Zero forcing, linear and quantum controllability for systems evolving on networks

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Abstract

We study the dynamics of systems on networks from a linear algebraic perspective. The control theoretic concept of *controllability* describes the set of states that can be reached for these systems. Under appropriate conditions, there is a connection between the quantum (Lie theoretic) property of controllability and the linear systems (Kalman) controllability condition. We investigate how the graph theoretic concept of a zero forcing set impacts the controllability property. In particular, we prove that if a set of vertices is a zero forcing set, the associated dynamical system is controllable. The results open up the possibility of further exploiting the analogy between networks, linear control systems theory, and quantum systems Lie algebraic theory. This study is motivated by several quantum systems currently under study, including continuous quantum walks modeling transport phenomena. Additionally, it proposes zero forcing as a new notion in the analysis of complex networks.

1 Introduction

This paper deals with several concepts from different fields such as linear algebra, graph theory and quantum and classical (linear) control theory. In the context of dynamics and control of systems on networks, it establishes a connection between a notion of graph theory (zero forcing) and concepts in control theory (quantum and classical controllability). We review these different concepts before we introduce the technical content of the paper and give physical motivation for our study.

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1.1 Background

For a dynamical system with a *control input*, the property of *controllability* describes to what extent one can go from one state to another with the evolution corresponding to an appropriate choice of the control. If all the possible state transfers can be obtained within a natural set (the phase space), then the system is said to be *controllable.*

For several classes of systems, controllability has been described in detail and controllability tests are known. In particular, for *linear systems*

$$\dot{\mathbf{x}} = A\mathbf{x} + \sum_{j=1}^{s} \mathbf{b}_j u_j, \tag{1}$$

$A \in \mathbb{R}^{n\times n}$, $\mathbf{b}_j \in \mathbb{R}^n$, $j = 1, 2, \ldots, s$, where both the state $\mathbf{x} \in \mathbb{R}^n$ and the control functions $u_j = u_j(t)$ enter the right hand side linearly, several equivalent conditions of controllability are known. The classical Kalman controllability condition (see, e.g., [15]) says the system (1) is controllable if and only if the $n \times (ns)$ matrix

$$\widetilde{W}(A, B) := [\mathbf{b}_1, A\mathbf{b}_1, \ldots, A^{n-1}\mathbf{b}_1, \ldots, \mathbf{b}_s, A\mathbf{b}_s, \ldots, A^{n-1}\mathbf{b}_s],$$

has full rank n, where $B := [\mathbf{b}_1 \quad \mathbf{b}_2 \quad \cdots \mathbf{b}_s]$. In this case, for any prescribed state transfer $\mathbf{x}_0 \to \mathbf{x}_1 (\in \mathbb{R}^n)$ and interval $[0, T]$, there exists a control $\mathbf{u}(t) = [u_1, \ldots, u_s]^T$ such that the corresponding solution $\mathbf{x}(t)$ of (1) satisfies $\mathbf{x}(0) = \mathbf{x}_0$ and $\mathbf{x}(T) = \mathbf{x}_1$. For quantum mechanical systems which are closed (i.e., not interacting with the environment) and finite dimensional, one considers the *Schrödinger equation*

$$i\frac{d}{dt}|\psi\rangle = H(\mathbf{u})|\psi\rangle, \tag{2}$$

where $|\psi\rangle \in \mathbb{C}^n$ is the quantum state and the Hamiltonian matrix $H = H(\mathbf{u})$ is Hermitian and depends on a control $\mathbf{u} = \mathbf{u}(t)$ which in some cases can be assumed to be a switch between different Hamiltonians. If (2) is a system linear in the state $|\psi\rangle$, the solution of (2) is $|\psi(t)\rangle = X(t)|\psi(0)\rangle$ where $X = X(t)$ is the solution of the *Schrödinger matrix equation*

$$i\dot{X} = H(\mathbf{u})X \tag{3}$$

with initial condition equal to the $n \times n$ identity matrix I_n. Since $H = H(\mathbf{u})$ is Hermitian for every value of $\mathbf{u}$ and therefore $-iH$ is skew-Hermitian, the solution of (3) is forced to be unitary at every time t. In this context, the system is called completely controllable if for any unitary matrix X_f in $SU(n)$[1] there exists a control function $\mathbf{u} = \mathbf{u}(t)$ and an interval $[0, T]$ such that the corresponding solution $X = X(t)$ of (3) satisfies $X(0) = I_n$ and $X(T) = X_f$.

At the beginning of the development of the theory of quantum control, it was realized (see e.g., [11]) that system (3) has a structure familiar in geometric control theory [13] and therefore controllability conditions developed there can be directly applied. In particular, the Lie algebra rank condition [14] says that a necessary and sufficient condition for complete controllability of system (3) is that the Lie algebra generated by the matrices $\{iH(\mathbf{u})\}$ (as $\mathbf{u}$ varies in the set of admissible values for the control) is $su(n)$ or $u(n)$.[2] This has given rise to a comprehensive approach to

[1] Following standard notation, $SU(n)$ is the special unitary group, i.e., the matrix group of $n\times n$ unitary matrices having determinant 1.

[2] Following standard notation, $u(n)$ is the Lie algebra of $n \times n$ skew-Hermitian matrices and $su(n)$ is the Lie algebra of $n \times n$ skew-Hermitian matrices with zero trace.

quantum control based on the application of techniques of Lie algebras and Lie group theory [7].

In recent years there has been considerable interest in the study of control systems, both classical and quantum, which are naturally modeled on networks. Often one tries to relate the controllability of these systems to topological or graph theoretic properties of the network. For quantum systems, the nodes of the network may represent energy levels or particles which are interacting with each other. For these systems, the application of the Lie algebra rank condition to determine controllability can become cumbersome and subject to errors when the dimension of the system becomes large. It is preferable to have criteria based on graph theoretic properties of the network not only because they are typically checked more efficiently but also because they give more insight in the dynamics of the system. Work in this direction has been done in [2], [5], [18]. In this context, a relevant property of a graph G and a subset S of its vertices is the capability of this set to 'infect' all the vertices of the graph, as explained in the next paragraph.

Every graph discussed is simple (no loops or multiple edges), undirected, and has a finite nonempty vertex set. Consider a graph G and color each of its vertices black or white. A vertex v is said to *infect*, or *force* a vertex w if v is black, w is white, w is a neighbor of v, and w is the only white neighbor of v. In the case where infection of w has occurred, we change the color of w to black and continue the iterative procedure. The set S is called a *zero forcing set* if this procedure, starting from a graph where only the vertices in S are black, leads to a graph where *all* vertices are black. An example of a zero forcing (infection) process is shown in Figure 1, indicated by arrows; the set of black vertices is a zero forcing set.

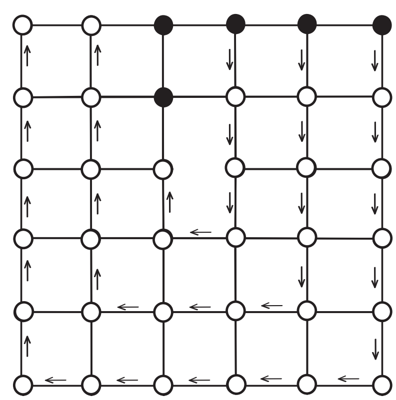

Figure 1: A zero forcing set and the process by which it can infect all vertices.

For a real symmetric $n \times n$ matrix $A = [a_{kj}]$, the *graph* of A, denoted $\mathcal{G}(A)$, is the graph with vertices $\{1, \ldots, n\}$ and edges $\{kj : a_{kj} \neq 0 \text{ and } k \neq j\}$. Observe that $G = \mathcal{G}(A_G) = \mathcal{G}(L_G)$, where A_G and $L_G = D_G - A_G$ denote the adjacency matrix of G and the Laplacian matrix of G, respectively (here D_G is the diagonal matrix of degrees). Zero forcing has been studied in detail in the context of linear algebra. This is because the size of the minimum zero forcing set of a given graph G, which is called the *zero forcing number* $\mathrm{Z}(G)$, is an upper bound to the maximum nullity (or maximum co-rank) over any field of G [3]; the maximum nullity is taken over all symmetric matrices A such that $\mathcal{G}(A) = G$ (see [8] for background on the problem of determining maximum nullity).

Zero forcing appears then to be a valuable concept in the study of graph-theoretic properties that are captured by generalized adjacency matrices. Indeed, there are important classical parameters introduced with this purpose, e.g., the Colin de Verdiére number, the Haemers bound, etc. It has to be remarked that questions about the maximum nullity of a graph are generally difficult problems and the zero forcing number does not constitute an exception: it was shown in [1] that there is no poly-logarithmic approximation algorithm for the zero forcing number.

1.2 Contribution of the paper and physical motivation

In this paper, we consider the dynamics of a system defined on a network and relate the above notions and criteria of controllability with the graph theoretic concept of zero forcing. Abstractly, we consider a graph G and a subset $S = \{j_1, \ldots, j_s\}$ of its vertices $V(G) = \{1, \ldots, n\}$. The dynamics are that of a quantum system (3) where the Hamiltonian is allowed to take the values $\{A, \mathbf{e}_{j_1}\mathbf{e}_{j_1}^T, \ldots, \mathbf{e}_{j_s}\mathbf{e}_{j_s}^T\}$. Here A is the adjacency matrix A_G of G, Laplacian matrix L_G of G, or more generally a real symmetric matrix such that $\mathcal{G}(A) = G$ with all nonzero off-diagonal entries of A having the same sign (which is the typical situation in transport models). The vectors $\{\mathbf{e}_{j_1}, \ldots, \mathbf{e}_{j_s}\}$ are the characteristic vectors[3] of the vertices in S. In this way, we can associate a linear system (1) with A and $\mathbf{b}_1 = \mathbf{e}_{j_1}, \ldots, \mathbf{b}_s = \mathbf{e}_{j_s}$. The main result of the present paper says that controllability in the quantum sense, expressed by the Lie algebra rank condition, and controllability in the sense of linear systems, expressed by the Kalman rank condition, are equivalent conditions. Moreover, if the set S (corresponding to $\mathbf{e}_{j_1}, \ldots, \mathbf{e}_{j_s}$) is a zero forcing set, then these equivalent controllability conditions are true (the converse is false). The first of these results is along the same lines as the main result of [10] which considers the case of quantum dynamics switching between the Hamiltonian A and $\mathbf{z}\mathbf{z}^T$, where $\mathbf{z} = \sum_{j \in S} \mathbf{e}_j$, and establishes the connection between controllability (quantum and linear). As mentioned above, these characterizations avoid lengthy calculations of the Lie algebra generated by a given set of Hamiltonians and replace them with more easily verified graph theoretic and linear algebra tests.

On physical grounds, our motivation for considering a Hamiltonian specified by a matrix with the given graph comes from the study of *continuous time quantum walks* which model transport phenomena in many physical and biological systems [6]. A recent review is given in [4]. Most of the studies consider this sole Hamiltonian and concern the statistical (diffusion) properties of the dynamics. We add here the Hamiltonians $\mathbf{e}_j\mathbf{e}_j^T$ where $\mathbf{e}_j$ is the characteristic vector of a given node of the network and study the nature of the states that the resulting dynamics can achieve, in particular whether an arbitrary (unitary) state transfer can be achieved between the states of the quantum system. The Hamiltonians $\mathbf{e}_j\mathbf{e}_j^T$ model a prescribed energy difference between the corresponding node and all the other nodes of the network which are assumed to be at the same energy level. Therefore the dynamics is the alternating of a diffusion process (modeled by the Hamiltonian A) and a rearrangement of the energies of the various states by selecting one of the states as high energy state and all the other at the same (lower) energy.

Theoretical research in network theory has focused on a number of discrete time, deterministic diffusion processes on graphs. While zero forcing has not been studied

[3]The vector $\mathbf{e}_j$ has the jth entry equal to one and every other entry equal to zero and is also called the jth *standard basis vector*.

in this context, there are two directions of research that are closely related: as it was already noted in [1], the threshold model introduced for studying influence in social networks shares with zero forcing certain issues underlying its computational complexity [16]; the model of complex networks controllability recently proposed in [17] also makes a natural use of the Kalman rank condition and it singles out certain combinatorial properties to determine when the condition is satisfied. Determining whether zero forcing has a place in the metrology of complex networks is a point worth further interest.

The paper is organized as follows. In Section 2 we introduce notation and give background and basic results concerning Lie algebras that will be used in the following sections. The connection between quantum (Lie algebraic) controllability and the Kalman criterion for linear systems is established in Section 3. There we also prove the converse of the main result of [10]. The relation with the zero forcing property is established in Section 4, and Section 5 contains concluding remarks.

2 Lie algebra terminology and preliminary results

Standard material on Lie algebras can be found in [12]. For $A_1, \dots, A_k \in \mathbb{C}^{n\times n}$, $\langle A_1, \dots, A_k\rangle_{[\cdot,\cdot]}$ denotes the real Lie algebra generated by $A_1, \dots, A_k$ under addition, real scalar multiplication, and the commutator operation. Let $\mathcal{H}_n(\mathbb{R})$ denote the real vector space of symmetric matrices. For $A \in \mathcal{H}_n(\mathbb{R})$, the notation $A = [a_{kj}]$ means for $k < j$ the (k, j) and (j, k) entries of A are both a_{kj}. Observe that $A = [a_{kj}] \in \mathcal{H}_n(\mathbb{R})$ can be expressed as

$$A = \sum_{k=1}^{n} a_{kk}\mathbf{e}_k\mathbf{e}_k{}^T + \sum_{k<j} a_{kj}(\mathbf{e}_k\mathbf{e}_j{}^T + \mathbf{e}_j\mathbf{e}_k{}^T).$$

The following proposition is well known (a proof appears in [10]). It provides a link between an appropriate Lie algebra of real matrices and the Lie algebra rank condition of quantum control theory, thereby allowing us to work with real matrices only. Recall that the Lie algebra consisting of all real $n\times n$ matrices is denoted by $gl(n, \mathbb{R})$, $sl(n, \mathbb{R})$ denotes the Lie algebra of real $n \times n$ matrices with zero trace, $u(n)$ denotes the Lie algebra of all skew-Hermitian (complex) $n \times n$ matrices, and $su(n)$ denotes the Lie algebra of all skew-Hermitian (complex) $n \times n$ matrices with zero trace. All these Lie algebras are considered as vector spaces over the field of real numbers.

Proposition 2.1. *For $A_1, \dots, A_k \in \mathcal{H}_n(\mathbb{R})$,*

$$\langle A_1, \dots, A_k\rangle_{[\cdot,\cdot]} = gl(n, \mathbb{R}) \iff \langle iA_1, \dots, iA_k\rangle_{[\cdot,\cdot]} = u(n).$$

The next lemma is used in the proof of Theorem 3.7 in the next section.

Lemma 2.2. *Let $A, B_1, \dots, B_s \in \mathcal{H}_n(\mathbb{R})$, with $s \geq 1$. Define $\mathcal{L} := \langle A, B_1, \dots, B_s\rangle_{[\cdot,\cdot]}$ and let $\hat{\mathcal{L}}$ denote the smallest ideal of $\mathcal{L}$ that contains $B_i, i = 1, \dots, s$. If $\mathcal{L} = gl(n, \mathbb{R})$ and $\operatorname{tr} B_k \neq 0$ for some B_k, then $\hat{\mathcal{L}} = gl(n, \mathbb{R})$.*

Proof. For $n = 1$ the result is clear, so assume $n \geq 2$, $\mathcal{L} = gl(n, \mathbb{R})$, and $\operatorname{tr} B_k \neq 0$ for some B_k. Observe that $\mathcal{L} := \langle A, B_1, \dots, B_s\rangle_{[\cdot,\cdot]}$ is spanned by A and $\hat{\mathcal{L}}$. Since $\mathcal{L} = gl(n, \mathbb{R})$, we have

$$[gl(n, \mathbb{R}), gl(n, \mathbb{R})] = [\operatorname{span}(A) + \hat{\mathcal{L}}, \operatorname{span}(A) + \hat{\mathcal{L}}] \subseteq \hat{\mathcal{L}}.$$

It is known that $[gl(n,\mathbb{R}), gl(n,\mathbb{R})] = sl(n,\mathbb{R})$, because $[gl(n,\mathbb{R}), gl(n,\mathbb{R})]$ is a nonzero ideal in $sl(n,\mathbb{R})$ and $sl(n,\mathbb{R})$ is a simple Lie algebra. Since $\dim sl(n,\mathbb{R}) = n^2 - 1$ and $B_k \notin sl(n,\mathbb{R})$, $\dim \hat{\mathcal{L}} \geq n^2$. Thus $\hat{\mathcal{L}} = gl(n,\mathbb{R})$. $\square$

The next lemma is used in the proof of Theorem 3.1 in the next section. Let $\mathcal{L}$ be a Lie algebra, $A \in \mathcal{L}$, and let $\mathcal{K}$ be a subspace of $\mathcal{L}$. Recall that the operation ad_A is defined as $ad_A(B) := [A, B]$, and the *normalizer* of $\mathcal{K}$ is

$$N_{\mathcal{L}}(\mathcal{K}) = \{A \,:\, [A, B] \in \mathcal{K} \text{ for all } B \in \mathcal{K}\}.$$

It follows from the Jacobi identity that $N_{\mathcal{L}}(\mathcal{K})$ is a subalgebra of $\mathcal{K}$ [12, p. 7].

Lemma 2.3. *Let $A, L \in \mathcal{H}_n(\mathbb{R})$. Assume $\langle iA, iL\rangle_{[\cdot,\cdot]} = u(n)$ and define*

$$\mathcal{S} := \operatorname{span}(\{ad_{iA}^{k_1}\, ad_{iL}^{k_2}\, \cdots\, ad_{iA}^{k_{s-1}}\, ad_{iL}^{k_s}\, [iA, iL]\}), \tag{4}$$

where s and $k_1, \ldots, k_s$ are nonnegative integers. Then $\mathcal{S} = su(n)$.

Proof. First note that $[iA, iL] \neq 0$ because we have assumed that iA and iL generate $u(n)$. Clearly $iA, iL \in N_{u(n)}(\mathcal{S})$. Since $N_{u(n)}(\mathcal{S})$ is a subalgebra of $u(n)$ and iA and iL generate $u(n)$, $N_{u(n)}(\mathcal{S}) = u(n)$. Thus $\mathcal{S}$ is an ideal of $u(n)$. Notice that $\mathcal{S} \subseteq su(n)$ since $[iA, iL]$ is skew-Hermitian with zero trace and iA and iL are skew-Hermitian. Since $\mathcal{S}$ is an ideal of $u(n)$, $\mathcal{S}$ is an ideal of $su(n)$, and $\mathcal{S} \neq \{0\}$. Since $su(n)$ is a simple Lie algebra, by definition it has only the trivial ideals $\{0\}$ and $su(n)$. Therefore $\mathcal{S} = su(n)$. $\square$

For $A \in \mathcal{H}_n(\mathbb{R})$ and $Z = \{\mathbf{z}_1, \ldots, \mathbf{z}_s\} \subset \mathbb{R}^n$, the *real Lie algebra generated by A and Z* is defined as

$$\mathcal{L}(A, Z) := \langle A, \mathbf{z}_1\mathbf{z}_1{}^T, \ldots, \mathbf{z}_s\mathbf{z}_s{}^T\rangle_{[\cdot,\cdot]}. \tag{5}$$

3 Controllability and walk matrices

For $A \in \mathcal{H}_n(\mathbb{R})$ and $Z = \{\mathbf{z}_1, \ldots, \mathbf{z}_s\} \subset \mathbb{R}^n$, the *extended walk matrix* of A and Z is the $n \times (ns)$ real matrix

$$\widetilde{W}(A, Z) := [\mathbf{z}_1, A\mathbf{z}_1, \ldots, A^{n-1}\mathbf{z}_1, \ldots, \mathbf{z}_s, A\mathbf{z}_s, \ldots, A^{n-1}\mathbf{z}_s]. \tag{6}$$

A special case is when $Z = Z_S := \{\mathbf{e}_j : j \in S\}$ (with $\mathbf{e}_j$ denoting the j-th standard basis vector) for some subset $S \subseteq V(G)$ for a graph G and A is the adjacency matrix A_G of the graph. In this case, the relevant walk matrix is $\widetilde{W}(A_G, Z_S)$.

For $s = 1$ the connection between the walk matrix $\widetilde{W}(A, Z)$ in (6) and the Lie algebra $\mathcal{L}(A, Z)$ in (5) was studied in [10]. It was shown [10, Lemma 1] that $\operatorname{rank} \widetilde{W}(A, \{\mathbf{z}\}) = n$ implies $\mathcal{L}(A, \{\mathbf{z}\}) = gl(n,\mathbb{R})$, or equivalently, $\langle iA, i\mathbf{z}\mathbf{z}^T\rangle_{[\cdot,\cdot]} = u(n)$ (cf. Proposition 2.1). The next theorem states that the converse of this result is also true.

Theorem 3.1. *Consider a matrix A in $\mathcal{H}_n(\mathbb{R})$ and a vector $\mathbf{z} \in \mathbb{R}^{n\times n}$. Then, $\langle iA, i\mathbf{z}\mathbf{z}^T\rangle_{[\cdot,\cdot]} = u(n)$ (or equivalently $\mathcal{L}(A, \{\mathbf{z}\}) = gl(n,\mathbb{R})$) implies that $\operatorname{rank} \widetilde{W}(A, \{\mathbf{z}\}) = n$.*

Proof. The equivalence of the hypotheses is justified by Proposition 2.1. The result is clear if $n = 1$, so assume $n \geq 2$. We use a contradiction argument. Assume the rank of the walk matrix $\widetilde{W}(A, \{\mathbf{z}\})$ is less than n but $\langle iA, iL\rangle_{[\cdot,\cdot]} = u(n)$, where $L := \mathbf{z}\mathbf{z}^T$. There exists a vector $\mathbf{x} \in \mathbb{C}^n$ such that $\mathbf{x}^*\widetilde{W}(A, \{\mathbf{z}\}) = 0$. Consider the rank 1 matrix $D := \mathbf{x}\mathbf{x}^*$. We claim that D commutes with every matrix in $\mathcal{S}$, where $\mathcal{S}$ is as in (4). To see this, notice that from (4), all elements in $\mathcal{S}$ are linear combinations of monomials of the form $M = A^{k_1}L^{k_2}A^{k_3}\cdots L^{k_{p-1}}A^{k_p}$, for some $p \geq 1$, $k_j \geq 0$, and L appearing at least once with exponent greater than zero. When multiplying D with M, with D on the left, write M as $A^{k_1}LY$ for some matrix Y, so we have

$$DM = DA^{k_1}LY = \mathbf{x}\mathbf{x}^*A^{k_1}\mathbf{z}\mathbf{z}^*Y = 0, \tag{7}$$

which follows immediately from the condition $\mathbf{x}^*\widetilde{W}(A, \{\mathbf{z}\}) = 0$ for $n - 1 \geq k_1 \geq 0$, and by using the Cayley-Hamilton theorem for $k_1 \geq n$. Analogously, when multiplying D on the right of M, we write M as QLA^{k_p}, for some matrix Q, and we have

$$MD = QLA^{k_p}D = Q\mathbf{z}\mathbf{z}^*A^{k_p}\mathbf{x}\mathbf{x}^* = 0, \tag{8}$$

since $\mathbf{x}^*A^{k_p}\mathbf{z} = 0$ also implies $\mathbf{z}^*A^{k_p}\mathbf{x} = 0$. Therefore D commutes with all elements of $\mathcal{S}$.

Observe that since $su(n)$ is simple, $su(n)$ is an irreducible representation of $su(n)$. Therefore, since D commutes with all elements of $\mathcal{S}$, it follows from Schur's Lemma that D must be a scalar multiple of the identity [12, p. 26]. However this is not possible since D has rank 1. This gives the desired contradiction and thus completes the proof. $\square$

We study the generalization of this result to multiple vectors ($s \geq 1$) but for matrices A and vectors $\mathbf{z}_1, \ldots, \mathbf{z}_s$ related to a connected graph G. In particular, $\mathcal{G}(A) = G$, all nonzero off-diagonal entries of A have the same sign, and $\mathbf{e}_{j_1}, \ldots, \mathbf{e}_{j_s}$ will be the characteristic vectors associated to a subset S of the vertices. In the next section we will relate this to the zero forcing property of the set S. In the context of graphs, it is important to consider multiple vectors because if G is a graph and $\operatorname{rank} A_G \leq |G| - 2$, then $\operatorname{rank} \widetilde{W}(A_G, \{\mathbf{z}\}) < n$ for any one vector $\mathbf{z}$. On the other hand we will see that if S is a zero forcing set for G and $\mathcal{G}(A) = G$, then $\mathcal{L}(A, \{\mathbf{e}_j : j \in S\}) = \mathcal{H}_n(\mathbb{R})$ (see Theorem 4.1 below).

The next definition extends the definition given in [9] (and implicitly in [10]) of an associative algebra that links the walk matrix and controllability.

Definition 3.2. For $A \in \mathcal{H}_n(\mathbb{R})$ and $Z = \{\mathbf{z}_1, \ldots, \mathbf{z}_s\} \subset \mathbb{R}^n$, define

$$P(A, Z) := \{A^m\mathbf{z}_k{\mathbf{z}_j}^TA^\ell : 1 \leq k, j \leq s, 0 \leq m, \ell \leq n - 1\}.$$

Remark 3.3. For $A \in \mathcal{H}_n(\mathbb{R})$ and $Z = \{\mathbf{z}_1, \ldots, \mathbf{z}_s\} \subset \mathbb{R}^n$, the associative algebra generated by $P(A, Z)$ is equal to $\operatorname{span} P(A, Z)$, because

$$(A^m\mathbf{z}_k{\mathbf{z}_j}^TA^\ell)(A^g\mathbf{z}_p{\mathbf{z}_q}^TA^h) = ({\mathbf{z}_j}^TA^{\ell+g}\mathbf{z}_p)A^m\mathbf{z}_k{\mathbf{z}_q}^TA^h \text{ and } {\mathbf{z}_j}^TA^{\ell+g}\mathbf{z}_p \in \mathbb{R}.$$

Lemma 3.4. *For $A \in \mathcal{H}_n(\mathbb{R})$ and $Z = \{\mathbf{z}_1, \ldots, \mathbf{z}_s\} \subset \mathbb{R}^n$,* $\operatorname{rank} \widetilde{W}(A, Z) = n$ *if and only if* $\operatorname{span} P(A, Z) = \mathbb{R}^{n\times n}$*.* [4]

[4]As a vector space, $\mathbb{R}^{n\times n}$ is the same as $gl(n, \mathbb{R})$. We use the latter notation when we want to stress the Lie algebra structure on $gl(n, \mathbb{R})$.

Proof. Clearly $\operatorname{rank} \widetilde{W}(A,Z) = n$ if and only if $\operatorname{range} \widetilde{W}(A,Z) = \mathbb{R}^n$. First assume $\operatorname{rank} \widetilde{W}(A,Z) = n$. For any matrix $M \in \mathbb{R}^{n\times n}$ with $\operatorname{rank} M = r$, there exist vectors $\mathbf{x}^{(q)}, \mathbf{y}^{(q)}$, $q = 1, \dots r$, such that $M = \sum_{q=1}^{r} \mathbf{x}^{(q)} {\mathbf{y}^{(q)}}^T$. Since $\operatorname{range} \widetilde{W}(A,Z) = \mathbb{R}^n$, each $\mathbf{x}^{(q)}$ is expressible as a linear combination of the columns of $\widetilde{W}(A,Z)$, i.e., as a linear combination of vectors of the form $A^m \mathbf{z}_k$, and similarly for $\mathbf{y}^{(q)}$. Thus each $\mathbf{x}^{(q)} {\mathbf{y}^{(q)}}^T$, and hence M, is expressible as a linear combination of $A^m \mathbf{z}_k {\mathbf{z}_j}^T A^\ell$. Thus the matrices of the form $A^m \mathbf{z}_k {\mathbf{z}_j}^T A^\ell$ span $\mathbb{R}^{n\times n}$.

For the converse, observe that if $B = \{\mathbf{b}_1, \dots, \mathbf{b}_r\}$ is a basis for $\operatorname{range} \widetilde{W}(A,Z)$, then

$$\operatorname{span} P(A,Z) = \operatorname{span}(\{\mathbf{b}_k {\mathbf{b}_j}^T : 1 \le k, j \le r\}).$$

If $n > r = \operatorname{rank} \widetilde{W}(A,Z)$, then $\dim \operatorname{span} P(A,Z) \le r^2 < n^2 = \dim \mathbb{R}^{n\times n}$, so the matrices in $P(A,Z)$ cannot span $\mathbb{R}^{n\times n}$. □

The *distance* between two distinct vertices u and v of a connected graph G, denoted by $d(u,v)$ is the minimum number of edges in a path from u to v.

Lemma 3.5. *Let $A \in \mathcal{H}_n(\mathbb{R})$ such that $\mathcal{G}(A)$ is connected and all nonzero off-diagonal entries of A have the same sign. If $k, j \in \{1, \dots, n\}$ and $k \ne j$, then $(A^{d(k,j)})_{kj} \ne 0$.*

Proof. Let $d := d(k,j)$. The entry $(A^d)_{kj}$ is a sum of terms which are each the product of d nonzero entries of A. Since d is the distance between k and j, only off-diagonal entries can appear in this product. Thus every term has the same sign and $(A^d)_{kj} \ne 0$. □

Lemma 3.6. *Let $A \in \mathcal{H}_n(\mathbb{R})$ be such that $\mathcal{G}(A)$ is connected and all nonzero off-diagonal entries of A have the same sign. Let $S \subseteq \{1, \dots, n\}$ and $Z = \{\mathbf{e}_j : j \in S\}$ be the subset of standard basis vectors. Then* $\operatorname{span} P(A,Z) \subseteq \mathcal{L}(A,Z)$.

Proof. The proof of Lemma 1 in [10] shows that for any real symmetric matrix A and vector $\mathbf{z}$, $A^m \mathbf{z}\mathbf{z}^T A^\ell \in \mathcal{L}(A, \{\mathbf{z}\})$ for all $m, \ell \in \{0, \dots, n-1\}$. Applying this, we obtain that $A^m \mathbf{e}_j {\mathbf{e}_j}^T A^\ell \in \mathcal{L}(A,Z)$ for all $j \in \{1, \dots, s\}, m, \ell \in \{0, \dots, n-1\}$. The result will follow if we are able to show that $A^m \mathbf{e}_k {\mathbf{e}_j}^T A^\ell \in \mathcal{L}(A,Z)$ for all $k, j \in \{1, \dots, s\}, m, \ell \in \{0, \dots, n-1\}$, with k different from j.

Consider the distance $d(k,j)$ between the nodes k and j in $\mathcal{G}(A)$, which is $\le n-1$ because $\mathcal{G}(A)$ is connected. From the fact that both $\mathbf{e}_k \mathbf{e}_k^T$ and $A^{d(k,j)} \mathbf{e}_j \mathbf{e}_j^T$ are in $\mathcal{L}(A,Z)$, we have in $\mathcal{L}(A,Z)$,

$$[\mathbf{e}_k {\mathbf{e}_k}^T, A^{d(k,j)} \mathbf{e}_j {\mathbf{e}_j}^T] = \mathbf{e}_k {\mathbf{e}_k}^T A^{d(k,j)} \mathbf{e}_j {\mathbf{e}_j}^T - A^{d(k,j)} \mathbf{e}_j {\mathbf{e}_j}^T \mathbf{e}_k {\mathbf{e}_k}^T = ({\mathbf{e}_k}^T A^{d(k,j)} \mathbf{e}_j) \mathbf{e}_k {\mathbf{e}_j}^T.$$

It follows from Lemma 3.5 that ${\mathbf{e}_k}^T A^{d(k,j)} \mathbf{e}_j \ne 0$, and so $\mathbf{e}_k {\mathbf{e}_j}^T \in \mathcal{L}(A,Z)$.

Then

$$\begin{aligned}
[A^m \mathbf{e}_k {\mathbf{e}_k}^T, \mathbf{e}_k {\mathbf{e}_j}^T] &= A^m \mathbf{e}_k {\mathbf{e}_k}^T \mathbf{e}_k {\mathbf{e}_j}^T - \mathbf{e}_k {\mathbf{e}_j}^T A^m \mathbf{e}_k {\mathbf{e}_k}^T \\
&= A^m \mathbf{e}_k {\mathbf{e}_j}^T - ({\mathbf{e}_j}^T A^m \mathbf{e}_k) \mathbf{e}_k {\mathbf{e}_k}^T.
\end{aligned}$$

So, $A^m \mathbf{e}_k {\mathbf{e}_j}^T \in \mathcal{L}(A,Z)$. Similarly, $\mathbf{e}_k {\mathbf{e}_j}^T A^\ell \in \mathcal{L}(A,Z)$. Finally,

$$\begin{aligned}
[A^m \mathbf{e}_k {\mathbf{e}_k}^T, \mathbf{e}_k {\mathbf{e}_j}^T A^\ell] &= A^m \mathbf{e}_k {\mathbf{e}_k}^T \mathbf{e}_k {\mathbf{e}_j}^T A^\ell - \mathbf{e}_k {\mathbf{e}_j}^T A^{m+\ell} \mathbf{e}_k {\mathbf{e}_k}^T \\
&= A^m \mathbf{e}_k {\mathbf{e}_j}^T A^\ell - ({\mathbf{e}_j}^T A^{m+\ell} \mathbf{e}_k) \mathbf{e}_k {\mathbf{e}_k}^T.
\end{aligned}$$

So, $A^m \mathbf{e}_k {\mathbf{e}_j}^T A^\ell \in \mathcal{L}(A,Z)$. □

The following theorem establishes the connection between quantum Lie algebraic controllability and the rank condition for an extended walk matrix modeled on a graph.

Theorem 3.7. *Let $A \in \mathcal{H}_n(\mathbb{R})$ such that $\mathcal{G}(A)$ is connected and all the nonzero off-diagonal elements of A have the same sign. Let $S \subseteq \{1, \ldots, n\}$ and $Z = \{\mathbf{e}_j : j \in S\}$ be a subset of standard basis vectors. Then* $\operatorname{rank} \widetilde{W}(A, Z) = n$ *if and only if* $\mathcal{L}(A, Z) = gl(n, \mathbb{R})$.

Proof. By Lemma 3.4, $\operatorname{span} P(A, Z) = \mathbb{R}^{n\times n}$ if and only if $\operatorname{rank} \widetilde{W}(A, Z) = n$, so it suffices to show that $\operatorname{span} P(A, Z) = \mathbb{R}^{n\times n}$ if and only if $\mathcal{L}(A, Z) = gl(n, \mathbb{R})$. By Lemma 3.6, $\operatorname{span} P(A, Z) \subseteq \mathcal{L}(A, Z)$, so $\operatorname{span} P(A, Z) = \mathbb{R}^{n\times n}$ implies $\mathcal{L}(A, Z) = gl(n, \mathbb{R})$. For the converse, assume $\mathcal{L}(A, Z) = gl(n, \mathbb{R})$. Then, by Lemma 2.2, $\hat{\mathcal{L}} = gl(n, \mathbb{R})$, where $\hat{\mathcal{L}}$ is the smallest ideal of $\mathcal{L}(A, Z)$ that contains $\mathbf{e}_j\mathbf{e}_j{}^T, j = 1, \ldots, s$. It is clear that $\hat{\mathcal{L}} \subseteq \operatorname{span} P(A, Z)$, so $\operatorname{span} P(A, Z) = \mathbb{R}^{n\times n}$. □

Corollary 3.8. *Let $A \in \mathcal{H}_n(\mathbb{R})$ such that $\mathcal{G}(A)$ is connected and all the nonzero off-diagonal elements of A have the same sign, and let $S \subseteq \{1, \ldots, n\}$. Then* $\operatorname{rank} \widetilde{W}(A, \{\mathbf{e}_j : j \in S\}) = n$ *if and only if $\langle iA, \{i\mathbf{e}_j\mathbf{e}_j{}^T : j \in S\}\rangle_{[\cdot,\cdot]} = u(n)$, i.e., the quantum system associated with the Hamiltonians iA and $i\mathbf{e}_j\mathbf{e}_j^T$, $j = 1, \ldots, s$, is controllable.*

Observe that for any connected graph G, the adjacency matrix A_G and the Laplacian matrix L_G satisfy the hypotheses of Theorem 3.7 and Corollary 3.8.

The result of [10] for the case $s = 1$ showing that $\operatorname{rank} \widetilde{W}(A, \{\mathbf{z}\}) = n$ implies $\langle iA, i\mathbf{z}\mathbf{z}^T\rangle_{[\cdot,\cdot]} = u(n)$, (and the converse proved in Theorem 3.1 in this paper) were proved in reference to systems on graphs. The proofs however go through for an arbitrary symmetric matrix A and vector $\mathbf{z}$. It is natural to ask whether the conditions on the matrix A that we have used in Theorem 3.7 are really necessary. To this purpose, we can observe that the result is not true if we give up either of the hypotheses that 1) $\mathcal{G}(A)$ is connected or 2) the off-diagonal entries of A have the same sign, as shown in the next two examples.

Example 3.9. To see the necessity of assuming that $\mathcal{G}(A)$ is connected, consider a block diagonal matrix $A = \begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix}$ with A_1 and A_2 symmetric matrices of dimensions n_1 and n_2, respectively, with $n_1 + n_2 = n$, and $\mathbf{z}_1$ and $\mathbf{z}_2$ two vectors that have zeros in the last n_2 or first n_1 entries, respectively, and such that the corresponding matrices $\widetilde{W}(A_1, \{\mathbf{z}_1\})$ and $\widetilde{W}(A_2, \{\mathbf{z}_2\})$ have ranks n_1 and n_2, respectively. In this case, the walk matrix $\widetilde{W}(A, \{\mathbf{z}_1, \mathbf{z}_2\})$ has rank n, but the Lie algebra generated by A, $\mathbf{z}_1\mathbf{z}_1^T$, and $\mathbf{z}_2\mathbf{z}_2^T$ contains only block diagonal matrices.

Example 3.10. To see the necessity of assuming that all nonzero off-diagonal entries of A have the same sign, consider $A = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$, and $Z = \{\mathbf{e}_1, \mathbf{e}_3\}$. It is straightforward to verify that the walk matrix $\widetilde{W}(A, \{\mathbf{e}_1, \mathbf{e}_3\})$ has rank 4. However, $\operatorname{rank} \mathcal{L}(A, \{\mathbf{e}_1, \mathbf{e}_3\}) \leq 8$, as can be seen as follows. Let

$$\mathcal{L} := \operatorname{span}(\begin{bmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{bmatrix}, \begin{bmatrix}0&0&0&0\\0&1&0&0\\0&0&0&0\\0&0&0&1\end{bmatrix}, \begin{bmatrix}0&0&0&0\\0&0&0&0\\0&0&1&0\\0&0&0&0\end{bmatrix}, \begin{bmatrix}0&0&0&0\\1&0&0&0\\0&0&0&0\\1&0&0&0\end{bmatrix},$$
$$\begin{bmatrix}0&1&0&1\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{bmatrix}, \begin{bmatrix}0&0&0&0\\0&0&0&0\\0&1&0&-1\\0&0&0&0\end{bmatrix}, \begin{bmatrix}0&0&0&0\\0&0&1&0\\0&0&0&0\\0&0&-1&0\end{bmatrix}, \begin{bmatrix}0&0&0&0\\0&0&0&1\\0&0&0&0\\0&1&0&0\end{bmatrix}).$$

Since $[B,C] \in \mathcal{L}$ for all $B, C \in \mathcal{L}$, $\mathcal{L}$ is a Lie subalgebra of $gl(4,\mathbb{R})$. Clearly $\dim \mathcal{L} \le 8$ and $\mathcal{L}(A, \{\mathbf{e}_1, \mathbf{e}_3\}) \subseteq \mathcal{L}$.

4 Zero forcing and controllability

The *neighborhood* of $v \in V(G)$ is $N(v) = \{w \in V(G) : w \text{ is adjacent to } v\}$.

Theorem 4.1. *Let $A \in \mathcal{H}_n(\mathbb{R})$ such that $\mathcal{G}(A)$ is connected and all the nonzero off-diagonal entries of A have the same sign. Let $V := \{1, 2, \ldots, n\}$ be the set of vertices for $\mathcal{G}(A)$, and $S \subseteq V$ be a zero forcing set of $\mathcal{G}(A)$. Then*

$$\mathcal{L}(A, \{\mathbf{e}_j {\mathbf{e}_j}^T : j \in S\}) = gl(n, \mathbb{R}).$$

Proof. After a (possibly empty) sequence of forces, denote by T the set of currently black vertices, and assume that for all $k \in T$, $\mathbf{e}_k {\mathbf{e}_k}^T \in \mathcal{L} := \mathcal{L}(A, \{\mathbf{e}_j {\mathbf{e}_j}^T : j \in S\})$. The hypotheses of Lemma 3.6 are satisfied for $Z = \{\mathbf{e}_j : j \in T\}$, so for all $k, \ell \in T$, $\mathbf{e}_k {\mathbf{e}_\ell}^T \in \mathcal{L}$.

If $T \neq V$, then there is a vertex $u \in T$ that has a unique neighbor w outside T. For that u we have

$$[\mathbf{e}_u \mathbf{e}_u^T, A] = \sum_{m \in N(u)} \tilde{a}_{um} (\mathbf{e}_u \mathbf{e}_m^T - \mathbf{e}_m \mathbf{e}_u^T),$$

where $\tilde{a}_{um} := a_{um}$ if $u < m$ and $\tilde{a}_{um} := a_{mu}$ if $m < u$. For all $m \in N(u)$ such that $m \neq w$, $m \in T$, so $\mathbf{e}_u {\mathbf{e}_m}^T, \mathbf{e}_m {\mathbf{e}_u}^T \in \mathcal{L}$. Thus $\mathbf{e}_u \mathbf{e}_w^T - \mathbf{e}_w \mathbf{e}_u^T \in \mathcal{L}$. Since

$$[\mathbf{e}_u {\mathbf{e}_u}^T, \mathbf{e}_u {\mathbf{e}_w}^T - \mathbf{e}_w {\mathbf{e}_u}^T] = \mathbf{e}_u {\mathbf{e}_w}^T + \mathbf{e}_w {\mathbf{e}_u}^T,$$

$\mathbf{e}_w \mathbf{e}_u^T, \mathbf{e}_w \mathbf{e}_u^T \in \mathcal{L}$. Then

$$[\mathbf{e}_w \mathbf{e}_u^T, \mathbf{e}_u \mathbf{e}_w^T] = \mathbf{e}_w \mathbf{e}_w^T - \mathbf{e}_u \mathbf{e}_u^T$$

so $\mathbf{e}_w \mathbf{e}_w^T \in \mathcal{L}$. Since S is a zero forcing set, we obtain $\mathbf{e}_\ell {\mathbf{e}_m}^T \in \mathcal{L}$ for all $\ell, m \in V = \{1, \ldots, n\}$, and thus we conclude that $\mathcal{L} = gl(n, \mathbb{R})$. □

Applying Proposition 2.1 we obtain the next corollary.

Corollary 4.2. *If G is a connected graph, $A \in \mathcal{H}_n(\mathbb{R})$, all the nonzero off-diagonal entries of A have the same sign, and $S \subseteq V$ is a zero forcing set of G, then $\langle iA, \{i\mathbf{e}_j {\mathbf{e}_j}^T : j \in S\}\rangle_{[\cdot,\cdot]} = u(n)$ and the corresponding quantum system is controllable.*

Note that the converse of Theorem 4.1 is false.

Example 4.3. Consider the path on four vertices P_4 with the vertices numbered in order. The set $\{\mathbf{e}_2\}$ is not a zero forcing set for P_4. However,

$$\widetilde{W}(A_{P_4}, \{\mathbf{e}_2\}) = \begin{bmatrix} 0 & 1 & 0 & 2 \\ 1 & 0 & 2 & 0 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 1 & 0 \end{bmatrix} \text{ and } \operatorname{rank} \widetilde{W}(A_{P_4}, \{\mathbf{e}_2\}) = 4,$$

so $\mathcal{L}(A_{P_4}, \{\mathbf{e}_2\}) = gl(n, \mathbb{R})$ by Theorem 3.7.

5 Conclusion

Motivated by the control and dynamics of systems modeled on networks both classical and quantum, we have established a connection between various tests of controllability and the notion of zero forcing in graph theory. Lie algebraic quantum controllability is necessary and sufficient for linear (Kalman-like) controllability of an associated system and both notions are implied by the zero forcing property of the associated set of vertices. Linear systems have a very well developed theory [15] and it is an open question to investigate to what extent this analogy can be further used to discover properties of quantum systems and systems on networks.

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