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Diagonal entries of the average mixing matrix

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Abstract

We study the diagonal entries of the average mixing matrix of continuous quantum walks. The average mixing matrix is a graph invariant; it is the sum of the Schur squares of spectral idempotents of the Hamiltonian. It is non-negative, doubly stochastic and positive semidefinite. We study the graphs for which the trace of the average mixing matrix is maximum or minimum and we classify those which are maximum. We give two constructions of graphs whose average mixing matrices have constant diagonal.

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1 Introduction

We consider a quantum process on an underlying graph, and its average behaviour over time. Let X be a graph on n vertices with adjacency matrix A. We use Δ to denote the $n \times n$ diagonal matrix with $\Delta_{i,i}$ equal to the valency of the vertex i. The matrix $\Delta - A$ is the *Laplacian*, denoted $L(X)$, and $\Delta + A$ is known as the *signless Laplacian* of X.

A continuous random walk on a graph X is given by the 1-parameter family of matrices

$$\exp(t(A - \Delta)).$$

Physicists are concerned with quantum analogs. If B is a linear combination of A and Δ, the 1-parameter family of matrices

$$U(t) = \exp itB$$

determines a *continuous quantum walk* on the vertices of X. We say that $U(t)$ is the *transition matrix* of the walk, and refer to B as the *Hamiltonian*. (Usually B is the adjacency matrix, the next most common choice is the Laplacian. If X is regular, then the adjacency matrix and the two Laplacians provide the same information.) Kay [8] provides a useful survey of continuous quantum walks.

Our overall aim is to establish connections between properties of a continuous quantum walk and properties of the underlying graph. In this paper we focus on a matrix derived from $U(t)$, the *mixing matrix* of the walk, which we define by

$$M(t) = U(t) \circ \overline{U(t)}.$$

(Here $\circ$ denotes the Schur product of two matrices.) The *average mixing matrix*, denoted $\widehat{M}$, is defined as follows:

$$\widehat{M}(X) = \lim_{T \to \infty} \frac{1}{T} \int_0^T M(t)\, dt. \tag{1.1}$$

The average mixing matrix is, intuitively, a distribution that the quantum walk adheres to, on average, over time, and thus may be thought of as a replacement for a stationary distribution, since, unlike their random counterparts, quantum walks do not converge to any distribution. Earlier work on this matrix appears in [1, 3, 4, 6].

The average mixing matrix is doubly stochastic and positive semidefinite. In this paper, we investigate its diagonal entries. The diagonal entry of the transition matrix gives the amplitude of the walk returning to vertex v; more technically, $|U^t_{v,v}|^2$ is the probability of measuring at vertex v at time t, having started at vertex v. Thus, we may consider the diagonal entries of the average mixing matrix to be the average probabilities of returning to a vertex, having started at that vertex.

Here, we study the graphs which attain the maximum and minimum of the trace of $\widehat{M}$ with respect to the Laplacian and adjacency matrices. We find that, amongst all graphs on n vertices, K_n maximizes the trace of the average mixing matrix with respect to the Laplacian matrix. We also investigate the graphs whose average mixing matrices, with respect to the adjacency matrix, have constant diagonal, and we give a construction for non-regular graphs with such a property. Tables summarizing the results of some of our computations are provided.

2 The Average Mixing Matrix

Let X be a graph on n vertices and let $B \in \{A(X), L(X)\}$. Let $\theta_1, \dots, \theta_d$ be the distinct eigenvalues of B and, for $r = 1, \dots, d$, let E_r be the idempotent projection onto the θ_r eigenspace of B; the spectral decomposition of B is as follows:

$$B = \sum_{r=1}^{d} \theta_r E_r.$$

The following is an important theorem, as it allows us to understand the average mixing matrix.

Theorem 2.1. *[6] Let X be a graph and let $B \in \{A(X), L(X)\}$. Let*

$$B = \sum_{r=1}^{d} \theta_r E_r$$

be the spectral decomposition of B. The average mixing matrix of X with respect to B is

$$\widehat{M}_B(X) = \sum_{r=1}^{d} E_r \circ E_r. \qquad \square$$

By way of example, we consider the complete graph K_n, with the adjacency matrix as Hamiltonian. Here $n-1$ is a simple eigenvalue and the asssociated eigenspace is spanned by the constant vectors; the projection is

$$E_1 = \frac{1}{n} J.$$

The second eigenvalue of K_n is -1, with multiplicity $n-1$. Since the spectral projections sum to I, the second projection is

$$E_2 = I - \frac{1}{n} J.$$

Hence the average mixing matrix of K_n is

$$\frac{1}{n^2} J \circ J + \left(I - \frac{1}{n} J\right) \circ \left(I - \frac{1}{n} J\right) = \left(1 - \frac{2}{n}\right) I + \frac{2}{n^2} J.$$

We will use $\widehat{M}_B(X)$ to denote the average mixing matrix of X, with the matrix B as the Hamiltonian of the quantum walk. We will denote by $\overline{X}$ the complement of a graph X. We will write $J_{j,k}$ for the $j \times k$ matrix with all entries equal to 1; when $j = k$, we will write J_j for convenience. For the Laplacian matrix of connected graphs, the average mixing matrix is the same as the complement, except when the complement is not connected; we will give the explicit relation between $\widehat{M}_L(\overline{X})$ and $\widehat{M}_L(X)$ for completeness, in Lemma 3.2.

3 Laplacians

Lemma 3.1 summarizes some basic properties of Laplacian eigenvalues, which can be found in any standard algebraic graph theory text, including [5].

Lemma 3.1. *Let X be a graph on n vertices and $L := L(X)$ be the Laplacian matrix of X. Suppose the distinct eigenvalues of L are $\theta_0 \leq \cdots \leq \theta_d$, with corresponding projections $E_0, \ldots, E_d$ onto the eigenspaces of L.*

(i) For every i, we have that $n - \theta_i$ is an eigenvalue of $L(\overline{X})$.

(ii) $\theta_0 = 0$ and the multiplicity of 0 as an eigenvalue of L is equal to the number of connected components of X.

(iii) The multiplicity of n as an eigenvalue of X is $c - 1$, where c is the number of connected components of the complement of X.

(iv) If X has c components $C_1, C_2, \ldots, C_c$ and the vertices of X are ordered $(x_{i_1}, \ldots, x_{i_{|C_i|}})_{i=1}^c$, then

$$E_0 = \begin{pmatrix} \frac{1}{|C_1|}J_{|C_1|} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \frac{1}{|C_2|}J_{|C_2|} & & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \frac{1}{|C_c|}J_{|C_c|} \end{pmatrix}$$

where $\mathbf{0}$ denotes an all zero matrix of the appropriate order.

Lemma 3.2. *Let X be a connected graph on n vertices and $L := L(X)$ be the Laplacian matrix of X. Suppose the distinct eigenvalues of L are $\theta_0 < \cdots < \theta_d$, with corresponding projections $E_0, \ldots, E_d$ onto the eigenspaces of L. If $\overline{X}$ has c components $C_1, C_2, \ldots, C_c$ and the vertices of X are ordered $(x_{i_1}, \ldots, x_{i_{|C_i|}})_{i=1}^c$, then*

$$\widehat{M}_L(\overline{X}) = \widehat{M}_L(X) - \frac{1}{n^2}J_n + \begin{pmatrix} \frac{1}{|C_1|^2}J_{|C_1|} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \frac{1}{|C_2|^2}J_{|C_2|} & & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \frac{1}{|C_c|^2}J_{|C_c|} \end{pmatrix} \tag{3.1}$$

where $\mathbf{0}$ denotes an all zero matrix of the appropriate order.

Proof. Observe that

$$L(X) + L(\overline{X}) = -J + nI.$$

As in the statement of the lemma, let the distinct eigenvalues of L be denoted by $\theta_0 < \cdots < \theta_d$, with corresponding projections $E_0, \dots, E_d$ onto the eigenspaces of L. If $i \neq 0$, then $L(\overline{X})E_i = (n - \theta_i)E_i$ and thus, since $\sum_{i=0}^{d} E_i = I_n$

$$L(\overline{X}) = 0 \cdot E_0 + \sum_{i=1}^{d} (n - \theta_i)E_i. \tag{3.2}$$

If $\overline{X}$ is connected, then $\theta_i \neq n$ for any i and thus (3.2) is the spectral decomposition of $L(\overline{X})$.

For the more general result, we suppose that $\overline{X}$ has c components

$$C_1, C_2, \dots, C_c$$

and the vertices of X are ordered $(x_{i_1}, \dots, x_{i_{|C_i|}})_{i=1}^{c}$. Since $\theta_d = n$, we obtain that

$$L(\overline{X}) = 0 \cdot (E_0 + E_d) + \sum_{i=1}^{d-1} (n - \theta_i)E_i. \tag{3.3}$$

We see that $E_0 + E_d$ is idempotent and thus (3.3) is the spectral decomposition of $L(\overline{X})$ and the lemma follows. □

In particular, Lemma 3.2 implies that if $\overline{X}$ is connected, then

$$\widehat{M}_L(X) = \widehat{M}_L(\overline{X}).$$

Corollary 3.3. *Let X be a graph on n vertices and $L := L(X)$ be the Laplacian matrix of X. If $\overline{X}$ has c components $C_1, C_2, \dots, C_c$, then*

$$\operatorname{tr}(\widehat{M}_L(\overline{X})) = \operatorname{tr}(\widehat{M}_L(X)) - \frac{1}{n} + \sum_{i=1}^{c} \frac{1}{|C_i|}.$$

Proof. This follows from taking the trace of both sides of (3.1). □

4 An Ordering

For symmetric, square matrices A and B, we write $A \succcurlyeq B$ if $A - B$ is positive semidefinite. The relation $\succcurlyeq$ is a useful partial ordering on matrices. We briefly investigate some of its properties when applied to average mixing matrices.

Lemma 4.1. *Let X and Y be graphs on the same vertex set. If each spectral idempotent of $A(Y)$ is the sum of spectral idempotents of $A(X)$, then $\widehat{M}_A(Y) \succcurlyeq \widehat{M}_A(X)$. Similarly, if each spectral idempotent of $L(Y)$ is the sum of spectral idempotents of $L(X)$, then $\widehat{M}_L(Y) \succcurlyeq \widehat{M}_L(X)$.*

Proof. We have

$$(E+F)^{\circ 2} = E^{\circ 2} + F^{\circ 2} + 2E \circ F.$$

If E and F are positive semidefinite, so are the three terms in the sum above, whence

$$(E+F)^{\circ 2} \succcurlyeq E^{\circ 2} + F^{\circ 2}.$$

We apply this iteratively and, using Theorem 2.1, the lemma follows. □

Lemma 4.1 has many consequences, some of which will be explored in the next section. For now, we give a lemma about the products of graphs, which uses the same basic idea in the proof. Recall that $X \,\square\, Y$ denotes the Cartesian product of graphs X and Y and $X \times Y$ denotes the categorical (or direct) product of X and Y.

Lemma 4.2. *Let X and Y be graphs.*

(a) $\{\widehat{M}_A(X \,\square\, Y), \widehat{M}_A(X \times Y)\} \succcurlyeq \widehat{M}_A(X) \otimes \widehat{M}_A(Y)$*; and*

(b) $\{\widehat{M}_L(X \,\square\, Y), \widehat{M}_L(X \times Y)\} \succcurlyeq \widehat{M}_L(X) \otimes \widehat{M}_L(Y)$.

Proof. Let $E_1, \dots, E_\ell$ and $F_1, \dots, F_k$ be the respective spectral idempotents of X and Y. Then each spectral idempotent of $X \,\square\, Y$ is a sum of idempotents of the form $E_r \otimes F_s$. To complete the proof that

$$\widehat{M}_A(X \,\square\, Y) \succcurlyeq \widehat{M}_A(X) \otimes \widehat{M}_A(Y),$$

note that

$$(E_r \otimes F_s)^{\circ 2} = E_r^{\circ 2} \otimes F_s^{\circ 2}.$$

This argument will also hold when we use the direct product instead of Cartesian product. The proof of part (b) also follows similarly. □

If P is a permutation matrix and $A(Y) = P^T A(X) P$, then

$$\widehat{M}(Y) = P^T \widehat{M}(X) P.$$

This indicates that the partial ordering on average mixing matrices using $\succcurlyeq$ cannot generally correspond to a useful ordering on graphs.

5 Application to Quantum Walks using the Laplacian

We will use Lemma 4.1 to show that K_n maximizes the trace of the average mixing matrix with respect to the Laplacian matrix, amongst all graphs on n vertices.

Note that, for graphs X and Y, we denote by $X + Y$ the disjoint union of X and Y.

Lemma 5.1. *Let X be a connected graph on n vertices. Then*

$$\widehat{M}_L(K_n) \succcurlyeq \widehat{M}_L(X).$$

More generally, if X has m connected components $C_1, \dots, C_m$ with $c_1, \dots, c_m$ vertices respectively, then

$$\widehat{M}_L(K_{c_1} + \cdots + K_{c_m}) \succcurlyeq \widehat{M}_L(X).$$

Proof. Let I and J be the $n \times n$ identity and all ones matrix, respectively. We observe that

$$L(K_n) = nI - J = 0\left(\frac{1}{n}J\right) + n\left(I - \frac{1}{n}J\right). \tag{5.1}$$

We see that the right side of (5.1) gives the spectral decomposition of $L(K_n)$.

Any connected graph X on n vertices has $\frac{1}{n}J$ as a spectral idempotent and so the sum of the other spectral idempotents of X must be equal to $I - \frac{1}{n}J$. Thus we have obtained that each spectral idempotent of $L(K_n)$ is the sum of spectral idempotents of $L(X)$, and so

$$\widehat{M}_L(Y) \succcurlyeq \widehat{M}_L(X)$$

by Lemma 4.1. The more general statement follows from considering the connected components separately and recalling that, for graphs X and Y,

$$\widehat{M}_L(X+Y) = \begin{pmatrix} \widehat{M}_L(X) & 0 \\ 0 & \widehat{M}_L(Y) \end{pmatrix}$$

and the lemma follows. □

Corollary 5.2. *Let X be a connected graph on n vertices. Then*

$$\operatorname{tr}(\widehat{M}_L(K_n)) \geq \operatorname{tr}(\widehat{M}_L(X)),$$

and equality holds if and only if X is isomorphic to K_n. More generally, if X has m connected components $C_1, \dots, C_m$ with $c_1, \dots, c_m$ vertices respectively, then

$$\operatorname{tr}(\widehat{M}_L(K_{c_1} + \cdots + K_{c_m})) \geq \operatorname{tr}(\widehat{M}_L(X)).$$

Equality holds if and only if X is isomorphic to $K_{c_1} + \cdots + K_{c_m}$.

Proof. Recall the following property from elementary linear algebra: if $A \succcurlyeq B$, then $\operatorname{tr}(A) \geq \operatorname{tr}(B)$. We immediately obtain for any connected graph X on n vertices that

$$\operatorname{tr}(\widehat{M}_L(K_n)) \geq \operatorname{tr}(\widehat{M}_L(X)).$$

Note that for positive semidefinite matrices A and B, if $A \succcurlyeq B$ and $\operatorname{tr}(A) = \operatorname{tr}(B)$, then $\operatorname{tr}(A - B) = 0$ and $A - B \succcurlyeq 0$ and so $A - B = 0$. Thus, if

$$\operatorname{tr}(\widehat{M}_L(K_n)) = \operatorname{tr}(\widehat{M}_L(X))$$

then

$$\widehat{M}_L(K_n) = \widehat{M}_L(X)$$

and thus X is isomorphic to K_n.

The more general statement follows if we consider the connected components separately. □

From (5.1), we can see that

$$\widehat{M}_L(K_n) = \left(\frac{1}{n}J\right)^{\circ 2} + \left(I - \frac{1}{n}J\right)^{\circ 2} = \left(1 - \frac{2}{n}\right)I + \frac{2}{n^2}J$$

and so

$$\operatorname{tr}(\widehat{M}_L(K_n)) = n - 2 + \frac{2}{n}.$$

Note that $\operatorname{tr}(\widehat{M}_L(\overline{K_n})) = \operatorname{tr}(I) = n$.

6 Eigenspace Refinement

Similar to Section 5, we look at implications of Lemma 4.1 for the average mixing matrix with respect to the adjacency matrix.

Lemma 6.1. *If X has an equitable partition with parts of size $a_1, \ldots, a_m$, then the eigenspaces of X refine the eigenspaces of the disjoint union of $K_{a_1}, \ldots, K_{a_m}$.*

Proof. This follows because every eigenvector of X is either constant, or sums to 0 on each part of the equitable partition. □

The trace of $\widehat{M}_A(K_n)$ is

$$\frac{1 + (n-1)^2}{n} = \frac{n^2 - 2n + 2}{n}.$$

Thus, with Lemma 4.1, we obtain the following:

Lemma 6.2. *If X has an equitable partition with parts of size $a_1, \ldots, a_m$, then*

$$tr\widehat{M}_A(X) \leq \sum_{j=1}^{m} \frac{a_j^2 - 2a_j + 2}{a_j}$$

Proof. Let $Y = K_{a_1} \cup \ldots \cup K_{a_m}$, the disjoint union of complete graphs. By the previous lemma, we see that the eigenspaces of X refine those of Y and thus

$$\operatorname{tr} \widehat{M}_A(X) \leq \operatorname{tr} \widehat{M}_A(Y).$$

We see that

$$\operatorname{tr}(\widehat{M}(Y)) = \sum_{r=1}^{m} \operatorname{tr}(\widehat{M}(K_{a_r})) = \sum_{r=1}^{m} \frac{a_r^2 - 2a_r + 2}{a_r}$$

and the result follows. □

We see that $a_1 + \cdots + a_m = n$. Thus

$$\sum_{j=1}^{m} \frac{a_j^2 - 2a_j + 2}{a_j} = \sum_{j=1}^{m} \left(a_j - 2 + \frac{2}{a_j} \right)$$
$$= n - 2m + 2 \sum_{j=1}^{m} \frac{1}{a_j}.$$

Corollary 6.3. *If X is a regular graph on n vertices, then*

$$\operatorname{tr} \widehat{M}_A(X) \leq \operatorname{tr} \widehat{M}_A(K_n).$$

7 Constant Diagonal

For this section, we will use $\widehat{M}(X)$ to denote $\widehat{M}_A(X)$.

We consider graphs whose average mixing matrices with respect to the adjacency matrix have constant diagonal. These matrices are easy to work with because of the following trivial lemma.

Lemma 7.1. *Let M be a positive semidefinite matrix. If M has a constant diagonal, then $M_{u,u} \geq M_{u,v}$. Furthermore, if M has a constant diagonal and $M_{u,u} = M_{u,v}$, then $Me_u = Me_v$.*

Proof. A 2×2 principal submatrix of M is the Gram matrix of two vectors, in our case of the same length. Hence the result is a slightly disguised version of Cauchy-Schwarz. □

A graph is *walk-regular* if the number of closed walks at vertex v of length k is c_k, a constant independent of the choice of vertex, for every k. Equivalently, X is walk-regular if $A(X)^k$ has a constant diagonal for every k. We refer to [5] for further details.

Lemma 7.2. *If X is a walk-regular graph, then $\widehat{M}(X)$ has a constant diagonal.*

Proof. Since the eigenprojections of $A(X)$ are polynomials in $A(X)$, we get that they are matrices with constant diagonals. Thus, $\widehat{M}(X)$ is a sum of matrices with constant diagonals. □

It is surprising that these are not the only graphs whose average mixing matrices have constant diagonals. We will consider rooted products of graphs.

Let X be a graph with vertices $\{v_1, \dots, v_n\}$ and let Y be a disjoint union of rooted graphs $Y_1, \dots, Y_n$, rooted at $y_1, \dots, y_n$, respectively. The *rooted product* of X and Y, denoted $X(Y)$, is the graph obtain by identifying v_i with the root vertex of Y_i. The rooted product was first introduced by Godsil and McKay in [7]. We will

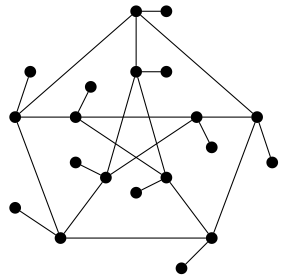


Figure 1: The rooted product of the Petersen graph with K_2.

consider the special case where Y is a sequence of n copies of K_2. In this case, we will write $X(K_2)$ to denote the rooted product. Figure 1 showed the rooted product of the Petersen graph with K_2, which is not walk-regular but whose average mixing matrix has a constant diagonal, by Corollary 7.5.

In [4], the authors consider the rooted product of X with K_2. The results Lemma 3.3 and Theorem 3.4 there are stated under the assumption that their eigenvalues of X are simple, but the proofs make no use of this assumption. We state the results for general graphs here and provide a brief proof. Note that the eigenvalues of such graphs are given in [7] and in [2], where they appear as a special case of Theorem 3.1; here, in order to analyse the average mixing matrix, we also need the explicit form of the spectral idempotents, which we give in the next lemma,

Lemma 7.3. *Let X be a graph and let $F_1, \dots, F_d$ the orthogonal projections onto the eigenspaces of $A(X)$ with corresponding eigenvalues $\lambda_1, \dots, \lambda_d$. Then, the eigenvalues of the adjacency matrix of $X(K_2)$ are $\{\mu_i, \nu_i\}_{i=1,d}$ where μ_i, ν_i are the roots of $t^2 - \lambda_i t - 1 = 0$. For $\mu \in \{\mu_i, \nu_i\}$, the projection onto the μ-eigenspace is*

$$\frac{1}{\mu^2+1}\begin{pmatrix} \mu^2 F_i & \mu F_i \\ \mu F_i & F_i \end{pmatrix}.$$

Proof. The eigenvalues of $X(K_2)$ are given in [7]. Fix i and $\mu \in \{\mu_i, \nu_i\}$.

$$E := \frac{1}{\mu^2+1}\begin{pmatrix} \mu^2 F_i & \mu F_i \\ \mu F_i & F_i \end{pmatrix}.$$

Observe that $E^2 = E$ and

$$\begin{aligned} A\left(X(K_2)\right)E &= \frac{1}{\mu^2+1}\begin{pmatrix} A & I \\ I & 0 \end{pmatrix}\begin{pmatrix} \mu^2 F_i & \mu F_i \\ \mu F_i & F_i \end{pmatrix} \\ &= \frac{1}{\mu^2+1}\begin{pmatrix} (\lambda\mu^2+\mu)F_i & (\lambda\mu+1)F_i \\ \mu^2 F_i & \mu F_i \end{pmatrix} \\ &= \frac{\mu}{\mu^2+1}\begin{pmatrix} (\lambda\mu+1)F_i & \frac{(\lambda\mu+1)}{\mu}F_i \\ \mu F_i & F_i \end{pmatrix}. \end{aligned}$$

Recall that $\mu^2 - \lambda\mu - 1 = 0$ and so $\lambda\mu + 1 = \mu^2$. We obtain that

$$A\left(X(K_2)\right)E = \mu E$$

and the lemma follows. □

n	number of graphs on n where $\widehat{M}_A(X)$ has constant diagonal	number of graphs on n where $\widehat{M}_L(X)$ has constant diagonal	number of walk-regular graphs on n vertices
2	2	2	2
3	2	2	2
4	7	5	4
5	3	3	3
6	15	12	8
7	4	4	4
8	48	59	14
9	12	9	9

Table 1: Graphs whose average mixing matrix has a constant diagonal with respect to the adjacency matrix and Laplacian adjacency matrix.

Theorem 7.4. *[4] Let X be a graph and let $F_1, \ldots, F_d$ be the orthogonal projections onto the eigenspaces of $A(X)$ with corresponding eigenvalues $\lambda_1, \ldots, \lambda_d$. Then*

$$\widehat{M}(X(K_2)) = \begin{pmatrix} \widehat{M}(X) - N & N \\ N & \widehat{M}(X) - N \end{pmatrix}$$

where

$$N = \sum_{i=1}^{d} \left(\frac{2}{\lambda_i^2 + 4} \right) (F_i \circ F_i).$$

Corollary 7.5. *If X is a walk-regular graph and Y is the rooted graph of X with K_2, then $\widehat{M}(X)$ has constant diagonal.*

Proof. Note that for a walk-regular graph X, matrices $\widehat{M}(X)$ and N both have constant diagonal, and thus the corollary follows. □

Two sources of graphs whose average mixing matrices have constant diagonals are walk-regular graphs and their rooted products with K_2. A computation on graphs up to 9 vertices reveals that there are other graphs with the property. Figure 2 shows three graphs X_1, X_2, X_3 on 6 vertices such that $\widehat{M}(X_i)$ has constant diagonal, but X_i is not a walk-regular graph nor a walk-regular graph rooted with K_2. Table 1 shows the numbers of graphs whose average mixing matrix has constant diagonal with respect to the adjacency matrix and the Laplacian matrix.

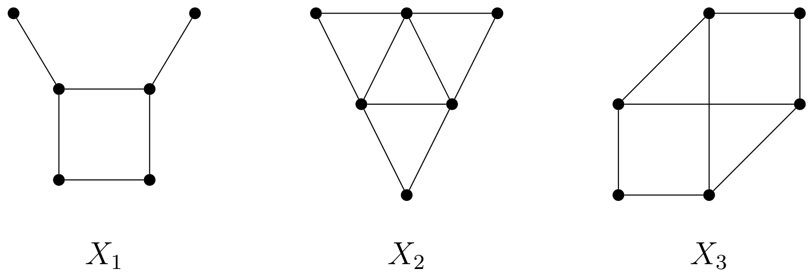


Figure 2: Graphs X_1, X_2, X_3 on 6 vertices such that $\widehat{M}(X_i)$ has constant diagonal.

8 Trace computations

We have determined the graphs attaining the maximum and minimum trace with respect to the average mixing matrices. In particular, Tables 2, 3, and 4 show the minimum with respect to $\widehat{M}_L$ and the minimum and maximum with respect to $\widehat{M}_A$.

n	3	4	5	6	7	8
$\max_X \operatorname{tr}(\widehat{M}_A(X))$	$1^2/_3$	$2^1/_2$	$3^2/_5$	$4^1/_3$	$5^2/_7$	$6^1/_4$
Graphs	K_3	K_4	K_5	K_6	K_7	K_8

Table 2: Graphs on n vertices attaining the maximum trace with respect to $\widehat{M}_A$ for $n = 3, 4, 5, 6, 7, 8$.

9 Open problems

In Section 7, we looked at graphs whose average mixing matrix has constant diagonal and gave two constructions for such graphs: walk-regular graphs and their rooted products with K_2. It seems surprising that this property can occur for graphs which are not regular, but the computational results suggest that there would be other constructions for such graphs. Such constructions would be interesting.

Based on the computations summarized in Table 2 and on Corollary 6.3, we also make the following conjecture.

Conjecture 9.1. *The complete graph on n vertices attains the maximum trace with respect to the $\widehat{M}_A$ for all n.*

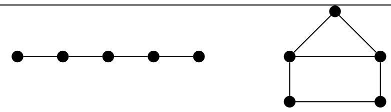
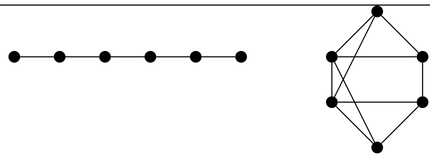
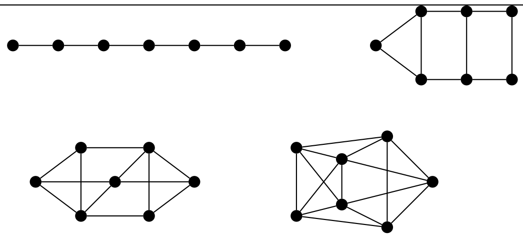
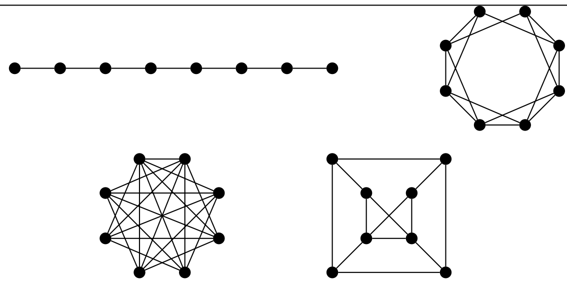
n	$\min_X \operatorname{tr}(\widehat{M}_L(X))$	Graphs
3	$1^1/_3$	
4	$1^1/_4$	
5	$1^2/_5$	
6	$1^1/_3$	
7	$1^3/_7$	
8	$1^3/_8$	

Table 3: Graphs on n vertices attaining the minimum trace with respect to $\widehat{M}_L$ for $n = 3, 4, 5, 6, 7, 8$.

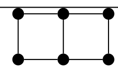
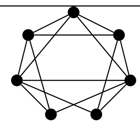
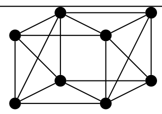
n	$\min_X \operatorname{tr}(\widehat{M}_A(X))$	Graphs
3	$1^1/_4$	
4	$1^1/_5$	
5	$1^1/_3$	
6	$1^1/_4$	
7	1.349025083599055	
8	$1^{29}/_{185}$	

Table 4: Graphs on n vertices attaining the minimum trace with respect to $\widehat{M}_A$ for $n = 3, 4, 5, 6, 7, 8$.

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