Pendant vertices in complex networks: Separable graphs and control localization of weighted trees

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Two topics in complex networks

- Separable graphs in quantum mechanics

- Control localization in weighted trees


I think I can safely say that nobody understands quantum mechanics.

(Richard Feynman)
Quantum information processing

- The peculiarities of quantum physics promise to deliver revolutionary applications.
- *Quantum computing*: superposition of states allow many computations to be performed in parallel. Can solve “hard” problems such as integer factorization in polynomial time.
- This could render well known cryptographic algorithms such as RSA obsolete.
- Fortunately, quantum cryptography can provide unbreakable crypto-systems. Relies on the fact that observation modifies the state and thus can detect eavesdropping.
Entanglement in quantum mechanics

- An important ingredient in creating the myriad of unintuitive phenomena in quantum physics is *entanglement of quantum states*.

- Entanglement has emerged as a crucial resource in applications of quantum mechanics such as:
  1. Quantum computation
  2. Quantum teleportation
  3. Quantum cryptography/secure communications
  4. Quantum dense coding
  5. and many others

http://www.acm.org/crossroads/xrds11-3/qcrypto.html

http://physicsworld.com/cws/article/print/1658
Entanglement in quantum mechanics

- On the other hand, entanglement with the *environment* is undesirable in quantum computing as it leads to *decoherence*, causing a collapse of the superimposed state.

http://brneurosci.org/subjectivity.html
What is entanglement?

- Roughly speaking, entanglement is when two subsystems cannot be described independently.
- This is responsible for the phenomenon whereby two subsystems can influence each other even though they are spatially separated.

Entangled photons

http://physicsworld.com/cws/article/indepth/11360/1/smallphotons

Density matrix formulation of quantum mechanics (Von Neumann, 1927)

- The state of a quantum mechanical systems is associated with a *density* matrix: a complex matrix that is Hermitian, positive definite and has unit trace.

- We say a density matrix of order \( n = pq \) is bipartite *separable* if it can be written as:

\[
A = \sum_i c_i B_i \otimes C_i, \quad c_i \geq 0, \quad \sum_i c_i = 1
\]

where \( B_i \) and \( C_i \) are density matrices of order \( p \) and \( q \) resp.

- A density matrix is bipartite *entangled* if it is not bipartite separable.

- Determining whether a density matrix is entangled or not is NP-hard [Gurvits, 2003].

- Of interest are simple criteria for entanglement and separability.
Partial transpose

- Decompose a density matrix $A$ into $p^2$ submatrices of order $q$

$$A = \begin{pmatrix}
A^{1,1} & A^{1,2} & \cdots & A^{1,p} \\
A^{2,1} & A^{2,2} & \cdots & A^{2,p} \\
\vdots & \vdots & \ddots & \vdots \\
A^{p,1} & A^{p,2} & \cdots & A^{p,p}
\end{pmatrix}$$

- The partial transpose $A^{TB}$ is defined as:

$$A^{TB} = \begin{pmatrix}
(A^{1,1})^T & (A^{1,2})^T & \cdots & (A^{1,p})^T \\
(A^{2,1})^T & (A^{2,2})^T & \cdots & (A^{2,p})^T \\
\vdots & \vdots & \ddots & \vdots \\
(A^{p,1})^T & (A^{p,2})^T & \cdots & (A^{p,p})^T
\end{pmatrix}$$
Peres-Horodecki necessary condition for separability

- [Peres, 1996]: If the density matrix is separable, then its partial transpose is positive semidefinite (PPT).

- This condition is also sufficient for separability in the cases of \((p=2,q=2)\) and \((p=2,q=3)\) [Horodecki et al, 1996], but not a sufficient condition in general for larger values of \(p,q\).

- If the density matrix has zero row sums, this is reduced to:
  
  [Wu, 2006]: If a density matrix with zero row sums is separable, then its partial transpose has zero row sums.
Laplacian matrices of graphs

- The Laplacian matrix of a graph is defined as $L = D - A$, where $D$ is the diagonal matrix of vertex degrees and $A$ is the adjacency matrix.

- Properties of Laplacian matrices:
  1. Singular
  2. Positive semidefinite (all eigenvalues are nonnegative).
  3. Symmetric
  4. Trace is positive (for nonempty graphs)

- This means that a Laplacian matrix with its trace normalized to 1 can be considered as a density matrix.

- In 2006, Braunstein et al. first considered Laplacian matrices of graph as density matrices and studied the relationship between the graph and the corresponding quantum mechanical state expressed by the density matrix.
Laplacian matrices of graphs as density matrices

- **Graph** ↔ **Laplacian matrix** ↔ **Density matrix** ↔ **state of quantum system**

- How does graph properties correlate with quantum physical properties of the corresponding system?
- In this talk, we look at graphs whose normalized Laplacian matrix is entangled or separable.
- This depends on the vertex labeling, i.e. we consider labeled graphs.
- We’ll call such a labeled graph *entangled* or *separable*.

[Image of graph with adjacency matrix and quantum state visualizations]
Separability of Laplacian matrices

- How many labeled graphs correspond to separable or entangled density matrices?
- We can ignore the empty graph since it has trace 0.
- Number of nonempty labeled graphs of n vertices is
  \[ L(n) = 2\frac{n(n-1)}{2} - 1 \]

- Definition: a square matrix is \textit{line sum symmetric} if the sum of the \( i \)-th row is equal the sum of the \( i \)-th column for all \( i \).
- Theorem [Wu, 2006]: A normalized Laplacian matrix \( A \) is separable if \( A^{i,j} \) is line sum symmetric for all \( i,j \).
Number of separable and entangled graphs

- Definition: $L_s(p,q)$ and $L_e(p,q)$ are the number of nonempty labeled graphs corresponding to separable and entangled density matrices of $n = pq$ vertices.

\[ L_s(p,q) + L_e(p,q) = L(n) = 2^{n(n-1)/2} - 1 \]

- Definition: Let $N_s(n)$ denote the number of $n$ by $n$ 0-1 matrices that are line sum symmetric and $N_e(n)$ denote the number of $n$ by $n$ 0-1 matrices that are not line sum symmetric.

\[ N_s(n) + N_e(n) = 2^{n^2} \]

The first few values of $N_s(n)$ are: 2, 8, 80, 2432, 247552, 88060928, 112371410944, 523858015518720, 9041009511609073664, 583447777113052431515648 (OEIS sequence A229865).
Number of labeled graphs with at least one pendant vertex

- Definition: Let $M_n(i)$ denote the number of symmetric $n$ by $n$ 0-1 matrices such that
  - There is at least one row with a single 1
  - The diagonal entries are 0
  - There are $2i$ nonzero elements in the matrix.

These matrices are the set of adjacency matrices of labeled graphs of $n$ vertices and $i$ edges with at least one vertex of degree 1 (i.e. has at least one pendant).

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OEIS A245796
Some properties of $M_n(i)$

- **Theorem:** $M_n(i) = 0$ if $i > \frac{(n-1)(n-2)}{2} + 1$. For $j \geq 0, n \geq 4 + j$,

  $$M_n\left(\frac{(n-1)(n-2)}{2} - j + 1\right) = n(n - 1) \binom{n-1}{j}$$

- For $i \leq 3$, $M_n(i)$ is equal to the number of labeled bipartite graphs with $n$ vertices and $i$ edges.

  $$M_n(1) = \frac{n(n-1)}{2}, \quad M_n(2) = \frac{(n+1)n(n-1)(n-2)}{8}, \quad M_n(3) = \frac{((n+1)(n+2)+2)n(n-1)(n-2)(n-3)}{48}$$
Lower bound for $L_s(p, q)$

- $L$ is separable if $q$ by $q$ submatrices $A^{i,j}$ are all line sum symmetric.
- In upper triangular part of $L$, there are $p(p-1)/2$ of them, resulting in $N_s(q) \frac{p(p-1)}{2}$ combinations.
- There are $pq(q-1)/2$ remaining entries (edges) which form $2^{\frac{pq(q-1)}{2}}$ combinations.

$$L_s(p, q) \geq 2^{\frac{pq(q-1)}{2}} N_s(q) \frac{p(p-1)}{2} - 1$$
Lower bound for $L_e(p, q)$

- $L$ is entangled if the partial transpose does not have zero row sums.
- Replace each $A_{i,j}$ with 0 if it is line sum symmetric and 1 otherwise. This results in a $p$ by $p$ 0-1 matrix $B$. If $B$ is the adjacency matrix of a graph with $i$ edges and at least one pendant vertex, then the partial transpose of $L$ does not have zero sums. There are $M_p(i)N_e(q)^iN_s(q)^{\frac{p(p-1)}{2}-i}$ such combinations.

- As before, there are $pq(q-1)/2$ remaining entries which form $2^{\frac{pq(q-1)}{2}}$ combinations.

$$L_e(p, q) \geq \sum_{i=1}^{\frac{(p-1)(p-2)+1}{2}} M_p(i)N_e(q)^iN_s(q)^{\frac{p(p-1)}{2}-i}2^{\frac{pq(q-1)}{2}}$$
Upper and lower bounds for numbers of separable and entangled graphs

- Theorem [Wu, 2014]:

\[
L_s(p, q) \geq 2 \frac{pq(q-1)}{2} N_s(q) \frac{p(p-1)}{2} - 1
\]

\[
L_s(p, q) \leq L(pq) - \sum_{i=1}^{\frac{(p-1)(p-2)+1}{2}} M_p(i)N_e(q)^i N_s(q) \frac{p(p-1)}{2} - i \frac{pq(q-1)}{2}
\]

\[
L_e(p, q) \leq L(pq) - 2 \frac{pq(q-1)}{2} N_s(q) \frac{p(p-1)}{2} - 1
\]

\[
L_e(p, q) \geq \sum_{i=1}^{\frac{(p-1)(p-2)+1}{2}} M_p(i)N_e(q)^i N_s(q) \frac{p(p-1)}{2} - i \frac{pq(q-1)}{2}
\]
Upper and lower bounds for numbers of separable graphs

- When $p = 2$, the upper and lower bounds coincide and we have exact values for $L_s(2, q)$ and $L_e(2, q)$
  \[ L_s(2, q) = 2^q (q-1) N_s(q) - 1 \]
  \[ L_e(2, q) = 2^q (q-1) N_e(q) \]

- This is a consequence of the fact that the line sum symmetry condition for entanglement and separability is both necessary and sufficient when $p = 2$. 
Control localization in dynamical systems connected via a weighted tree

- Joint work with Prof. Ravindra Bapat (Indian Statistical Institute)

Control in dynamical systems coupled via a network

Consider state equations of the form:

\[
\frac{dx_i}{dt} = f(x_i, t) - \alpha \left( \sum_j L_{ij} D(t) x_j + c_i D(t) (x_i - u(t)) \right)
\]

where \( u(t) \) is the target trajectory and \( c_i \) are scalar control strengths.

- \( c_i > 0 \) if control is applied to the \( i \)-th system, and \( c_i = 0 \) otherwise.

- Under what conditions will the state trajectories \( x_i \) all follow the target trajectory \( u(t) \)?

- If \( u(t) \) is the trajectory of an unforced system, i.e. \( du/dt = f(u, t) \), and using a virtual state \( x_{n+1} = u \), we can rewrite this as:

\[
\frac{dx_i}{dt} = f(x_i, t) - \alpha \left( \sum_j \tilde{L}_{ij} D(t) x_j \right)
\]

- Where \( \tilde{L} = \begin{pmatrix} L + C & c \\ 0 & 0 \end{pmatrix} \) with \( C \) a diagonal matrix and \( c \) a vector with \( c_i \)’s as entries.
Control in dynamical systems coupled via a network

- This reduces the control problem into a synchronization problem.
- For the case when L is symmetric, it was shown that $\lambda_1(L + C)$, the smallest eigenvalue of L+C, is proportional to a sufficient condition for when the states of the coupled system follow $u(t)$.
- Thus we will study how $\lambda_1(L + C)$ depends on L and on C.
- In particular, consider the case where L is the Laplacian matrix of a graph. How does $\lambda_1(L + C)$ depends on properties of the graph.
Properties of $\lambda_1(L + C)$

- Let $p$ be the number of nonzero $c_i$’s.

- Theorem: $\lambda_1(L + C) \leq \frac{\sum c_i}{n}$. If $p < n$, then $\lambda_1(L + C) \leq \lambda_{p+1}(L)$

- Let $\kappa = \lim_{c_i \to \infty} \lambda_1(L + C)$, i.e. the limiting case where the nonzero control is arbitrary large.

- Theorem: $\kappa = \lambda_1(M)$, where $M$ is the matrix obtained from $L$ by deleting the rows and columns corresponding to nonzero $c_i$’s.
The case of a weighted tree

- Suppose $L$ is the Laplacian matrix of a tree with positive weights.
- Fiedler characterizes these trees based on $y$, the eigenvector corresponding to $\lambda_2$, the second smallest eigenvalue of $L$.
- There are two possibilities:
  - There exists a vertex $i$ such that $y_i = 0$. In this case, there is a unique vertex $k$ (called the characteristic vertex) such that $y_k = 0$ and $k$ is adjacent to a vertex with a nonzero entry. This is called a type-I tree.
  - No entry of $y$ is zero. There exists a unique edge $e = (i,j)$ such that $y_i y_j < 0$. $e$ is called a characteristic edge and $i$ and $j$ are called characteristic vertices. This is a type-II tree.
Only one $c_i$ is nonzero, $c_i \to \infty$

- Consider the case where only one system receives control. 
  \[ \lambda_1 (L + C) \leq \lambda_2 (L) \]
- Where should the control be applied to maximize or minimize $\kappa$?
- Theorem [Bapat and Wu, 2014]: $\kappa$ is maximized only when control is applied to the characteristic vertex and minimized only when control is applied to a pendant vertex.
Only one $c_i$ is nonzero, finite $c_i$

- Theorem [Bapat and Wu, 2014]: $\lambda_1 (L + C)$ is maximized at exactly one vertex, or at 2 vertices which must be adjacent. There exists a pendant vertex at which $\lambda_1 (L + C)$ is minimized.

- Numerical experiments support the following conjecture:

- Conjecture: For a diagonal matrix $C$ with one nonzero entry and Laplacian matrix $L$ of a weighted tree, $\lambda_1 (L + C)$ is maximized when the nonzero entry of $C$ occurs on a characteristic vertex.

- We found type-II trees where $\lambda_1 (L + C)$ is maximized at one of the characteristic vertex, but not the other.
Separability of Laplacian matrices

- Vertex degree condition is \textit{not} a sufficient condition for separability of Laplacian matrices [Hildebrand et al., 2008].
- However, vertex degree condition (and thus also PPT) is \textit{necessary} and \textit{sufficient} for separability when p=2 [Wu, 2006].
- Circulant graphs with canonical vertex labelling are separable [Braunstein et al.,]
Effect of graph operations on separability

- Tensor products of graphs result in a separable Laplacian matrix [Braunstein et al., 2006].

- Any type of products of graphs (Cartesian, lexicographical, tensor, strong, modular, etc.) result in a separable Laplacian matrix [Wu, 2009].

- Corollary: complete graphs are separable since complete graphs are strong products of complete graphs.

- Sums of graphs preserve separability but union of graphs does not preserve separability [Wu, 2009].
A sufficient condition for separability

- *Theorem:* If the number of edges from vertex \((u,v)\) to vertices of the form \((w,\bullet)\) is the same as the number of edges from \((w,v)\) to vertices of the form \((u,\bullet)\), then the density matrix is separable [Wu, 2006].
Invariance of separability under graph isomorphism

- Separability and entanglement are not invariant under graph isomorphism in general.
- Braunstein et al. ask the question: For which graphs are these properties invariant under graph isomorphism?
- Partition graphs into 3 classes:
  1. \( E \): normalized Laplacian matrix is entangled under all vertex labellings
  2. \( S \): normalized Laplacian matrix is separable under all vertex labellings
  3. \( SE \): normalized Laplacian matrix is entangled for some vertex labellings and separable for others.
- It turns out that each of these 3 classes are nonempty for each \( n \).
- For \( p=2 \), vertex degree condition can be used to determine \( E \), \( S \), and \( SE \).
Partitions for 2 x 2
Partition for 2 x 3

- $S$ is the complete graph $K_6$
- These following 6 graphs and their complements form $E$
Characterization of the set S

- For $n > 4$, $S$ consists of the complete graph $K_n$ [Wu, 2009].
- For all non-complete graphs, there exists a vertex labelling such that the resulting density matrix is entangled.
Characterization of the set \(SE\) and \(E\)

- For \(n > 4\) and \(p \mid r\), complete bipartite graphs \(K_{r,n-r}\) and their complements belong to class \(SE\).
- For \(r < q\) and \(p \mid r\), complete bipartite graphs \(K_{r,n-r}\) and their complements belong to class \(E\) [Wu, 2008].
- Complete characterization of \(SE\) and \(E\) is still an open problem.
References

Characterization of the set SE and E

- For $n > 4$ and $p | r$, complete bipartite graphs $K_{r,n-r}$ and their complements belong to class SE.
- For $r < q$ and $p | r$, complete bipartite graphs $K_{r,n-r}$ and their complements belong to class E [Wu, 2008].
- Complete characterization of SE and E is still an open problem.

http://www.cs.berkeley.edu/~sequin/SCULPTS/CHS_minisculpts/TangleKnots/PentafoilTangle4.JPG
Theoretical foundations of synchronization, consensus and control in systems coupled via a complex networks

- Relate the ability to reach synchronization with Laplacian eigenvalues of the graph.

- Leverage concepts in algebraic graph theory: e.g. Algebraic connectivity of directed graphs, diameter, eccentricity.

- Some “common-sense” results:
  - Synchronization can be achieved in a network of connected dynamical systems if the diffusive coupling is strong enough.
  - Control can be achieved in a network of dynamical systems if and only if sufficiently strong forcing is applied to roots of trees in a spanning directed forest of the interaction graph of L.
Partial transpose graph

- Arrange vertices on a \( p \) by \( q \) grid
- Each vertex has a label \((u,v)\), \( u \in \{1,\ldots, p\} \), \( v \in \{1,\ldots, q\} \).
- The *partial transpose graph* has the same vertex set and \(((u,v),(w,t))\) is an edge of the partial transpose graph if and only if \(((u,t),(w,v))\) is an edge of the original graph.
- Graphically, this corresponds to mirroring each edge around a horizontal axis through its middle.
Quantum states

- A pure state can be described by a state vector.
- A mixture of pure states is a mixed state. A mixed state can be viewed as:
  1. a statistical mixture of a number of pure states (i.e. experiments where the parameters are random)
  2. an ensemble of pure states (a large number of pure states with different proportions for each pure state).
- A mixed state cannot be expressed as a state vector.
- We need another structure to capture the properties of a mixed state.
Partial transpose graph

- Adjacency matrix of partial transpose graph is partial transpose of adjacency matrix.
- [Braunstein et al., 2006] introduced the vertex degree criterion:
  - Each vertex has the same degree as its counterpart in the partial transpose graph
  and showed that it is a necessary condition for separability
- It turns out this condition is as strong as the PPT condition.
- For Laplacian matrices of graphs,
  - Vertex degree condition \(\leftrightarrow\) Peres-Horodecki PPT condition \(\leftrightarrow\) partial transpose of Laplacian has zero row sums [Wu, 2006].
Separability of Laplacian matrices

- Separability is not invariant under graph isomorphism. Vertex labelling is important.

- In [Braunstein et al, 2006] it was shown that:
  1. The complete graph is separable under all vertex labellings.
  2. The star graph is entangled under all vertex labellings.
  3. The Petersen graph is separable or entangled depending on the vertex labelling.