacency matrix $A(\vec{G}) \equiv B$ such that any one of the (equivalent) conditions (a), (b), (c), (d), (e), (f), or (g) of Theorem 1 is satisfied.*

Stevanović and Stevanović [1] have investigated dinormal graphs, utilizing their defining characteristic as that associated to condition (e) in the preceding Theorems 1 and 2. They noted a simple cycle with “clockwise” orientation as a prototypical example (see also [3]), and gave further examples. And they established that $A(\vec{G})$ and $A(\overleftarrow{G})$ commute (i.e., condition (a)) as a consequence of their condition (e).

3 Generation of dinormal graphs

Given a group Γ , let S be a set of generators. Then, the associated Cayley digraph $\text{Cay}(\Gamma; S)$ has the adjacency matrix

$$A(\text{Cay}(\Gamma; S))_{g,h} = \begin{cases} 1, & \text{if } g \in hS; \\ 0, & \text{otherwise} \end{cases} \quad (g, h \in \Gamma), \tag{1}$$

where $hS := \{hs \mid s \in S\}$. Evidently,

$$A(\text{Cay}(\Gamma; S)) = \sum_{s \in S} D^\Gamma(s), \tag{2}$$

where $D^\Gamma(s)$ is the “permutation representation” of Γ , which is such that the (g, h) -th element is $= 1$, if $g = sh$, and otherwise is $= 0$. Further, $S^\dagger := \{s^{-1} \mid s \in S\}$ is also a set of generators and

$$A(\text{Cay}(\Gamma; S^\dagger)) = [A(\text{Cay}(\Gamma; S))]^\dagger. \tag{3}$$

Indeed, the example providing [3] the Stevanovićs’ motivation for their considerations [1] is found with what is in fact such a Cayley graph $\text{Cay}(C_n; S)$, where $S = \{c\}$ and $\{C_n = \{c^p \mid p \in [1, n]\}$ is the cyclic group of order n with its generator c . More generally, we have:

Proposition 3 *Let Γ be a commutative group and let none of the s in a generating set S be an involution. Then, removal of the directions from the edges of $\text{Cay}(\Gamma; S)$ gives a dinormal graph. For $S = \{s_1, s_2, \dots, s_p\}$, the 2^p possible sets $\tilde{S} := \{\tilde{s}_i \mid i \in [1, p]\}$ with $\tilde{s}_i = s_i$ or $\tilde{s}_i = s_i^{-1}$ each generate the same dinormal graph when directions are removed from $\text{Cay}(\Gamma; \tilde{S})$.*

Proof First, note that since no $s \in S$ is involutory, no arc in $\text{Cay}(\Gamma; S)$ has its reverse in $\text{Cay}(\Gamma; S)$. As a consequence of commutativity of Γ , members of S commute as

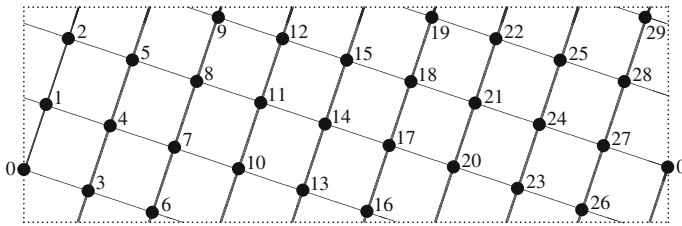


Fig. 1 The toroidal Cayley graph $\text{Cay}(C_{30}; \{c, c^3\})$ on 30 vertices; $n_{\text{cyc}} = 1$, $L = 30$, $n_{\text{long}} = 1$, and $n_{\text{tran}} = 9$

also do their permutation representatives and, since A and A^\dagger are sums of commuting group-element representations, A and A^\dagger also commute, and they are normal. The “union” of the 2 Cayley graphs of S and S^\dagger then is dinormal. \square

Another example is $\text{Cay}(C_7, \{c, c^3\})$, where c is a generator of the cyclic group C_7 . See Fig. 1 in [1]. In fact, one finds further such examples listed by Stevanović and Stevanović [1]: their \vec{G}_4 is $\text{Cay}(C_6; \{c, c^4\})$; their \vec{G}_5 is $\text{Cay}(C_7; \{c^2, c^3\})$; and their \vec{G}_9 is $\text{Cay}(C_8; \{c, c^3\})$.

4 Square-net toroidal graphs

Toroidal graphs based on the square-planar network are possible and are expressible as Cayley graphs which are dinormal. Indeed, in chemistry, there are numerous square-net structures based [4] on oxalate coordinating ligands interconnecting pairs of transition-metal ions. Now when one takes a product of 2 mutually commuting cyclic groups, C_a and C_b , say, with generators c_a and c_b , the dinormal graph $\text{Cay}(C_a C_b; \{c_a, c_b\})$ is a “standard” toroidal graph: It is a torus based on the $|C_a|$ by $|C_b|$ square grid, in this case with simplest “nonhelical boundary conditions”. This is also a direct sum of cyclic graphs of sizes $|C_a|$ and $|C_b|$, and so is also covered in the Stevanović’s “NEPS product” case. But there are also toroidal graphs with “twisted” or “helical” boundary conditions, which perhaps are not covered in the NEPS construction. *E. g.*, the Stevanović do not identify their graphs \vec{G}_4 , \vec{G}_5 or \vec{G}_9 as arising from NEPS products. Clearly, also our Cayley graph construction does not include their general NEPS cases, as NEPS graphs sometimes lead to nonregular dinormal graphs. Cayley graphs $\text{Cay}(C_p, \{c, c^a\})$ may be viewed as helical graphs. For instance, for $\text{Cay}(C_{30}, \{c, c^3\})$ imagine part C of the graph arising from the generator c ; let this cycle C be helically embedded on the surface with G turns around the cylindrical body of the torus before it comes back to itself, as in Fig. 1 above. There, the nodes c^m are labeled just by the exponent m , the c -bonds are in bold-face, and the c^3 -bonds in lighter face. Another example, $\text{Cay}(C_{28}, \{c, c^{15}\})$ is also depicted in Fig. 2, with a similar labeling of nodes and edges. Here, the main cycle generated by c traverses twice around the cylindrical length of the torus. Finally, yet another example is given in Fig. 3, for $\text{Cay}(C_{24}, \{c^2, c^3\})$. Here, there are 2 disjoint cycles winding their way around the cylindrical length of the torus, each being connected by the generator c^2 , one cycle containing all the “odd” vertices and one the “even”. At the same time, the second

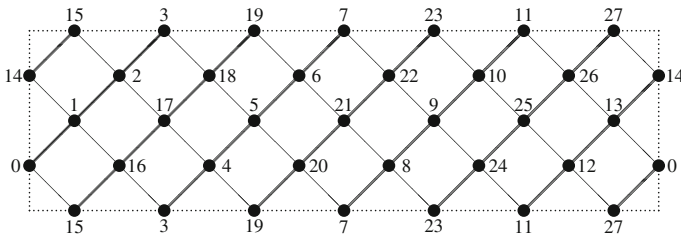


Fig. 2 The toroidal Cayley graph $\text{Cay}(C_{28}; \{c, c^{15}\})$ on 28 vertices; $n_{\text{cyc}} = 1$, $L = 28$, $n_{\text{long}} = 2$, and $n_{\text{tran}} = 7$

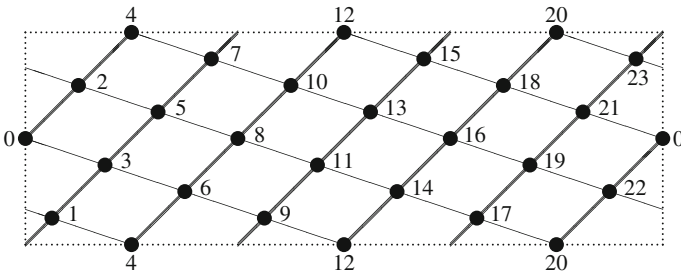


Fig. 3 The toroidal Cayley graph $\text{Cay}(C_{24}; \{c^2, c^3\})$ on 24 vertices; $n_{\text{cyc}} = 2$, $L = 12$, $n_{\text{long}} = 1$, $n_{\text{tran}} = 3$

generator c connects from one of these cycles to the other. Overall, we imagine that such Cayley graphs generate all graphically distinct toroidal square-grid graphs.

Indeed, we may make a conjecture about the set T_4 of topologically distinct graph embeddings for such square-net graphs embedded on a torus \mathcal{T} . Here, by “topologically distinct” we mean to distinguish those embeddings on \mathcal{T} which are homomorphically distinct via a homeomorphism which preserves not only the graph G but also \mathcal{T} and the space \mathbb{E}^3 in which \mathcal{T} is embedded.

Conjecture 4 *The topologically distinct members of T_4 are uniquely specified by:*

- * the number n_{cyc} of straight cycles winding around \mathcal{T} ;
- * the length L of such a cycle;
- * the number n_{long} of times such a cycle winds around in the longitudinal direction;
- * the number n_{tran} of times such a cycle winds around in the transverse direction.

Here $n_{\text{cyc}} \geq 1$, $n_{\text{long}} \geq 0$, $n_{\text{tran}} \geq 0$, $n_{\text{long}} + n_{\text{tran}} \geq 1$, and $G = \text{Cay}(C_{Ln_{\text{cyc}}}; \{C^{n_{\text{cyc}}}, c^{n_{\text{cyc}}+1}\})$, where c is a generator of $C_{Ln_{\text{cyc}}}$.

Notably, not all the parameters (particularly, n_{long} and n_{tran}) appear in the specification of the (unembedded) G . Again, these G are generally dinormal.

5 Dinormality and phasing

A *phased* graph G obtained from an ordinary graph has [5] an adjacency matrix A with general modulus 1 values in place of the unit entries of the unphased case, but subject

to the constraint that A is Hermitian. The definition of a dinormal (unphased) graph is extended to phased ones, with B and B^\dagger having disjoint sets of nonzero elements such that $A(G) = B + B^\dagger$.

Proposition 5 *Suppose that G has a dinormal partitioning $A = B + B^\dagger$, with the eigenvalues of B being $\beta_j = \rho_j \exp(i\theta_j) (1 \leq j \leq n)$. If U is a diagonal unitary matrix and $B_U := UB_U^*$, then the phased graph \hat{G} with the adjacency matrix $\hat{A} = \exp(i\theta)B_U + \exp(-i\theta)B_U^*$ has eigenvalues $2\rho_j \cos[i(\theta + \theta_j)] (1 \leq j \leq n)$, the same as A .*

Proof Since A is dinormal, B and B^\dagger commute as then also do B_U and B_U^\dagger , and yet further also do $e^{i\theta}B_U$ and $e^{-i\theta}B_U^\dagger$. Thence, application of Theorem 1 gives the eigenvalues of A as the sums of those of $e^{i\theta}B_U$ and $e^{-i\theta}B_U^\dagger$. Further, the eigenvalues of B and B^\dagger are the same, whence those of $e^{i\theta}B_U$ are those of B multiplied by $e^{i\theta}$. Similarly, the eigenvalues of $e^{-i\theta}B_U^\dagger$ are $e^{-i\theta}$ times those of B^\dagger , which are complex conjugates of those of B . Thence, each (real) eigenvalue λ of B corresponds to one $\lambda e^{i\theta} + \lambda e^{-i\theta}$ of A . □

Proposition 6 *Suppose that $\text{Cay}(\Gamma; S)$ is as in Proposition 3. Then, the phased graph G with*

$$A(G) = \sum_{s \in S} \left[e^{i\theta_s} D^\Gamma(s) + e^{-i\theta_s} D^\Gamma(s^{-1}) \right]$$

is dinormal.

Proof Since Γ is Abelian, the $s \in S$ commute, as then also do corresponding permutation representations $D^\Gamma(s)$. The $e^{i\theta_s} D^\Gamma(s)$ and $e^{-i\theta_s} D^\Gamma(s^{-1})$, $s \in S$, then all commute, as also do $\sum_{s \in S} e^{i\theta_s} D^\Gamma(s) = B$ and $B^\dagger = \sum_{s \in S} e^{-i\theta_s} D^\Gamma(s^{-1})$. □

6 Conclusion

In conclusion, the naming and characterizing of dinormal graphs is here enhanced, and a method for their generation is found, which along with the Stevanović and Stevanović’s NEPS-sum method for building new dinormal graphs from old ones reveals a wide range of such graphs, including a range of square toroidal graphs. Further, an application is found to further understand phased graphs [4].

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References

1. D. Stevanović, S. Stevanović, On relation between spectra of graphs and their digraph decompositions. Publications de l’Institut Mathématique, Nouvel série **85**(99), 47–54 (2009)
2. R.A. Horn, C.R. Johnson, *Matrix Analysis* (Cambridge University Press, New York, 1985)

3. I. Gutman, P.J. Plath, On molecular graphs and digraphs of annulenes and their spectra. *J. Serb. Chem. Soc.* **66**, 237–241 (2001)
4. See several of the articles in issue # 1 of *Chem. Rev.* **98** (1998)
5. D.J. Klein, V.R. Rosenfeld, Phased graphs and graph energies. *J. Math. Chem.* accepted